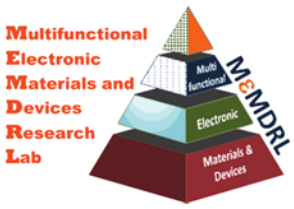
The Fourteenth International Meeting on Ferroelectricity

BOOK OF ABSTRACTS

San Antonio, Texas, USA

September 4th – 8th, 2017

SPONSORSHIP



PREFACE

The Fourteenth International Meeting on Ferroelectricity is held on September 4th to 8th, 2017 in San Antonio, Texas, USA. Over the past half century, since this series started (in 1965, at Prague, Czechoslovakia) the meeting is held every four years in different locations around the world, IMF has provided the platform to bring together researchers from academia, industry and government laboratories to share their knowledge in the field and to present the development of novel applications of ferroelectricity in various interdisciplinary and cross-coupled research areas. As a result, the IMF series has nurtured several special Symposia and Conferences in related fields and accelerated the rapid growth and extended interests in the field of ferroelectrics around the globe. The major themes and drives of these premier meetings have been to present the recent developments in the new understandings of fundamentals, advances in the field and bringing out the novel emerging cross-coupled effects among various characteristics of materials such as semiconductors, biosystems, and so on. Over the decades the conference has provided extensive and cumulative understanding of a large family of novel ferroic materials. The previous thirteen IMFs spread over the last fifty years have successfully established the field by serving its goals to the targeted research community.

The Fourteenth International Meeting on Ferroelectricity (IMF-2017) Organization committee is pleased to welcome you and thanks for your participation and support to continue this important tradition of the Ferroelectrics Community.

Amar S. Bhalla
George W. Taylor
On behalf of
The IMF2017 Organization Committee

General Chairs
Bhalla, Amar S. – USA
Taylor, George – USA

Local Chair
Guo, Ruyan – USA

Related Activities
Guo, Ruyan – USA
Santos, Ivair A. – Brazil
Cótica, Luiz F. – Brazil

Organizing Committee
Guerra, José – Brazil
Betal, Soutik – USA
Dutta, Moumita – USA
Young, Brandon – USA
Gamboa, Bryan – USA
Meng, Li – USA
Flynn, Paul – USA

Program Committee
Saxena, Avadh – USA
Fulay, Pradeep P. – USA
Katiyar, Ram – Puerto Rico
Prasankumar, Rohit – USA
Tidrow, Steven – USA
Chen, Chong-lin – USA
Jia, Quanxi – USA
Priya, Shashank – USA
Belleiche, Laurent – USA
Salamo, Greg – USA
Lorenz, Bernd – USA

International Program Contributors
Roleder, Krystian – Poland
Katiyar, Ram – Puerto Rico
Yimnirunn, Rattikorn – Thailand
Garcia, Ducinei – Brazil
Santos, Ivair A. – Brazil
Cótica, Luiz F. – Brazil
Guerra, José – Cuba/Brazil
Chen, Xioming – China
Maiti, Tanmoy – India
Gupta, Vinay – India
Lin, Yuan – Australia
Kim, S. S. – South Korea
Suvorov, Danilo – Slovenia
Mitic, Vojislav V. – Serbia

Publication
Bhalla, Amar S. – USA
Taylor, Deb – USA
Santos, Ivair A. – Brazil
Guerra, Jose – Brazil

Financial Matters
Bhalla, Amar S. – USA
Taylor, George – USA
Guo, Ruyan – USA

International IMF Advisory Board
Bhalla, Amar S. – USA
Baik, S. G. – Korea
Banys, Juras – Lithuania
Eiras, José A. – Brazil
Glazer, Mike – United Kingdom
Glinchuck, Maya – Ukraine
Gonzalo, Julio A. – Spain
Gregg, John – Northern Ireland
Hlinka, Jiri – Czech Republic
Kleemann, Wolfgang – Germany
Kreisel, Jens – Luxemburg
Lang, Sidney B. – Israel
Maglione, Mario – France
Michel, Dieter – Germany
Migoni, Ricardo – Argentina
Noda, Yukio – Japan
Noh, Tae Won – Korea
Noheda, Beatriz – Netherland
Ren, Wei – China
Roleder, Krystian – Poland
Setter, Nava – Switzerland
Sigov, Alexander – Russia
Sternberg, Andris – Baltic States
Taylor, George W. – USA
Tello, Manuel L. – Spain
Tseng, Tsueng-Yuen – Taiwan
Tsurumi, Takaaki – Japan
Vakhrushev, Sergey – Russia
Yao, Xi – China
Ye, Zuo-Guang – Canada

Special Events

Memorial and Honoring Sessions

The IMF2017 will be honoring the following distinguished researchers who past away in recent years:

Leslie Eric Cross (1923-2016)

The international ferroelectric community is very sad to learn that Professor L. Eric Cross passed away at his home in University Park, Pennsylvania, USA on December 28 2016, at the age of 93. Professor Eric Cross's research career spanned over more than six decades. It covered basic and applied research on ferroelectrics and related materials that enabled multidisciplinary applications of ferroelectrics as sensors and actuators. Respected by colleagues worldwide, Dr. Cross was revered for his groundbreaking work as a scientist, researcher, lecturer and mentor.

Jan Fousek (1930-2016)

Professor Jan Fousek passed away on September 4th, 2016. He was one of the most prominent researchers in the field of ferroelectricity over the past 50 years. Due to his pioneering work in ferroelectric domains and domain walls, optical and electro-optical properties of improper and pseudoproper ferroelectrics, as well as ferroelectric phase transition studies, Professor Fousek had influenced generations of ferroelectric-related researchers around the world.

Hans Schmid (1931-2015)

Professor Hans Schmid, Professor Emeritus of Chemistry at the University of Geneva, passed away on April 2nd, 2015. Professor Schmid had a pioneering and very important contribution in the field of multiferroic materials. He reported the synthesis of the first single crystal that presented simultaneously ferroelectric, ferroelastic and (weak) ferromagnetic behavior.

Women at the Frontier of Ferroelectrics

Over the past few decades the field of "ferroelectrics and device applications" has expanded quite rapidly. The research field has grown into several multiferroics based applications and now becoming a well-recognized field touching the multidisciplinary boundaries of various emerging multifunctional technologies, devices as well as electronic materials research. Geographically, it is being researched in most of the developed and developing economies and to some extent in several other countries. In recent years the participation and role of women researchers in this research field has been growing in many

ways as: enhanced contributions to the various funded research programs in academic institutions, successful technologists, entrepreneurs and in several other similar responsible roles. With the recognition of these facts it is very desirable to further promote and highlight the role of women scientists in this important field of science and technology. In this sense, during the IMF2017 meeting, we will hold a special recognition and discussion event "Women at the Frontier of Ferroelectrics," that will take place on Thursday, September 7th, from 12:30 to 13:40 over the lunch time.

Cultural Event

The IMF2017 San Antonio local organizers have made a special arrangement to offer all participants experience of *Fiesta Noche del Rio* performance. The show will take place at Arneson River Theatre from 20:30 to 22:00 on Tuesday, September 5th.

IMF2017 Banquet at ITC

The 14th International Ferroelectric Meeting has arranged a special evening for the IMF2017 attendees, combining exposure to Texan cultures and the conference banquet. It will be held at the UTSA's Institute of Texan Cultures (ITC), a Smithsonian affiliated institute. Snacks and drinks (cash bar) will be served between 17:30 to 18:30 for participants to enjoy the many exhibitions and collections of the ITC. Dinner is to start at 18:30.

The Fourteenth International Meeting on Ferroelectricity (IMF2017)
Monday, September 4th to Friday September 8th, 2017
at the Grand Hyatt San Antonio,
San Antonio, Texas, USA

Tuesday, September 5th, 2017

08:30 - 09:00	**OPENING SESSION**			
09:00 - 09:50	**Plenary 01 - 185.** Systems with defects of "random local field" or "random local anisotropy" types: validity of the Imry-Ma theorem - **Sigov, Alexander**			
09:50 - 10:20	**COFFEE BREAK**			
	ORAL SESSION – ROOM 1	ORAL SESSION – ROOM 2	ORAL SESSION – ROOM 3	ORAL SESSION – ROOM 4
	Theory I	**Dielectrics I**	**Relaxors I**	**Ferroics/Multiferroics I**
KEYNOTE 10:20 - 10:50	**187.** (INVITED) Non-linearity of ferroelectric oxides and possible applications in neuromorphic computing? - **Demkov, Alex**	**94:** (INVITED) Photovoltaic properties of some lead free (KNN) and lead-based (PFN) multiferroics - **Eiras, José A.**	**21.** (INVITED) Ferroic superglasses: Relaxor ferroelectric PMN versus CoFe superspin glass - **Kleemann, Wolfgang**	**177.** (INVITED) Ferroionic states: coupling surface electrochemistry with bulk ferroelectricity- **Kalinin, Sergei**
INVITED 10:50 - 11:15	**231.** (INVITED) First-principles based Landau-Devonshire potential for $BiFeO_3$ - **Marton, Pavel**	**256.** (INVITED) Role of Li for $BaTiO_3$ based lead-free piezoelectric ceramics - **Li, Guorong**	**379.** (INVITED) Multiple length scales in relaxor ferroelectrics - **Ohwada, Kenji**	**69.** (INVITED) Spin-lattice coupling in the potential multiferroic $SmFeO_3$ - **Kreisel, Jens**
11:15 - 11:30	**58.** First-principles study of $(Ba,Ca)(Ti,Zr)O_3$ solid solutions - **Amoroso, Danila**	**104.** Structure, dielectric and ferroelectric properties of NBT- and KNN- based perovskite ceramics - **Politova, Ekaterina**	**8.** The Polar Nano Regions-to-Relaxor Transition in PMN and PSN, $Pb_{1-x}Sc_{1/2}Nb_{1/2}O_{3-x}$; x = bulk concentration of nearest neighbor [Pb- O] divacancies - **Burton, Benjamin**	**154.** Lattice dynamics, dielectric properties and phase transitions of $Ag_{1-x}Li_xNbO_3$ ceramics - **Kania, Antoni**
11:30 - 11:45	**88.** Fluctuations and topological defects in proper ferroelectrics - **Prokhorenko, Sergei**	**116.** In search for artificial MPBs: dielectric spectroscopy of $BaTiO_3$ – $KNbO_3$ composites - **Ivanov, Maksim**	**406.** Observation of positive and negative magnetodielectric effects in relaxor $PbCo_{1/3}Nb_{2/3}O_3$ Ceramic - **Pandey, Adityanarayan H.**	**388.** Large remnant polarization and enhanced magnetic properties in non-quenched $Bi(Fe,Ga)O_3$-$(Ba,Ca)(Zr,Ti)O_3$ multiferroic ceramics - **Liang, Ruihong**
11:45 - 12:00	**113.** Modelling the photostriction of ferroelectric materials from first-principles - **Paillard, Charles**	**207.** Tuning optical responses with strain in multiferroelectrics and ferroelectrics - **Yang, Yurong**	**62.** $BaZr_{0.5}Ti_{0.5}O_3$: lead-free relaxor ferroelectric or dipolar glass - **Kutnjak, Zdravko**	**366.** Structure-Property Relationships in Multiferroic Compounds - **Cotica, Luiz F.**
12:00 - 12:15	**151.** First-principle prediction of novel multiferroic phases in epitaxial (111) $BiFeO_3$ films - **Xu, Changsong**	**385.** Understanding the Reason for Large Dielectric Response in Pb-free $(1-x)BaZr_{0.2}Ti_{0.8}O_3$-$(x)Ba_{0.7}Ca_{0.3}TiO_3$ Ferroelectric Ceramics - **Gao, Jinghui**	**68.** Permittivity of relaxor BNT (0.925)BT(0.075)x%Mn ceramics found from impedance spectroscopy - **Schmidt, V. Hugo**	**337.** Neutron diffraction studies of multiferroic $BiCoO_3$ - **Taddei, Keith**
12:15 - 12:30	**338.** Zone-boundary phonon instabilities investigated with neutron scattering combined with nharmonic first-principles simulations - **Delaire, Olivier**	**430.** (INVITED) Exploring $BiFeO_3$-based solid solutions and heterolayers for multifunctional applications - **Wang, John/Chung, JingYang**	**10.** Improving the optical properties of poly(vinylidene fluoride) (PVDF) films by doping with Nd^{3+} compound: Synthesis and characterization – **Falcão, Evaristo A.**	**397.** On the microstructure in the charge-glass state of $Pb_{1-x}Sr_xCrO_3$ - **Mori, Shigeo**

12:30 - 13:50	**LUNCH**			
	Room 1	Room 2	Room 3	Room 4
	Domains I	Design and Simulation I	Growth Materials I	Electrocalorics I
KEYNOTE 13:50 - 14:20	**258.** (INVITED) Domain wall engineering: concept, challenges - **Hlinka, Jiri**	**175.** (INVITED) Accelerated discovery and design of ferroelectrics through statistical learning methods - **Rajan, Krishina**	**145.** (INVITED) Processing and properties of next generation textured piezoelectric ceramics - **Messing, Gary**	**55.** (INVITED) Multicaloric effects in multiferroics - **Planes, Antoni**
INVITED 14:20 -14:45	**418.** (INVITED) Towards ferroelectric domain wall electronics - **Gregg, Marty**	**171.** (INVITED) Simulation of topological domains in hexagonal $RMnO_3$ patterns and kinetics of domain walls- **Liu, Jun-Ming**	**361.** (INVITED) Optical and electrooptical properties of rare earth doped transparent ferroelectric ceramics - **Garcia, Ducinei**	**395.** (INVITED) Some guidelines for improving caloric responses using ferroelectrics - **Dkhil, Brahim**
14:45 -15:00	**368.** First-principles theory of domain wall dynamics in improper ferroelectric hexagonal manganites - **Artyukhin, Sergey**	**84.** Microscopic origins of the large piezoelectricity of lead-free $(Ba,Ca)(Zr,Ti)O_3$ - **Nahas, Yousra**	**421.** Simulation , Growth and Properties Characterization of Large Size $Pb(In_{1/2}Nb_{1/2}O_3)$ - $Pb(Mg_{1/3}Nb_{2/3}O_3)$ -$PbTiO_3$ Single Crystal - **Xu, Zhuo**	**64.** Antiferroelectric and lead-free ferroelectric materials as electrocaloric coolants - **Rozic, Brigita**
15:00 -15:15	**205.** Ultrafast and high-resolution imaging of polarization switching in ferroelectrics - **Kalinin, Sergei**	**152.** Correlations in polarization switching kinetics in polycrystalline ferroelectrics - **Khachaturyan, Ruben**	**115.** Texture engineering: a convenient method to enhance the performance of piezoelectric ceramics - **Zhai, Jiwei**	**291.** Effect of Mn-addition on electrocaloric and dielectric properties of $0.9Pb(Mg_{1/3}Nb_{2/3})O_3$ - $0.1PbTiO_3$ ceramics - **Vrabelj, Marko**
15:15-15:30	**17.** Roles of electronic orbital hybridizations in rare-earth- substituted $BiFeO_3$ in the vicinity of morphotropic phase boundary - **Tu, Chi-Shun**	**440.** Pressure induced switching in ferroelectrics: on the junction between physics and electrochemistry - **Cao, Ye**	**312.** Giant piezoelectric voltage coefficient in grain-oriented modified-$PbTiO_3$ material- **Yan, Yongke**	129. Understanding the True Electrothermal Response of Ferroelectric Thin Films - **Hanrahan, Brendan**
15:30 -15:45	**137.** Impact of flexoelectricity and surface charges on the formation and properties of domain structures in thin ferroelectric films - **Vorotiahin, Ivan**	**92.** Designing Lead-Free antiferroelectrics for energy storage - **Xu, Bin**	**340.** Understanding processing-structure-property relationships in textured lead-free materials - **Maurya, Deepam**	**138.** Electrocaloric Effect, Dielectric, Ferroelectric and Piezoelectric properties in Normal and Relaxor phases of La-doped PZT65/35 - **Samanta, Shibnath**
15:45 -16:00	**319.** (INVITED) Structural Characterizations of Hardening in A-site Non-stoichiometric $(1--x)Bi_{0.5}Na_{0.5}TiO_3 - (x)BaTiO_3$ Lead Free Piezoelectric Ceramics - **Prasertpalichat, Sasiporn**	**214.** Coupling effect in Relaxor-Ferroelectric layered composite – phase field simulation and analytical solution - **Wang, Shuai**	**349.** A Novel High Curie Temperature Piezo-/ferroelectric Solid Solution of $Bi(Zn_{2/3}Ta_{1/3})O_3$ -$PbTiO_3$ - **Yuan, Yi**	**282.** Molten Salt Synthetic Method for Making Perovskite Nanoparticles - **Mao, Yuanbing**
16:00 -16:20	**25.** (INVITED) Science and technology of interface-engineered biocompatible piezoelectric oxide/ultrananocrystalline diamond (UNCD (TM)) films for a new generation of multifunctional/ biomedical MEMS/NEMS devices - **Auciello, Orlando**	**216.** Machine Learning guided Computational Search for Ruddlesden-Popper Oxides without Inversion Symmetry - **Balachandran, Prasanna V.**	**164.** (INVITED) Electromechanical Characterization of High-Coupling Textured PMN-PT and PMN-PZT Ceramics - **Blottman, John**	**TBD**

Wednesday, September 6th, 2017				
08:10 – 9:00	**MEMORIAL SESSION** Covered by Drs. Ruyan Guo, Jiri Hlinka and Manfred Fiebig			
09:00 - 09:50	**Plenary 02 - 244.** Large coupling ferroelectricity through polarization rotation - **Cohen, Ronald E.**			
09:50 - 10:20	**COFFEE BREAK**			
	Room 1	Room 2	Room 3	Room 4
	Theory II	Dielectrics II	Relaxors II	Ferroics/Multiferroics II
KEYNOTE 10:20 - 10:50	**241.** (INVITED) Polarization twist in perovskite ferrielectrics: A study on $(Bi,Na)TiO_3$-$BaTiO_3$ single crystals - **Noguchi, Yuji**	**176.** (INVITED) The bulk photovoltaic effect in the crystals without symmetry center and its application to the solar energy - **Fridkin, Vladimir**	**67.** (INVITED) On the relationship between materials properties and short-range order in highly piezoelectric lead-based relaxors - **Gehring, Peter**	**51.** (INVITED) $EuTiO_3$: a possible multiferroic with unusual magneto-optical properties and applications - **Bussmann-Holder, Annette**
INVITED 10:50 - 11:15	**285.** (INVITED) Role of random electric fields in lead-free relaxor ferroelectrics - **Ye, Zuo-Guang**	**390.** (INVITED) Thermodynamic stability of polar vortices in ferroelectric superlattices- **Chen, Long- Qing**	**183.** (INVITED) Manipulation of electric field effect by orbital switching - **Pan, Feng**	**36.** (INVITED) Strain-induced polar-to-nonpolar transitions in layered perovskites - **Rondinelli, James**
11:15 - 11:30	**364.** Spin-phonon couplings and lattice instabilities in complex oxides - **Hong, Jiawang**	**130.** Dynamics of acoustic phonons in niobium doped $PbZrO_3$ single crystals - **Kajewski, Dariusz**	**277.** Sintering and characterization of dielectric and thermal mechanical properties of $(Bi_{1/2}Na_{1/2})TiO_3$-$BaTiO_3$ ceramics - **Lente, Manuel H.**	**106.** Structural characterization of ferroic materials by advanced spectroscopy techniques - **Yimnirun, Rattikorn**
11:30 - 11:45	**391.** Elastic and Optical Properties of Ruddlestone-Popper perovskites - ab initio calculation - **Mamedov, Amirullah**	**215.** Porous ferroelectric ceramic with novel aligned pore structures for energy harvesting - **Zhang, Yan**	**11.** Super tetragonal ferroelectric phase of $BiFeO_3$ -$PbTiO_3$: A cause for several novel phenomena - **Ranjan, Rajeev**	**121.** Magnetoelectric properties of cement and mortar- **Andrzejewski, Bartlomiej**
11:45 - 12:00	**73.** Pecularities of antiferroelectric phase transitions in $PbZr_{0.71}Sn_{0.29}O_3$ crystal by Mössbauer effect. - **Jankowska-Sumara, Irena**	**243.** The influence of defect type and configuration on the electrical properties of PZT based ceramics - **Zeng, Jiangtao**	**321.** Observation of multiple phases and incommensurate transitions in bismuth and lead oxide based complex perovskites leading to high temperature relaxor behavior - **Dwivedi, Akansha**	**381.** Tunable magnetic pole inversion in multiferroic $BiFeO_3$-$DyFeO_3$ solid solution - **Wu, Jiangtao**
12:00 -12:15	**370.** Controlling Jahn-Teller Distortions through Hybrid-Improper Ferroelectricity in Rare-Earth Manganite Perovskites - **Schmitt, Michael M.**	**306.** In situ dielectric spectroscopy and Brillouin scattering study of lithium niobate. - **Piecha, Julita**	**170.** Lattice dynamics of $Na_{1/2}Bi_{1/2}TiO_3$ as studied by dielectric spectroscopy and Brillouin light scattering - **Lushnikov Sergey**	**194.** Development of an optical magnetic field sensorbased on Ce and Mn doped $BiFeO_3$ thin films using SPR technique - **Sharma, Anjali**
12:15 -12:35	**235.** (INVITED) Phonon Dynamics and Phase Transformations in Bismuth Titanate - **Nayak, Sanjeev**	**39.** (INVITED) Electromechanical Behavior of Strontium-Modified Lead Zirconate Titanate Ceramics - **Singh, Raj**	**111.** (INVITED) Probing short-range order in PZN-xPT and PMN-xPT relaxor ferroelectrics with neutron scattering - **Xu, Guangyong**	**331.** (INVITED) Magnetoelectric and magnetostriction properties in multiferroic composites: A phenomenological approach - **de Oliveira, Adilson J. A.**

12:30 - 13:50	LUNCH			
	Room 1	Room 2	Room 3	Room 4
	Domains II	Design and Simulation II	Growth Materials II	Electrocalorics II
KEYNOTE 13:50 -14:20	**178.** (INVITED) Insight into structure, properties, and mobility of ferroelectric domain walls - **Setter, Nava**	**74.** (INVITED) Atomistic simulations of relaxor ferroelectrics - **Bellaiche, Laurent**	**20.** (INVITED) Loss of elastic stability and formation of inhomogeneous states at phase transitions in thin films on substrates - **Levanyuk, Arkady**	**179.** (INVITED) Inverse barocaloric effects in ferroelectrics - **Moya, Xavier**
INVITED 14:20 -14:45	**402.** (INVITED) Domain walls of ferroelastic oxides as memristive devices - **Noheda, Beatriz**	**369.** (INVITED) Metallic ferroics: Coexistence of noncentrosymmetry, metallicity, electron correlation and magnetism - **Gopalan, Venkatraman/Stone, Greg**	**218.** (INVITED) Composition and crystallization control in lead-free ceramic and polymer ferroelectrics derived from non-crystalline precursors - **Yao, Kui**	**263.** (INVITED) Strontium titanate based double perovskites: A new paradigm for high temperature thermoelectrics - **Maiti, Tanmoy**
14:45 - 15:00	**387.** Electrostrain enhancement at an "invisible boundary" in a single ferroelectric phase - **Zhao, Luo**	**405.** Atomic-level understanding of the structure-property connections in perovskite-based ferroelectric systems - **Datta, Kaustuv**	**223.** Lithium niobate thin films of stoichiometric composition doped with Ho^{3+} ions - **Kokanyan, Edvard**	**161.** Abnormal electrocaloric effect in the presence of defect dipoles - **Ma, Yangbin**
15:00 -15:15	**182.** Large electrostrains in ferroelectric crystals/ceramics via reversible domain switching - **Li, Faxin**	**29.** Investigation of the Response of Nanoscale Ferroelectric Material through Molecular Dynamics Simulation - **Li, Meng**	**249.** X-ray spectroscopic evidence for the coexistence of ferroelectric and antiferrodistortive orders in $SrTiO_3$ thin films - **Lu, Cong**	**167.** (INVITED) Skyrmion dynamics in multiferroics in the presence of a temperature gradient - **Lin, Shizeng**
15:15 - 15:30	**226.** Polar nature at the domain boundary - **Yokota, Hiroko**	**18.** Impact of thermal vibrations on polarization reversal: a Monte-Carlo model- **Kliem, Herbert**	**296.** Effects of The Deposition Temperature of Nd-doped $Bi_4Ti_3O_{12}$ Thin Films Prepared by Pulsed Laser Deposition. - **Kim, Eun Young**	**419.** Flexocaloric and Multicaloric Effects in Ferroic Materials - **Saxena, Avadh**
15:30 - 15:45	**255.** Crystal Structure and Skin Effect in $(1-x)BiFeO_3$-$(x)PbTiO_3$ Single Crystals **Zhuang, Jian**	**269.** Strain and switching behavior in doped BZCT system - **Liu, Zhen**	**110.** Formation of epitaxial ferroelectric thin films on graphene: mechanism and properties - **Petrov, Peter**	**324.** Electrocaloric effect in aging ferroelectric samples - **Xu, Baixiang** Empty
15:45 - 16:00	**272.** Molecular Dynamics Simulations of Polarization Switching at Ferroelectric Domain Walls - **Zeng, Xiaowei**	**270**. Artificial synapses with ferroelectric tunnel junctions – **Garcia, Vincent**	**362.** Growth and characterization of PLD grown large area $PbZr_xTi_{1-x}O_3$ thin films - **Rath, Martando**	**407.** Direct measurements of electrocaloric $PbSc_{0.5}Ta_{0.5}O_3$ ceramics – **Avramenko, Alex**
16:00 - 16:20	**99.** (INVITED) Natural Domains of $BaTiO_3$ in Ultrahigh Vacuum, Air and Acid: Properties & Invariant Domain-Size Proving Intrinsic Screening - **Watanabe, Yukio**	**156.** (INVITED) Room-temperature relaxor ferroelectricity and photovoltaic effects in SnTiOx/Si thin film heterostructures - **Hong, Seungbum**	**357.** (INVITED) Structure and dielectric analysis of hybrid copolymers of PVDF/Metal-Organic frameworks composite film - **Manuspiya Hathaikarn**	**120.** (INVITED) Enhancement of Bulk Photovoltaic Effect in $BiFeO_3$ Thin Films by Mn Doping - **Nakashima, Seiji**

Thursday, September 7th, 2017				
08:10 - 09:00	**Plenary 03 - 208.** Guided materials design: Search for ferroelectrics with targeted properties - **Lookman, Turab**			
09:00 - 09:50	**Plenary 04 - 35.** Domain dynamics in multiferroics - **Fiebig, Manfred**			
09:50 - 10:20	**COFEEE BREAK**			
	Room 1	Room 2	Room 3	Room 4
	Theory III	Dielectrics III	Relaxors III	Ferroics/Multiferroics III
KEYNOTE 10:20 - 10:50	**233.** (INVITED) Critical dynamics and formation of the intermediate ferroelectric phase in the Zr-rich $PZr_{(1-x)}Ti_xO_3$ - **Vakhrushev, Sergey**	**433.** (INVITED) What determines a highly piezoelectric morphotropic phase boundary? - **Xiaobing Ren**	**56.** (INVITED) On the paraelectric behavior of water at T = T* = 60 ºC as a polar liquid - **Gonzalo, Julio A.**	**72.** (INVITED) Static and dynamic magnetoelectric coupling in multiferroics: A review - **Kamba, Stanislav**
INVITED 10:50 - 11:15	**50.** (INVITED) Hybrid improper ferroelectricity in Ruddlesden-Popper $A_3B_2O_7$ ceramics - **Liu, Xiao Q.**	**227.** (INVITED) Clausius – Mossotti relation fractal modification - **Mitic, Vojislav**	**189.** (INVITED) Defects and dielectric polarization in polar functional materials - **Liu, Yun**	**278.** (INVITED) Polarization and spin order pattern of multiferroic RMn_2O_5 based on a magnetic space group - **Noda, Yukio**
11:15 - 11:30	**134.** Experimental and theoretical determination of anharmonic soft phonons in the improper ferroelectric $YMnO_3$ - **Bansal, Dipanshu**	**276.** A study of the multiferroic state under high pressure across the phase diagram of $Mn_{(1-x)}Co_xWO_4$ for $0.05 > x > 0.17$ - **Gooch, Melissa**	**127.** Empirical correlations and a phenomenological description for relaxor dielectric response - **Grinberg, Ilya**	**268.** Effect of Magnetic and Electric Fields on Magnetization and Polarization of $BiMnO_3$ Multiferroics Film - **Alrub, Ahmad M. A. A.**
11:30 - 11:45	**181.** Pressure-induced transitions in ferroelectric single-crystal $PbZr_{0.54}Ti_{0.46}O_3$ - **Aihaiti, Muhetaer**	**122.** Highly resistive nanostructured $BiFeO_3$ monoliths by Spark- Plasma Sintering: A re-oxidation study - **Volnistem, Eduardo**	**186.** $Ba(Ga_x,Ta_x)Ti_{(1-2x)}O_3$: Induced diffuse phase transitions using charge compensated dipole pairs (Ga-Ta) introduced in barium titanate parent matrix - **K. Veerapandiyan, Vignaswaran**	**141.** Effects of cryomilling on ferroic properties of $BiFeO_3$ nanoparticles and bulk ceramics - **Dias, Gustavo S.**
11:45 - 12:00	**173.** The symmetry-mode decomposition, structural refinement and ferroelectricity of $(1-x)AgNbO_3$ -$(x)LiTaO_3$ - **Lu, Teng**	**372.** Synthesis, structure and piezo-/ferroelectric properties of a novel bismuth-containing ternary complex perovskite solid solution - **Liu, Zenghui/Ye Zuo-Gang**	**225.** Lattice dynamics, dielectric behaviour and acoustic waves in tetragonal tungsten-bronzes - **Buixaderas, Elena**	**83.** Improved Magnetic Properties, Dielectric and Structural Characterizations in Mn and Cr Doped $0.9BiFeO_3$ -$0.1BaTiO_3$ Compositions - **Gotardo, Ricardo**
12:00 - 12:15	**436**. (INVITED) The role of strain and surface charge in stabilizing ferroic domains and atomic-scale dipole moments - **Yachin, Ivry**	**257.** (INVITED) Large Magnetoelectric Couplings in Lead- free Nanocomposites - **Chen, Aiping**	**346.** The normal to diffuse phase transition crossover from thermal expansion analysis in calcium modified lead titanate – **Estrada/Flávia/Garcia, Ducinei**	**148.** The Effect of Time-dependent Magnetic Field on Electrical Polarization in Bismuth Ferrite - **Sayedaghaee, S. Omid**
12:15 - 12:30	**219.** Piezoelectric response induced phase transition in perovskite thin films - **Lee, Hyeon J.**	**TBD**	**373.** An exceptional hysteresis-strain- thermal stability combination of electrostrain via re-entrant relaxor- ferroelectric composite - **Fang, Minxia**	**439.** Metaferroics: Higher field effects in a Multiferroic - **Kumar, Pradeep**

12:30 - 13:50	LUNCH			
12:40 – 13:40	**Women at the Frontier of Ferroelectrics (Room 4) – Chairs: R. Guo, L.D. Madsen**			
	Room 1	Room 2	Room 3	Room 4
	Domains III	THz/IR/Raman I	Growth III	Energy Harvesting
KEYNOTE 13:50 - 14:20	**220.** (INVITED) Emergent chirality in oxide superlattices - **Ramesh, Ramamoorthy/Pedriac Shafer**	**34.** (INVITED) Ultrafast polarization dynamics in ferroelectric thin films - **Lindenberg, Aaron**	**174.** (INVITED) Crystalline phase, micro-structure and electrical properties of lead-free piezoelectric KNN-based films - **Ren, Wei**	**242.** (INVITED) The bulk photovoltaic effect in polar oxides for robust and efficient solar energy harvesting - **Rappe, Andrew**
INVITED 14:20 - 14:40	**415.** (INVITED) Atomic structure and dynamic behaviors of domain walls and polar vortices in multiferroic thin films - **Pan, Xiaoqing/Li, Linze**	**44.** (INVITED) Using intense THz pulses to probe and control dynamics in multiferroics - **Prasankumar, Rohit**	**140.** (INVITED) PLD growth of ultra-thin $SrTiO_3$ films on Si(100): coverage and thermal budget effects - **Suvorov, Danilo**	**441.** (INVITED) Defect engineered complex oxide thin films with anomalous multifunctionalities - **ChongLin Chen**
INVITED 14:40 - 15:00	**90.** (INVITED) Nanoscale domain structures in uniaxial ferroelectric single crystals - **Shur, Vladimir**	**288.** (INVITED) THz dielectric responses derived from dipole clusters of $BaTiO_3$ -based ferroelectrics - **Tsurumi, Takaaki**	**75.** (INVITED) Transmission electron microscopy of multifunctional hard coatings - **Jiang, Jiechao**	**425.** (INVITED) Room-temperature aerosol deposition of ferroelectric ceramic films for power inverters in electric drive vehicles - **U. Balu, Balachandran**
15:00 - 15:15	**375.** Direct observation of charged domain walls in hybrid improper ferroelectric $(Ca,Sr)_3Ti_2O_7$ - **Mori, Shigeo**	**229.** Terahertz dynamics of soft and central modes in ferroelectric superlattices - **Razumnaya, Anna**	**345.** Compressively strained lead titanate films - **Zubko, Pavlo**	**232.** Study of Electrocaloric Effect, Recoverable Energy Storage density, Dielectric and Piezoelectric Properties in Modified Barium Titanate - **Khatun, Nasima**
15:15 - 15:30	**153.** Electrical Control and Temperature Tuning of Chiral Phases in Electrotoroidic Nanocomposites - **Walter, Raymond**	**247.** Electric-field tuning of a planar terahertz metamaterial based on strained $SrTiO_3$ layers - **Kadlec, Christelle**	**365.** Long-range Stripe Nanodomains in Epitaxial (110)$BiFeO_3$ Thin Films on (100)$NdGaO_3$ Substrate - **Sharma, Yogesh**	**142.** Phase Transitions in Doped Hafnia Thin Films for Pyroelectric Applications - **Park, Min Hyuk**
15:30 - 15:45	**322.** Towards functional polar domain walls in ferroelastic $CaTiO_3$ - **Guennou, Mael**	**262.** Tunable terahertz range dielectric spectra of in domain-engineered ferroelectric nanostructures - **Hlinka, Jiri**	**76.** Microstructural development of hard Hf-B-Si-C-N coating at high temperatures - **Shen, Yi**	**188.** Flexible ferroelectric oxide films for mechanical energy harvesting - **Jung, JongHoon**
15:45 - 16:00	**66.** Probing ferroelectric domains with X-ray nanodiffraction - **Hadjimichael Marios**	**77.** Phonon-Polariton Dispersion Relation of Ferroelectric $LiTaO_3$ Crystals - **Kojima, Seiji**	**169.** Charged defects in ferroelectric oxides: investigation of doped $BaTiO_3$ thin films - **Castro Chavarria, Christopher**	**298.** Improved energy storage density and dielectric properties in La substituted $BaTi_{0.95}Sn_{0.05}O_3$ - **Kumar, R.**
16:00 - 16:15	**96.** Effect of electric field on local structure probed by angular dependence of Raman scattering - **Md Al, Helal**	**275.** Resonance Damping of the THz-frequency Transverse Acoustic Phonon in the Relaxor Ferroelectric $KTa_{1-x}Nb_xO_3$ - **Iolin, Eugene**	**112**. (INVITED) Direct synthesis of tetragonal $BaTiO_3$ nanoparticles by sonochemical and surface active etching method - **Vittayakorn, Naratip**	**TBD**

Friday, September 8th, 2017				
09:00 - 09:50	**Plenary 05 - 237.** Coupled multiple order parameters and their domain switching in magnetoelectrics - **Kimura, Tsuyos**			
09:50 - 10:20	**COFFEE BREAK**			
	Room 1	Room 2	Room 3	Room 4
	Theory IV	Dielectrics IV	Novel Materials	Ferroics/Multiferroics IV
KEYNOTE 10:20 - 10:50	**442.** (INVITED) NSMM Versus Goldschmidt's Factor Formalism a Scorecard - **Tidrow, Steven**	**48.** (INVITED) The macro- and nanoscale phenomena in $BaTiO_3$ single crystal - **Roleder, Krystian**	**408.** (INVITED) Developing novel multiferroic materials - **Dalal, Naresh**	**118.** (INVITED) The structure and phase transitions of $Na_{1/2}Bi_{1/2}TiO_3 - ATiO_3$ solid solutions - **Sternberg, Andris**
INVITED 10:50 - 11:10	**245.** (INVITED) Possibility of ferroelectricity in wurtzite-structured zinc oxide thin films - **Moriwake, Hiroki**	**180.** (INVITED) Remarkable ferroelectric properties in ultrafine $BaTiO_3$ nanocrystals - **Wang, Xiaohui**	**413.** (INVITED) Inducing ferroelectricity into the M_3CuCl_3 ($M = Ti^+, K^+$) family of quantum antiferromagnets - **Kinyon, Jared**	**135.** (INVITED) Atomic control of ferroelectricity in oxide thin films and heterostructures - **Noh, Tae Won**
INVITED 11:10 - 11:30	**221.** (INVITED) Ferroelectricity in κ - Al_2O_3 -type $(A,Fe)_2O_3$ (A = Al, Ga, Fe, Rh, In, Sc, and In) multiferroic oxides - **Itoh, Mitsuru**	**417.** (INVITED) Influences of nanogold addition on microchemical composition, domain structure and electrical properties of perovskite $BaTiO_3$ -based ceramics - **Ananta, Supon**	**382.** (INVITED) Phonon mode links ferroicities in multiferroic $[(CH_3)_2NH_2]Mn(HCOO)_3$ - **Musfeldt, Jan**	**12.** (INVITED) Modulation of Magnetoelectric Coupling in $BiFeO_3$ Mutiferroic Ceramics - **Chen, Xiang M.**
11:30 - 11:45	**123.** Critical scattering and incommensurate phase transition in antiferroelectric $PbZrO_3$ under pressure - **Burkovsky, Roman**	**105.** Evolution of surface charge through the ferroelectric- paraelectric phase transition in $BaTiO_3(001)$ - **Mathieu, Claire**	**400.** Nanoscale tailoring of oxygen vacancy distribution by mechanically loaded scanning probe - **Wang, Bo**	**31.** Multiferroicity in Haldane spin- chain compound Sm_2BaNiO_5 - **Upadhyay, Sanjay K.**
11:45 - 12:00	**280.** Lattice dynamics and dielectric relaxation in $PbMg_{1/3}Nb_{2/3}O_3$ relaxor from atomistic simulations - **Bokov, Alexei**	**238.** Phase Transition Behavior and Defect Chemistry of the $BaTi_{0.94}Sn_{0.06}O_3$ Ceramic investigated via In-situ extended X- ray absorption fine structure (EXAFS) technique - **Sukkha, Usa**	**157.** Electronic Structure of Lead-Free Organic-Inorganic Hybrid $CH_3NH_3X_{I3}$ Perovskite Materials - **Padchasri, Jintara**	**41.** Spin excitations in the Z -type hexaferrites $(Ba_xSr_{(1-x)})_3Co_2Fe_{24}O_{41}$ - **Kadlec, Filip**
12:00 - 12:15	**416.** Second order phase transitions in uniaxial ferroelectrics - **Lashley, Jason**	**393.** Mechanism of ferroelectric aging in donor&acceptor doped $BaTiO_3$ ceramics - **Zhou, Chao**	**197.** Coplanar waveguide resonator using PZT thin film - **Gupta, Reema**	**7.** Poly methyl methacrylate/ magnetite nano-composites - **Salwa, Abe El-Messieh**
12:15 - 12:30	**428.** Structure, bandgap modulation, and magnetic switching in Fe_2O_3-doped ferroelectric ceramics – **Li, Jun**	**43.** Rare-earth modified $BaTiO_3$ ferroelectric ceramics – Abnormal PTCR response - **de los Santos Guerra, José**	**274.** Novel Approach to Mitigate the Trade-Offs Between Fast Programming and Long Retention Times in Polymer Ferroelectric Memory - **Georgiou, Vasileia**	**3.** Synthesis and properties of $BiFeO_3$-based nanopowders - **Santos, Ivair**

12:30 - 13:50	**LUNCH**		
	Room 1	Room 2	Room 3
	Probe (Nanoscale)	THz/IR/Raman II	Applications
KEYNOTE 13:50 - 14:20	**209.** (INVITED) In-Situ transmission electron microscopy investigation of ferroelectric domain switching induced by external stimulation - **Liao, Xiaozhou**	**102.** (INVITED) Driving structural dynamics in mutiferroics and ferroelectrics with THz light - **Johnson, Steven**	**22.** (INVITED) Magnetoelectric gyrators for I-V conversion - **Viehland, Dwight**
INVITED 14:20 - 14:40	**70.** (INVITED) Magnetic resonance probing of ferroelectricity and magnetism in metal-organic frameworks - **Bertaina, Sylvain**	**246.** (INVITED) Surface plasmon resonance (SPR) based electro-optic and magneto-optic modulators - **Gupta, Vinay**	**146.** (INVITED) High-density ferroelectric random access memory using wall- current readout of binary information - **Jiang, Anquan**
INVITED 14:40 - 15:00	**192**. Surface acoustic wave devices for gas and biosensing applications - **Tomar, Chowdhuri Monika**	**236.** (INVITED) Micro-Raman spectroscopy of Doped-ZnO Ferromagnetic and Ferroelectric Nano-Materials with Multiple-Excitation wavelengths - **Sharma, Shiv**	**414.** (INVITED) Optimization of BST Phase Shifter Circuits for Beam-Steering Applications - **Subramanyam, Guru**
15:00 - 15:15	**287.** Imaging of non-collinear antiferromagnetic order and ferroelectric order in $BiFeO_3$ - **Fusil, Stephane**	**14.** Ferroics and multiferroics, for Terahertz device design - **Dutta, Moumita**	**193.** ZnO/Si Lamb wave SAW devices - **Ran, Lokesh**
15:15 - 15:30	**330.** Probing Local and Global Ferroelectric Phase Transition in Single Phase Multiferroic Thin Films - **Pradhan, Dhiren**	**377.** Second-harmonic phonon spectroscopy of the model oxide α-quartz- **Winta, Christopher J.**	**162.** Effect of mechanical and electrical strain on bilayer polymer nonvolatile memory devices - **Singh, Deepa**
15:30 - 15:45	**284.** Probing the domain structures and the extrinsic contributions in piezoelectric materials - **Zhang, Nan**	**401.** (INVITED) On the origin of ferroelectricity in $Hf_{0.5}Zr_{0.5}O_2$ thin films - **Wei, Yingfen**	**234.** Optimizing the performance of $(Ba,Sr)TiO_3$ tunable capacitors for high figures of merit - **Freeze, Christopher**
15:45 - 16:00	**344.** Chemical Phenomena of Local Polarization Reversal in Ferroelectric Thin Films - **Ievlev, Anton V.**	**252.** Dielectric and ferroelectric properties of rare earth doped lead zirconate titanate ceramics - **Bhattarai, Mohan**	**303.** Device physics of polymeric ferroelectric memory diodes - **Asadi, Kamal**
16:00 - 16:15	**TBD**	**TBD**	**53.** Magnetoelectric nanorobots for remote controlled dynamically targeted live cell manipulation - **Betal, Soutik**

Poster Session: Tuesday, September 5th, 2017 – 16:30-18:30h

Tu-S28-P-01
Electrochemical and structural characterization of *polyacrylonitrile* (PAN) based gel polymer electrolytes blended with tetrabutylamonium iodide for dye-sensitized solar cells
Faisal Chowdhury
Tu-S28-P-02
Effects of La^{3+} ions on the physical properties of $(Bi_{0.5}Na_{0.5})_{0.92}Ba_{0.08-3x/2}La_xTiO_3$ lead-free ceramics
Yanela Méndez-González, Aimé Peláiz-Barranco, José de los Santos Guerra, Pierre Saint-Grégoire, Arbelio Pentón-Madrigal
Tu-S28-P-03
Dielectric and structural analysis of three-layered ferroelectric perovskites
Yuslin González-Abreu, Aimé Peláiz-Barranco, Pierre Saint-Grégoire, Yaovi Gagou, José de los Santos Guerra
Tu-S28-P-04
Electromagnetic pulse protection circuits design of piezoelectric vibration acceleration sensor
Cui Hao, Denghua Li
Tu-S28-P-05
Piezoelectric stack transducer evaluation and comparison for optimized energy harvesting
Bryan Gamboa, Ruyan Guo, Amar Bhalla
Tu-S28-P-06
An Interpretation of relaxor behavior by the Weiss field approach
Andreas Leschhorn, Herbert Kliem
Tu-S28-P-07
Phase transition and ferroelectric properties of Aurivillius $Bi_4Ti_2Nb_{0.5}Fe_{0.5}O_{12}$
Cristian Lavado, Marcelo Stachiotti
Tu-S28-P-08
Fabrication and characterization of (Fe+Nb)-doped PZT thin films
Lucia Imhoff, Sebastian Barolin, Nora Pellegri, Marcelo Stachiotti
Tu-S28-P-09
Structural and electrical properties of $Mg_{0.05}Ba_{0.95}Zr_{0.1}Ti_{0.9}O_3$ ceramics
Ariel Di Loreto, Agustín Frattini, Rodrigo Machado, Marcelo Stachiotti
Tu-S28-P-10
Polarised-light and electron microscopy of the static domain structure of ferroic $Fe_3B_7O_{13}I$ boracite at room temperature
Guillermo Castellanos-Guzman, O. Jimenez, Carmen Miramontes-Corona, D. Mendoza, Oziel R.Camacho, Alan Y.Vargas-Aguilera
Tu-S28-P-11
$BiFeO_3$-$SrTiO_3$ thin film as new lead-free relaxor-ferroelectric capacitor with ultrahigh energy storage performance
Hao Pan, Yi Zeng, Yang Shen, Yuan-Hua Lin, Jing Ma, Liangliang Li, Ce-Wen Nan
Tu-S28-P-12
Ab-Initio study on the electronic properties of perovskite structure-based ferroelectrics
Abrahan Pablo Aslla-Quispe, Roberto Hiroki Miwa, José de los Santos Guerra
Tu-S28-P-13
Chrome influence on the physical properties of $Bi_{0.90}Ba_{0.10}Fe_{0.90}Ti_{0.10}O_3$ multiferroic ceramic system
Yalina García-Puente, Osmany García-Zaldívar, Aimé Peláiz-Barranco, Martin A. Hernández-Landaverde, Francisco Calderón Piñar, Sergio Díaz-Castañón, José de los Santos Guerra, Marcos A. Oliveira
Tu-S28-P-14
Study of the crystallization kinetics of ferroelectric nanocrystals into TeO_2-based glass system
Renato Cruvinel de Oliveira, Anielle Christine Almeida Silva, Noélio Oliveira Dantas, José de los Santos Guerra
Tu-S28-P-15
Li, La doped KNNT ceramics obtained by RTGG
Jorge Portelles, Juan Fuentes, Jose Juan Gervacio, Oscar Raymond, Jesus M Siqueiros, Jesus Heiras, Ma. de la Paz Cruz, Norma Palmero, Carlos Ostos
Tu-S28-P-16
Microwave dielectric properties of $Bi_2(Zn_{1/3}Nb_{2/3})_2O_7$ thin films by microwave sintering
Siyuan Dong, Meng Li, Ruyan Guo, Amar Bhalla, Xiaoli Wang
Tu-S28-P-17
Magnetoelectricity at nanoscale
Soutik Betal, Eduardo Ortega, Moumita Dutta, Amar Bhalla, Ruyan Guo
Tu-S28-P-18
Effect of oxygen flow rate on optical and electrical properties of flexible SnO_2/Ag/SnO_2 multilayer thin films on PET substrate
Guneik JANG, Taekeun Kim
Tu-S28-P-19
Dielectric and dilatometric studies of Rb_2ZnI_4 and its mixed systems
Toshihisa Yamaguchi, Masaaki Takashige
Tu-S28-P-20
Micro-Raman scattering, dielectric and DSC investigations of phase transitions behavior in the $PbHf_{1-x}Sn_xO_3$ single crystal
Irena Jankowska-Sumara, Maria Podgórna, Jae-Hyeon Ko, Andrzej Majchrowski
Tu-S28-P-21
Negative diploar heat capacity in relaxor ferroelectrics and dipolar glasses
Zdravko Kutnjak, Rasa Pirc
Tu-S28-P-22
Perovskite relaxor multiferroics in novel dielectric cooling designs
Brigita Rozic, Andraz Bradesko, Marko Vrabelj, Hana Ursic, Lovro Furlanovic, Uroš Plaznik, Barbara Malic, Tadej Rojac, Qiming Zhang, Andrej Kitanovski, Zdravko Kutnjak
Tu-S28-P-23
Piezoelectric properties and local structure analysis of $(1-x)(Na_{0.50}K_{0.45}Li_{0.05})NbO_3$-$(x)Ca(Zr_{0.50}Ti_{0.50})O_3$ solid solutions produced by malic acid complex solution method
Masafumi Kobune, Haruka Nagai, Takeyuki Kikuchi, Yasuhiro Yoneda
Tu-S28-P-24
Phase transitions in dense perovskite formate frameworks: EPR and dielectric study
Mantas Simenas, Sergejus Balciunas, Monika Trzebiatowska-Gusowska, Miroslaw Maczka, Georg Völkel, Andreas Pöppl, Juras Banys
Tu-S28-P-25
Preparation of $BiFeO_3$ thin films by MOCVD
Masaru Shimizu, Nao Yoshimura, Hironori Fujisawa, Seiji Nakashima
Tu-S28-P-26
Phase transition studies on the multiferroic $(1-x)BiFeO_3$-$(x)BaTiO_3$ solid solutions below room temperature
ARUN KUMAR, Dhananjai Pandey
Tu-S28-P-27
Synthesis and characteristics of high dielectric constant material: $BaCu_3Ti_4O_{12}$
Kalpana Parida, RNP Choudhary
Tu-S28-P-28
The defect and dielectric relaxation of Nb and Mn Co-doping $BaTiO_3$ ceramics
Yang Xiaojing [1], Liu Xiaobing [2], Ding Shihua [3]
Tu-S28-P-29
Defects and dielectric properties of BCZT ceramics doped with Nd
Ding Shihua, Peng Yong, Song Tianxiu
Tu-S28-P-30
Double hysteresis loops in $Pb(Zn_{1/3}Nb_{2/3})O_3$-$PbTiO_3$
Makoto Iwata, Yasutaka Kaiden, Yoshihiro Ishibashi
Tu-S28-P-31
Domain kinetics in KTP single crystals for periodical poling applications
Vladimir Shur, Andrey Akhmatkhanov, Elena Pelegova, Ekaterina Vaskina, Maria Chuvakova, Ekaterina Gachegova, Maxim Ivanov, Andrei Kholkin
Tu-S28-P-32
Formation of self-assembled domain structure at non-polar surfaces of $LiNbO_3$ by tip scanning without application of external field

Vladimir Shur, Anton Turygin, Denis Alikin, Jury Alikin
Tu-S28-P-33
Dynamics of ferroelectric polarization simulated by a second-order Landau model
Michael Richman, Paul Rulis, Anthony Caruso
Tu-S28-P-34
Multi-shell nanowires including ferroelectrics
Hironori Fujisawa, Yohei Takeuchi, Masaru Shimizu, Seiji Nakashima
Tu-S28-P-35
Effect of electric field on 180º domain switching in uniaxial $Ca_{0.30}Ba_{0.70}Nb_2O_6$ crystals studied by Brillouin Scattering
Md Aftabuzzaman, Md Al Helal, Jan Dec, Wolfgang Kleemann, Seiji Kojima
Tu-S28-P-36
Temperature dependent local structure of MFe_2O_4 (M = Ni and Mn) determined by *in-situ* X-ray absorption fine structure (EXAFS)
PINIT KIDKHUNTHOD
Tu-S28-P-37
Aging in relaxor ferroelectric systems
Jan Dec, Wolfgang Kleemann
Tu-S28-P-38
Large electro-mechanical energy conversion in PZT-PNN ceramics
Muangjai Unruan, Sujitra Unruan, Yutthapong Inkong, Rattikorn Yimnirun
Tu-S28-P-39
Effect of $BaZr_{0.4}Ti_{0.6}O_3$ addition on electrical and magnetic properties of Multiferroic (1-x)$BiFeO_3$-x$BaTiO_3$ ceramics
Sujitra Unruan, Rattikorn Yimnirun, Rungnapa Tipakontithikun, Muangjai Unruan
Tu-S28-P-40
Influence of humidity on electrophysical properties of pure silicon dioxide
Milovidova SD, Nguyen Hoai Thuong, Rogazinskaya OV, Sidorkin AS, Zolotukhina MA
Tu-S28-P-41
Local piezo-ferroelectric properties of highly textured $(K_{0.5}Na_{0.5})_{0.985}La_{0.005}NbO_3$ thin films
H´Linh H´Mok, Espiridión Martínez Aguilar, Jose Juan Gervacio Arciniega, Xavier Vendrell, Jesús M. Siqueiros, Oscar Raymond Herrera
Tu-S28-P-42
Dielectric properties of $BaTiO_3$ based composites
Sergejus Balčiūnas, Maksim Ivanov, Satoshi Wada, Jūras Banys
Tu-S28-P-43
Thermophysical properties of multiferroic bismuth ferrite with rare-earth elements
Suleiman Kallaev, Abumuslim Bakmaev, Zairbek Omarov, Alikber Bilalov, Larisa Reznichenko, Sedik Hazbulatov
Tu-S28-P-44
Effects of morphology and surface potential shift of mechanosynthesized $BiFeO_3$ nanoparticles on the visible-light catalysis for decontamination of organic dyes
Eduardo Volnistem, Raquel Bini, Gustavo Dias, Luiz Cótica, Ivair Santos
Tu-S28-P-45
Computational design of new semiconductor ferroelectric perovskite oxides
Ilya Grinberg, Jing Yang, Andrew Rappe
Tu-S28-P-46
Dielectric, piezoelectric and optical properties of a $PbZr_{1-x}Ti_xO_3$ single crystal
Iwona Lazar, Krystian Roleder, Andrzej Majchrowski, Dariusz Kajewski, Andrzej Soszyński, Janusz Koperski
Tu-S28-P-47
Resistivity of relaxor $BNT_{0.925}BT_{0.075}$x%Mn ceramics found from impedance spectroscopy
Noah Archer, Hugo Schmidt, Chi-Shun Tu
Tu-S28-P-48
Tailoring the properties of $BiFeO_3$ for applications through first-principles calculations
Espiridion Martinez Aguilar, H'Linh H'Mok, Maria Guadalupe Moreno Armenta, Jesus Maria Siqueiros Beltrones
Tu-S28-P-49
Study of the multiferroic ordering in $BiFeO_3$(012)/$La_{0.67}Sr_{0.33}MnO_3$(012) heterostructures by first principles calculations
H´Linh H´Mok, Espiridión Martínez Aguilar, Jordi Ribas Ariño, Jesús M. Siqueiros Beltrones, Oscar Raymond Herrera
Tu-S28-P-50
AC conductivity of multiferroic $BiFeO_3$ nanocrystalline ceramics
Sadyk Sadykov, Nariman Alikhanov
Tu-S28-P-51
Phase transformation induced bloating behavior in diopside glass-ceramics used for microwave dielectric materials
Kuei Chih Feng, Pin-Yi Chen, Cheng-Sao Chen, Chi-Shun Tu
Tu-S28-P-52
Structural characteristics and large electric-field-induced strains in strontium and manganese Co-doped 92.5%$(Bi_{0.5}Na_{0.5})TiO_3$-7.5%$BaTiO_3$ crystals
Cheng-Sao Chen, Pin-Yi Chen, Yi-Ping Syu, Kuei-Chih Feng, Chi-Shun Tu
Tu-S28-P-53
Universal energetic coupling in complex antiferroelectric and incommensurate perovskites
Kinnary Patel, Sergey Prosandeev, Yurong Yang, Bin Xu, Jorge Iñiguez, Laurent Bellaiche
Tu-S28-P-54
Ferroelectric domain structure and piezoelectric properties of highly textured $Pb(Fe_{0.5}Nb_{0.5})O_3$ thin films deposited by sputtering
José Juan Gervacio Arciniega, Mario Alberto Curiel Álvarez, C. I. Enrique Flores, Carlos E Ostos Ortiz, Reynaldo Font, F. J. Espinoza-Beltrán, Jesus M. Siqueiros Beltrones, Oscar Raymond Herrera
Tu-S28-P-55
Study of magnetoeletric coupling in $BiFe_{1-y}Co_yO_3$ compositons using ferroic characterizations
Anuar Mincache, Odair Oliveira, Eduardo Volnistem, Gustavo Dias, Ivair Santos, Luiz Cótica, Amar Bhalla, Ruyan Guo
Tu-S28-P-56
Indications of an enhanced magnetoelectric coupling in nanostructured $BiFeO_3$-$PbTiO_3$ compounds
Valdirlei Freitas, Ivair Santos, Luiz Cótica, Gustavo Sanguino Dias, Diana Navroski
Tu-S28-P-57
Switchable thin film bulk acoustic wave devices based on ferroelectric films
Anatoliy Mikhailov
Tu-S28-P-58
Magnetic and dielectric response of $Sr_{0.95}Nd_{0.05}Fe_{12-x}Al_xO_{19}$ (x = 0.36, 0.60, 0.84 and 1.08) obtained by hydrothermal synthesis
Andrzej Hilczer, Katarzyna Pasińska, Ewa Markiewicz, Adam Pietraszko, Bartłomiej Andrzejewski
Tu-S28-P-59
Magnetic and ferroelectric properties of sol-gel synthesized Al and Mn doped $GaFeO_3$ ceramics
NANDNI SHARMA, Ashish Mall, Rajeev Gupta, Ashish Garg, Sanjeev Kumar
Tu-S28-P-60
Synthesis, structural, microstructural and ferroic properties of $CoFe_2O_4$:$BaTiO_3$ nanocomposites
Denise Alanis, Raquel Bini, Eduardo Volnistem, Daniel Silva, Gustavo Dias, Ivair Santos, Ruyan Guo, Amar Bhalla, Luiz Cótica
Tu-S28-P-61
Size and shape effects in ferroelectric nanoparticles
Franco Di Rino, Marcelo Sepliarsky, Marcelo Stachiotti
Tu-S28-P-62
Background dielectric permittivity: material constant or a fitting parameter?
Arkady Levanyuk, Boris Strukov, Andres Cano
Tu-S28-P-63
Investigation of non-linear susceptibility of some relaxor ferroelectrics
Dziugas Jablonskas, Maksim Ivanov, Robertas Grigalaitis, Juras Banys

Tu-S28-P-64
Influence of the dynamic magnetization response in the magnetoelectric effect in multiferroic composites
Alexandre Gualdi, Fabio Zabotto, Ducinei Garcia, Amar Bhalla, Ruyan Guo, Paulo Cesar de Camargo, Adilson Jesus Aparecido de Oliveira
Tu-S28-P-65
Study of birefringence and electro-optic effect in SBN60 thin film
Surbhi Gupt, Ayushi Paliwal, Vinay Gupta, Monika Tomar
Tu-S28-P-66
Bipolar resistive switching in Pt/BFO/BTO/Pt sandwiched structures
Savita Sharma, Surbhi Gupta, VInay Gupta, Monika Tomar
Tu-S28-P-67
XPS resolved surface state analysis of ZnO and Ni doped ZnO films for quantum well applications
Sheetal Dewan, Monika Tomar, A.K. Kapoor, R.P. Tandon, Vinay Gupta
Tu-S28-P-68
Dielectric spectroscopy of barium titanate doped with Ce^{4+} at the Ti site
Dzmitry Adamchuk, Sarunas Svirskas, Juras Banys, Vincenzo Buscaglia
Tu-S28-P-69
Ferroelectric photovoltaic properties of multilayered PZT/BFO thin film system
Reema Gupta, Monika Tomar, Ashok Kumar, Vinay Gupta
Tu-S28-P-70
Studies on the effect of integration of metal nanoclusters on the electrical and ferroelectric properties of barium titanate thin film
Savita Sharma, Monika Tomar, Ashok Kuma, Vinay Gupta
Tu-S28-P-71
Relaxor behavior analysis of rare-earth modified PZT ferroelectric ceramics
Suzana Pereira Hessel, Atair Carvalho da Silva, Arthur Vinicius Oliveira Costa, Ruyan Guo, Amar S. Bhalla, José de los Santos Guerra
Tu-S28-P-72
Synthesis and characterization of $0.5Ba(Ti_{0.8}Zr_{0.2})O_3$–$0.5(Ba_{0.7}Ca_{0.3})TiO_3$ thin films grown by chemical solution deposition
Nadia Mamana, Maria Luz Santiago, Nora Pellegri, Marcelo Stachiotti
Tu-S28-P-73
Electrical properties of ceramic $Ba[(M_{0.05}Ta_{0.05})Ti_{0.9}]O_3$ with M = Sc, Cr, Mn, or Fe and $Ba[(M_{0.0333}Ta_{0.0666})Ti_{0.9}]O_3$ with M = Mn, Ni, or Cu
YuHsun Liao, V. K. Veerapandiyan, Steven M. Pilgrim, Walter A. Schulze, Steven C. Tidrow
Tu-S28-P-74
Dielectric relaxation anomalies in ferroelectric nanocomposites
Hoai Thuong Nguyen, Alexander Sidorkin, Svetlana Milovidova
Tu-S28-P-75
Dielectric properties of ferroelectric barium titanate - barium zirconate superlattices obtained using pulsed laser deposition
Alexander Sidorkin, Yaovi Gagou, Pierre Saint-Gregoire, Evgenii Vorotnikov, Lolita Nesterenko
Tu-S28-P-76
Effect of sintering temperature on relaxor ferroelectric behavior of BCZT ceramic prepared by sol-gel auto combustion
Piyaporn Jaimeewong, Xiaotong Wang, Zenghui Liu, ZuO-Guang Ye, Anucha Watcharapasorn
Tu-S28-P-77
On the structural and dielectric properties of nickel ferrite based multiferroic composites
Roney Junio de Portugal, Atair Carvalho da Silva, Soutik Betal, Moumita Dutta, Ruyan Guo, Amar S. Bhalla, José de los Santos Guerra
Tu-S28-P-78
Dielectric and piezoelectric properties of $(1-x)Ba(Zr_{0.2}Ti_{0.8})O_3$-$(x)(Ba_{0.7}Ca_{0.3})TiO_3$ ceramics
Panupong Jaiban, Pimpilai Wannasut, Suwapitcha Buntham, Anucha Watcharapasorn
Tu-S28-P-79
Temperature and composition-driven percolation in $BaTiO_3$-based relaxor ferroelectric solid solutions
Alexei Bokov, Jian Zhuang, Wei Ren, Zuo-Guang Ye
Tu-S28-P-80
Microscopic Description of the Ferroism properties in $AlFe_{1-x}A_xO_3$ (A= Mn or Co) and $Al_{1-x}Ga_xFeO_3$ Magnetoelectric Compositions
Guilherme Maia Santos, Luiz Fernando Cótica, José Eduardo Padilha, Ivair Aparecido dos Santos, Amar Bhalla, Ruyan Guo
Tu-S28-P-81
Temperature dependent local structure of $LiCoO_2$ determined by *in-situ* Co K-edge X-ray absorption fine structure
Chinawat Ekwongsa
Tu-S28-P-82
In-situ observation of an electric-field-induced lattice distortion of $BiFeO_3$ thin films
Seiji Nakashima, Osami Sakata, Hiroshi Funakubo, Takao Shimizu, Daichi Ichinose, Yasuhiko Imai, Hironori Fujisawa, Masaru Shimizu
Tu-S28-P-83
The evidence of giant Surface Flexoelectric Field in (111)-oriented $BiFeO_3$ thin film
tieying yang
Tu-S28-P-84
Pinched hysteresis behaviour in lead free ferroelectric ceramic BCT-BZT
Atal Bihari Swain
Tu-S28-P-85
Study on the interface behaviours between bismuth-based ceramics and electrodes
Xiukai Cai, Yuanxing Cai, Peng Deng, Zhiwei Xue, Sirui Cai
Tu-S28-P-86
NSMM Review – Part II: Development of structural relations using geometric considerations
YuHusn Liao, Vignaswaran K. Veerapandiyan, V. Mitic, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven Tidrow

Poster Session: Wedenesday, September 6th, 2017 – 16:30-18:30h.

We-S55-P-01
Preparation, characteristics and temperature as well as frequency dependence dielectric and complex impedance spectroscopic studies on composite multiferroic of $PbTiO_3$ – $SrFe_{12}O_{19}$
Krishan Kumar Bamzai
We-S55-P-02
Diisopropylammonium halides – new family of lead-free ferroelectric materials
Anna Piecha-Bisiorek, Ryszard Jakubas
We-S55-P-03
Order-disorder phenomenon in a ferroelectric Jahn-Teller phase transition
Jiri Hlinka
We-S55-P-04
Flexible crystals of perovskite-like coordination polymers with tunable and switchable organic guests
Magdalena Rok, Grazyna Bator
We-S55-05
We-S55-P-06
On the influence of the synthesis temperature on the fluorescence dependence of doped PVDF/Er films
Evaristo Falcao, Glauciane Leite, Eriton Botero, Ruyan Guo, Amar Bhalla
We-S55-P-07
Improvements of the PVDF fluorescence spectrum caused by Nd and Ce addition
Evaristo Falcao, Lais Aguiar, Eriton Botero, Claudio Carvalho, Ruyan Guo, Amar Bhalla
We-S55-P-08
Study of the phase transition in PLZT samples by the Interferometric Method
Evaristo Falcao, Ivair Santos, Jose Pereira, Alysson Steimacher, Antonio Medina, Mauro Baesso, Jose Eiras, Garcia Ducinei, Ruyan Guo, Amar Bhalla

We-S55-P-09
Temperature dependent magnetoelectric and magnetodielectric response of multiferroic cobalt ferrite and Pb(Zr,Ti)O3 multilayered structure
Brandon Young
We-S55-P-10
Upconversion in co-doped SBN for supercontinuum light generation
Moumita Dutta, Michael Williams, Rohit Prasankumar, Amar Bhalla, Ruyan Guo
Structure and properties of $Pb(Mg_{1/4}Nb_{1/2}Ti_{1/4})O_3$ nanodots from first principles
Abdullah Albarakati, Sergey Prosandeev, Dawei Wang, Laurent Bellaiche
We-S55-P-12
Physical, electrical and magnetic properties of ferrite modified PZT-based composite ceramics
Jiradtakeat Dechawuttikul, Anurak Prasatkhetragarn, Pongsakorn Jantaratana, Rattikorn Yimnirun
We-S55-P-13
Study on dielectric and magnetic properties of the organic-inorganic hybrid layered structure halide material
Yonghwan Kim, namjung hur
We-S55-P-14
Environmental friendly $SrTi_{1-x}Mo_xO_3$:15Nb perovskites for high temperature thermoelectric applications
Mandvi Saxena, Ritwik Banerjee, Tanmoy Maiti
We-S55-P-15
Relaxor ferroelectric $Ba_xSr_{2-x}TiCoO_6$ double perovskite material for high temperature thermoelectric application
Nirma Kumari, Mandvi Saxena, Pinku Roy, Tanmoy Maiti
Plasmonics and Perovskites Laboratory, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, Uttar
We-S55-P-16
Metal-like electrical conductivity in double perovskite $A_xSr_{2-x}TiMoO_6$ (A = La, Ba) oxides for high temperature thermoelectric power generation
Mandvi Saxena, Tanmoy Maiti
Plasmonics and Perovskites Laboratory, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, Uttar
We-S55-P-17
Gamma-ray irradiation effects on the ferroelectric domain structure of epitaxial $Pb(Zr_{0.52}Ti_{0.48})O_3$ thin films
Sang Don Bu, Sam Yeon Cho, Eun Young Kim
We-S55-P-18
Ferroelectric-based synapse devices with oxide heterostructure
Joonbong Lee, Hojin Lee, Yeogyun Yoon, Youjung Gill, Yunseok Kim, Taekjib Choi
We-S55-P-19
Enhanced thermoelectric figure of merit in environment friendly nanocomposite of $SrTi_{0.85}Nb_{0.15}O_3$ and graphene oxide for clean energy generation
Tanmoy Maiti, Pinku Roy, Farheen Anjum
We-S55-P-20
Synthesis of orthorhombic SnO_2 and effect of the cerium doping on the structural properties
Ernesto Pereira, Maria Helena Costa, Adilson de Oliveira
We-S55-P-21
Spectral insights of newly synthesized environmentally benign bismuth based lead free organic inorganic hybrid perovskite solar cell
Tanmoy Maiti, Pritam Dey, Harish Singh, Shubham Gautam
We-S55-P-22
Colossal change in thermopower with temperature driven p–n type conduction switching in La and Ca doped Sr_2TiFeO_6 double perovskites
Tanmoy Mait, Pinku Roy
We-S55-P-23
Ambient processing of P(VDF-TrFE)-based thin-film capacitors
Hamed Sharifi Dehsari, Jasper Michels, Kamal Asadi
We-S55-P-24
Ferroelectric response of phase pure PMN-PT thin films realized through pulsed laser deposition
Pius Augustine, Martando Rath, M.S. Ramachandra Rao[2]
We-S55-P-25
Highly resistive fast-sintered $BiFeO_3$ multiferroic magnetoelectric ceramics
Gustavo S. Dias, Luiz F. Cótica, Ivair A. Santos, Valdirlei F. Freitas, Fabiano Yokaichiya
We-S55-P-26
Dielectric and ferroelectric properties of $(1-(x/2))BaTiO_3$-$(1-(x/2))BiFeO_3$-$(x)LaFeO_3$ ceramics synthesized via solid-state reaction method with NaCl salt as the surface active agent.
Narit Triamnak, Kunyarat Aryuyuen, Kiratiporn Boonkham, Chanatorn Patadoung
We-S55-P-27
Physical characterizations of the high-bioactive PVDF-HAp ferroelectric composite
Valdirlei Freitas, Taiana Bonadio, Jaciele Rosso, Gustavo Dias, Luiz Cótica, Ivair Santos, Ludmilla Silva
We-S55-P-28
Effect of Nb doping in $BaSrZrTiO_3$
Anju Dixit
We-S55-P-29
Rapid detection of transient currents in ferroelectric nanocapacitors via Bayesian Inference
Suhas Somnath, Kody Law, Anna Morozovska, Petro Maksymovych, Yunseok Kim, Xiaoli Lu, Marin Alexe, Richard Archibald [2], Sergei Kalinin, Stephen Jesse, Rama Vasudevan
We-S55-P-30
Long-wave optic phonons in $PbNi_{1/3}Nb_{2/3}O_3$ crystals.
Alexander Fedoseev, Tatyana Smirnova, Sergey Lushnikov, Ram Katiyar
We-S55-P-31
Investigation on a giant magnetoelectric effect in a hexaferrite via neutron scattering techniques
Yan Wu, Huibo Cao, Young Sun
We-S55-P-32
Synthesis and characterization of the perovskite compound $YFe_xCr_{1-x}O_3$ ($0 < x < 1$)
Roberto Salazar, Friedrich E. Wagner, Antonio Lazo, Rubén Puga, Juan Z. Dávalos, Américo Orccohuancca, Héctor Loro
We-S55-P-33
Inorganic ferroelectric/dielectric nanocomposite thin films
Yomery Espinal, Brendan Hanrahan, Pamir Alpay

We-S55-P-34
Domain wall conductivity with a twist
Rama Vasudevan, Ye Cao, Nouamane Laanait, Anton Ievlev, Linglong Li, Jan-Chi Yang, Ying-Hao Chu, Long-Qing Chen, Sergei Kalinin, Petro Maksymovych
We-S55-P-35
Is ferroelastic $BiVO_4$ also antiferroelectric?
Nidal Banja, Hongjian Zhao, Jorge Iniguez, Mael Guennou
We-S55-P-36
Preparation, characterization and dielectric properties of Mg-doped $CaCu_3Ti_4O_{12}$ ceramics
Eduardo Antonelli, Leonardo Arruda
We-S55-P-37
Refractive indices and birefringence of lithium niobate as a function of temperature and wavelenght
Abdallah Albarakaty, Nasser Moustafa
We-S55-P-38
Molten salt synthesized $La_{1-x}Sr_xCoO_3$ as an efficient electrocatalyst for water splitting
Yuanbing Mao, Swati Mohan
We-S55-P-39
Structural analysis and thermoelectric properties of La-doped Sr_2CoMoO_6 double perovskites
Tanmoy Maiti, Khagesh Tanwar
We-S55-P-40
Sensing magnetic fields with an innovative smart probe composed by piezoelectric elements
José R D Pereira, Fernando J Gaiotto, Rogerio G Nespolo, Diogo Z Montanher, Ivair A Santos
We-S55-P-41

Phase transitions studies in (1-x)($Ba_{0.77}Ca_{0.23}$)TiO_3-x$Ba(Ti_{0.75}Zr_{0.15})O_3$ ceramics
Eduardo Antonelli, Renato Boschilia, Rangel Aredes, Andre Boaventura
We-S55-P-42
Magnetoelectric properties of epitaxial $Sr_{0.5}Ba_{0.5}MnO_3$ films
Temuujin Bayaraa, Yurong Yang, Jorge Íñiguez, Laurent Bellaiche
We-S55-P-43
Induced Magnetic-anisotropy by the remanent electric polarization of PMN-PT/$CoFe_2O_4$ multiferroics particulates composites
Korllvary R.C. Parra-Jimenez, Fábio L. Zabotto, Ducinei Garcia, Adilson J. A. de Oliveira
We-S55-P-44
Gradient-lead-excess crystallization process: A way to produce highly textured (111) PZT films
Alexander Sigov, Lyubov Delimova, Elena Guschina, Nina Zaitseva, Dmitry Seregin, Konstantin Vorotilov
We-S55-P-45
Dielectric polarization in $BaSrTiO_3$ films modulated by THz electric field
Mikhail Agranat, Elena Mishina, Alexander Sigov
We-S55-P-46
Estimation of dead layer at the PZT - Pt interface
Alexander Sigov, Yury Podgorny, Pavel Lavrov, Konstantin Vorotilov
We-S55-P-47
Effect of the rare earth ion substitution on structural, dielectric and magnetic properties of perovskite $Re_2Bi_2Fe_4O_{12}$(Re = Eu, Sm, La) ceramics
Javier Alonso Cuervo Farfán, Diego Seiti Fukano Viana, Flávio Paulo Milton, Ducinei Garcia, David Arsenio Landínez Téllez, Jairo Roa Rojas
We-S55-P-48
NSMM Review – Part I: Scorecard of NSMM *versus* Goldschmidt's Factor formalism
Vignaswaran K. Veerapandiyan, YuHusn Liao, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven C. Tidrow
We-S55-P-49
Ferroelectric property in nano-layered Hafnium oxide
Sita Dugu, Shojan Pavunny, Rajesh Katiyar, Ram S Katiyar
We-S55-P-50
Dielectric behavior of functional Paint/PMN-PT nanocomposite films
Ashok Batra, Bir Bohara, Mohan Aggarwal, Ravi Lal
We-S55-P-51
Investigation on the structural, dielectric, ferroelectric, and magnetic properties of BNTFCO ceramics
Margarita Correa, Claudia Zuluaga, Ram Katiyar
We-S55-P-52
NSMM Review – Part III: *Pm*3*m* coordination and temperature dependent *radii*
YuHusn Liao, Vignaswaran K. Veerapandiyan, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven C. Tidrow
We-S55-P-53
NSMM Review – Part IV: coordination and temperature dependent polarizabilities
Vignaswaran K. Veerapandiyan, YuHusn Liao, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven C. Tidrow

We-S55-P-54
Growth and characteristics of the $CH_3NH_3PbBr_3$ perovskite crystal for optoelectronic applications
Raja Surabhi, Ashok Batra, Kamala Bhat, Samuel Uba, Ashwith Chilvery
We-S55-P-55
NSMM Review – Part V: Polarization and volume induced structural phase transitions
Vignaswaran K. Veerapandiyan, YuHusn Liao, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven Tidrow
We-S55-P-56
NSMM Review – Part VI: Clausius – Mossotti relation incorporates Curie and Curie – Weiss laws
Vignaswaran K. Veerapandiyan, YuHusn Liao, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven C. Tidrow
We-S55-P-57
First principles studies in $Bi_{1-x}Nd_xFeO_3$ compositions
Gabriel H. Perin, Gustavo S. Dia, Ivair A. Santos, Ruyan Guo, Amar Bhalla, Jose E. Padilha, Luiz F. Cotica
We-S55-P-58
Probing the pore structure of a chiral periodic mesoporous organosilica using liquid crystals
jayalakshmi vallamkondu, P. Lemieux Robert
We-S55-P-59
Meso-kinetics of one time relaxation electrical processes in $BaTiO_3$ ceramics - Boltzmann-Poisson model
Vojislav V.Mitić, Zoran B.Vosika, Goran Lazović, Vesna Paunović, Ljubiša Kocić
We-S55-P-60
Preparation and characterization of PAN-EC-PC-TPAI-I_2 gel polymer electrolytes for dye-sensitized solar cells
Faisal Chowdhury
We-S55-P-61
We-S55-P-62
On the „inverted" phase transitions in ferroic crystals containing propylenediammonium cations
Janusz Przesławski, Matthew Crofton, Zbigniew Czapla
We-S55-P-63
The effect of fluorine doping on structural and dielectric properties of Diisopropylammonium bromide
Thirmal Chinthakuntla, Ratnamala Chatterjee, Simant Srivastav, Murugavel Pattukannu, Atalbihari Swain, Divyanshu Bhatnagar
We-S55-P-64
Dielectric and impedance spectroscopic studies of pristine and lanthanum substituted $YBiO_3$
Divyanshu Bhatnagar, Thirmal Chinthakuntla, Ratnamala Chatterjee
Magnetics and Advanced Ceramics Laboratory, Physics Department, Indian Institute of Technology Delhi, New Delhi, India
We-S55-P-65
Investigation of ferroelectric properties by using Monte Carlo simulations
Se-Hun Kim
We-S55-P-66
Multiple bandgaps of ferroelectric based two-dimensional phononic crystals slab with Archmedes and Fibonacci spiral holes
Amirullah Mamedov, Selami Palaz, Oral Oltulu, Ekmel Ozbay
We-S55-P-67
Electronic band structure and optical properties of $Gd_2(MoO_4)_3$: First Principle calculations
Amirullah Mamedov, Sevket Simsek, Gokay Ugur, Sule Ugur, Ekmel Ozbay
We-S55-P-68
High temperature thermoelectric properties of Sr-rich $Gd_{1-x}Sr_xMnO_3$ based manganites
Tanmoy Maiti, Ritwik Banerjee
We-S55-P-69
Structural and electrical properties of charge compensated dipole pairs substituted barium titanate
Vignaswaran Kaliyaperumal Veerapandiyan, Mackenzie Stevens, Steven Tidrow
We-S55-P-70
First Principles study of piezoelectric properties and morphotropic phase boundary of $AgNbO_3$-based solid solutions
Sittichain Pramchu, Atchara Jaroenjittichai, Yongyut Laosiritaworn
We-S55-P-71
Thickness dependence of dynamic phase diagram in ferroelectric films: Monte Carlo and Neural Network investigation
Wimalin Laosiritaworn, Yongyut Laosiritaworn
We-S55-P-72
Low-frequency noise characteristics of $CuInP_2S_6$ lamellar crystal
Andrius Dziaugys, Ilona Zamaraite
We-S55-P-73

Effects of MnO_2 doping on the electrical properties of 0.99BCZT-0.01Seeds ceramic systems
Piewpan Parjansri, Sukum Eitssayeam
We-S55-P-74
Phase relations in the Bi_2O_3-Mn_2O_3-M_2O_3 (M = Fe, Al, Ga) pseudo-ternary systems
Sreco Skapin, Amalija Golobic, Danilo Suvorov
We-S55-P-75
Sintering behavior, phase structure and electric properties of KNNTS-BKNZ ceramics with excessive alkali metals
Rui Nie, Xing Xing, Jiagang Wu, Qiang Chen, Wen Zhang, Jianguo Zhu, Dingquan Xiao
We-S55-P-76
Dielectric, Electrical Conduction, Piezoelectric and Impendence Analysis of Bi_3TiNbO_9 Piezoceramics with Ce-Modifications
Jing Yuan, Rui Nie, Jianguo Zhu
We-S55-P-77
Stress dependence of structure, electronic and optical properties of $BaTiO_3$ from WC, VdW-DF-C09 and HSE Functional calculations
Eleicer Ching-Prado
We-S55-P-78
Enhanced performance in AZO based transparent flexible TFTs due to oxygen vacancy in ZnO film with Zn-Al-O interface fabricated by atomic layer deposition
Yang Li, Huanhuan Wang, Jinzhu Wuand, Xiaohong Wu
We-S55-P-79
Anomalous dielectric behaviour in Cr^{3+} substituted $Ba_{0.90}Sr_{0.10}TiO_3$ ferroelectric ceramics
Parveen Kumar, Chandra Prakash, K.K. Raina
We-S55-P-80
Dielectric properties of HHTP-4H2O cold pressed pellets
Sergejus Balčiūnas, Anna Peterson, Maksim Ivanov, Jasper Adamson, Jūras Banys
We-S55-P-81
Dielectric and structural properties of PVDF-$NaNbO_3$- based cold sintered composites
Deepankar S. Gyan, Parth Sharma, Yash Tamrakar, Akansha Dwivedi
We-S55-P-82
Electrocaloric effects in the lead-free $Ba(Zr,Ti)O_3$ relaxor ferroelectric from atomistic simulations
Zhijun Jiang, Sergei Prokhorenko, Sergey Prosandeev, Yousra Nahas , Dawei Wang, Jorge Íñiguez, Emmanuel Defay, Laurent Bellaiche
We-S55-P-83
Direct imaging of the effect of screening of ferroic domains by means of UHV PFM
Cecile Saguy, Maya Barzilay, Itamar Holzman, Asaf Hershkovitz, Yachin Ivry

The Fourteenth International Meeting on Ferroelectricity (IMF2017)

Grand Hyatt San Antonio, Texas, USA, Sept. 4-8, 2017

Monday, September 4th, 2017 - Welcome Hall - 14:00 - 18:00

Welcome and Registration

Tuesday, September 5th, 2017 - Welcome Hall - 07:30 - 08:30

REGISTRATION

Tuesday, September 5th, 2017 - Plenary Room - 08:30 - 09:00

Plenary - OPENING

Tuesday, September 5th, 2017 - Plenary Room - 09:00 - 09:50

Plenary - PLENARY 01

Tu-S-O-01

(INVITED) Systems with defects of "random local field" or "random local anisotropy" types: validity of the Imry-Ma theorem

Alexander Sigov [1], Alexander Morosov [2], Alexey Berzin [1]

[1] *Moscow Technological University (MIREA), Moscow, Russia*
[2] *Moscow Institute of Physics and Technology (State University), Moscow, Russia*

After the classical paper by Imry and Ma [PRL 35,1399 (1975)], the viewpoint was firmly established in the literature that at space dimensions d<4 the introduction of an arbitrarily small concentration of defects of the "random local field" or “random easy axis” types into a system with continuous symmetry of the n-component vector order parameter (O(n) model) leads to the long-range order collapse and to the occurrence of a disordered state, which in what follows will be designated as the Imry-Ma state and the statement given above was named the Imry-Ma theorem. We demonstrate that this theorem is not universally true and propose the conditions of its applicability. An anisotropic distribution of the directions of defect-induced random local fields or random easy axes in the order parameter n-dimensional space gives rise to the effective anisotropy in the system. The effective anisotropy can be

both “easy axis” and “easy plane” types. The Imry-Ma theorem breaks down due to existence of the “easy axis” anisotropy induced by the defects designed initially for breaking down the long-range order. In the case of slightly anisotropic distribution of the fields or easy axes, there exists a critical concentration of defects, if exceeded, the Imry-Ma inhomogeneous state can exist as an equilibrium one. In the case of strongly anisotropic distribution, the Imry-Ma inhomogeneous state is completely suppressed and the state with the long-range ordering is realized at any defect concentration.

Keywords: defects, imperfect systems, order parameter, O(n) model, long-range ordering, phase diagram, Imry-Ma theorem.

Tuesday, September 5th, 2017 - Room1 - 10:20 - 10:50

keynote speaker - THEORY I

Tu-S-O-01

(INVITED) Non-linearity of ferroelectric oxides and possible applications in neuromorphic computing?

Alex Demkov

The University of Texas, Austin, United States

A recent discovery of growth methods that allow for growing transition metal oxides or TMOs directly on Si, created revolutionary opportunities in silicon photonics, a hybrid technology combining semiconductor logic with optical information technologies. I will discuss the recent progress in development and integration of nonlinear optical materials that will enable combining semiconductor logic with fast broadband optical. This combination advances the nonlinear optical materials for defense applications and telecom industries, where the benefits of reliability, smaller size and weight, and lower cost of ownership are compelling. In particular, neurocomputing may benefit from this technology. A typical neurocomputer is a network of simple artificial neurons that process information in parallel. The salient features of this paradigm, its massive connectivity and parallelism, are most naturally realized in optics, where analog inner products and simple point nonlinearities are precisely the computations needed. Optics and neural networks present an ideal match of requirements and capabilities. I will briefly discuss possible opportunities in neuromorphic computing created by integration of TMOs with silicon.

Keywords: integrated oxides, Pockels effect, Molecular Beam Epitaxy, neuromorphic computing

Tuesday, September 5th, 2017 - Room2 - 10:20 - 10:50

keynote speaker - DIELECTRICS I

Tu-S-O-01

(INVITED) Photovoltaic properties of some lead free (KNN) and lead-based (PFN) multiferroics

JOSE ANTONIO EIRAS

Federal University of São Carlos, Physics Department, São Carlos, Brazil

Single phase multiferroic materials, that present typical ferroelectric ordering coexisting with magnetic ordering, are being intensively investigated, viewing to the coupling between spontaneous polarization and magnetization (magnetoelectric effect - ME). Multiferroic and photovoltaics materials have traditionally been investigated separately, although the coupling between light absorption and ferroelectricity has been known for years. Multiferroics may present a bandgap that is significantly lower than that of classical ferroelectrics, due to the pronounced electron-electron coupling, allowing combining ferroelectric properties with a low bandgap semiconductor material offering excellent options to tune photovoltaic properties. The efficiency of light conversion to electric energy (photovoltaic effect) in these materials can be modified by new techniques of synthesis, by suitable doping and sample conformation. In this presentation will be presented discussed semiconductor e photovoltaic properties of some lead free (KNN) and led based (PFN) multiferroics bulk and thin films. High density bulk ceramics samples were obtained through conventional or Spark Plasma Sintering technique (SPS). Thin films were grown by RF sputtering. Electric dielectric and photovoltaic properties have been investigated submitting the samples to different oxidation treatments, which allow changing the amount of oxygen vacancies generated during the sintering. Transport properties of domains and domain walls were investigated macroscopically, with conventional I-V techniques, and microscopically, using conductive atomic force microscopy (c-AFM). UV-Vis spectra of surface reflection revealed a remarkable dependence of the light absorption and, consequently, in the optical bandgap on the processing procedure.

Keywords: Photovoltaics, Multiferroics, ferroelectrics, KNN, PFN.

Tuesday, September 5th, 2017 - Room3 - 10:20 - 10:50

keynote speaker - RELAXORS I

Tu-S-O-01

(INVITED) Ferroic superglasses: Relaxor ferroelectric PMN versus CoFe superspin glass

Wolfgang Kleemann [1], Jan Dec [2]

[1] *University Duisburg-Essen, Physics Department, Duisburg, Germany*
[2] *University of Silesia, Institute of Materials Science, Katowice, Poland*

The term ‘ferroic glass’ was coined [Ren, 2014] for strain, magnetic, and electric dipolar nanodomain states, which undergo glassy dynamic criticality as $T \dashrightarrow T_g$ and non-ergodicity at $T < T_g$. While these

features are also found in 'superdipolar glass' systems of matrix isolated magnetic nanoparticles as in $[Co_{80}Fe_{20}(0.9\ nm)/Al_2O_3(3\ nm)]_{10}$ multilayers [Bedanta, Petracic, Kleemann, 2015], the mesoscopic 'ferroic glasses' are generally more complex due to the much closer relationship of the nanodomains to the embedding matrix. This is shown for the archetypical relaxor $PbMg_{1/3}Nb_{2/3}O_3$ [Kleemann, Dec, 2016], where quenched electric random fields give rise to creation and growth of polar nanoregions (PNR) on cooling toward T_g with a spectrum of relaxation frequencies skewing from Lacroix-Béné to Cole-Davidson-type. It becomes replaced by relaxation and creep-like domain wall dynamics below T_g ~ 240 K, where the PNR percolate [Jeong *et al*., 2005; Koreeda *et al*., 2013] and form a ferroelectric microdomain state under the control of the ferroelectric F_{1u} soft lattice mode [Fu *et al*., 2012].

Keywords: random electric fields, polar nanoregions, superdipolar glass, percolation, domain wall dynamics

Tuesday, September 5th, 2017 - Room4 - 10:20 - 10:50

keynote speaker - FERROICS/MULTIFERROICS I

Tu-S-O-01

Ferroionic states: coupling surface electrochemistry with bulk ferroelectricity

Sergei Kalinin

Oak Ridge National Lab, Oak Ridge, United States

Ferroelectricity on the nanoscale has remained a subject of much fascination in condensed matter physics for the last several decades. It is well-recognized that stability of the ferroelectric state necessitates effective polarization screening, and hence screening mechanism and screening charge dynamics become strongly coupled to ferroelectric phase stability and domain behavior. We pose that in the nanoscale systems, the ferroelectric state is fundamentally inseparable from electrochemical state of the surface, leading to emergence of coupled electrochemical-ferroelectric states. I will present the results of experimental and theoretical work exploring the basic mechanisms of emergence of these coupled states including the basic theory and phase-field formulation for domain evolution. I further discuss the thermodynamics and thickness evolution of this state using analytical theory and phase-field modelling. These considerations further stimulate the development of the novel SPM modalities addressing time-dependent dynamics and chemical changes during SPM imaging. I will introduce the general data acquisition mode (GMode) of SPM, based on full data capture and subsequent information theory and physics based analysis of the data stream. I will further delineate the applications of in-situ SPM – time of flight secondary ion mass spectrometry (ToF SIMS) to map the changes in surface chemistry during tribological and local electrochemical experiments, including ferroelectric polarization switching and pressure-induced resistance changes in oxides. These analyses reconcile multiple prior studies, and set forward the predictive pathways for new generations of ferroelectric devices and applications.

Keywords: piezoresponse, ferroelectric surfaces, ToF-SIMS

Tuesday, September 5th, 2017 - Room1 - 10:50 - 11:15

Invited talk - THEORY I

Tu-S-O-01

(INVITED) First-principles based Landau-Devonshire potential for $BiFeO_3$

Pavel Marton [1, 2], Antonín Klíč [1], Marek Paściak [1], Jiří Hlinka [1]

1 Institute of Physics, Czech Academy of Sciences, Na Slovance 2, Praha, Czech Republic
2 Institute of Mechatronics and Computer Engineering, Technical University of Liberec, Studentská 2, Liberec, Czech Republic

BiFeO3 is a prototypical multiferroic material with large ferroelectric polarization and strong influence of the oxygen-octahedra tilts on its properties. Although properties of such material can be already efficiently studied with accurate first-principles and atomistic calculations and simulations, on the larger scale, e.g. for modelling of domain walls and their mutual interactions, it is still necessary to resort to simpler models. Among these the Landau approach has recently turned out to be extremely profitable. Although there are some parametrizations of Landau-type models [1,2,3], to our knowledge none of these is general enough to exceed limits of specific utilization for which they were developed. We present here a first-principles-based (zero temperature) parametrization of the Landau-Devonshire-type energy expansion of BiFeO3 [4] in terms of ferroelectric polarization, oxygen-octahedra tilts and mechanical strain. The scheme is based on extrapolation of the *R*3*c* structural distortion of the ground-state from the cubic reference state. This allows us to probe the energy surface for extended set of points in the parameter space and even those points, which would otherwise be difficult to access. We show that the acquired parametrization, despite simplicity of the adopted scheme, leads to tensorial properties in a sound agreement with available experimental and first-principles data. Where possible, we compare our results to the other parametrizations.

References

[1] Xue et al., Phys. Rev. B vol. 90, 220101 (2014).

[2] Popkov et al., Phys. Rev. B vol. 92, 140414 (2015).

[3] Kulagin et al., Physics of the Solid State vol. 57, 933 (2015).

[4] Marton et al., in preparation.

Keywords: BiFeO3, Landau-Devonshire potential, first-principles

Tuesday, September 5th, 2017 - Room2 - 10:50 - 11:15

Invited talk - DIELECTRICS I

Tu-S-O-01

(INVITED) Role of Li for $BaTiO_3$ based lead-free piezoelectric ceramics

Jiwei Lou [1], Xiaoming Chen [1], Jiangtao Zeng [1], Dokyun Kim [2], Liaoying Zheng [1], Zhenyong Man [1], Chul Hong Park [2], Guorong Li [1]

[1] *Key Laboratory of Inorganic Functional Materials and Devices, Shanghai Institute of Ceramics, Chinese Academy of Sciences,, Shanghai, China*
[2] *Department of Physics Education, Pusan National University, Pusan 609735, Pusan, Korea, Republic of (South)*

The Li^+-containing additives is an useful sintering aid to decrease the sintering temperature. Li ions can incorporate into the lattice of $BaTiO_3$ based ceramics during the sintering process. However, it is not clear where Li+ ions located in A or B site , which caused some confusion in understanding the nature of doping Li cations in the perovskite structure. In this report, the Li-doped $(Ba_{0.85}Ca_{0.15})(Ti_{0.9}Zr_{0.1})O_3$ (BCZT) and $BaTiO_3$ ceramics were investigated. It is found that the Li doping increases the activation energy of the ionic conduction and hardening the piezoelectric properties of BCZT ceramics. For $Ba_{1-x}Li_xTiO_{3-x/2}$, $BaTi_{1-x}Li_xO_{3-3x/2}$ and $BaTiO_{3+x}$+ $(x/2)Li_2CO_3$ ceramics (x = 0, 0.01, 0.03, 0.05, 0.07), the results show that Li^+ prefers to selectively substitute Ba^{2+} at A site then to substitute when the concentration of Li^+ is below 1%, then enters into B site for Ti^{4+} at B site in $BaTiO_3$+$(x/2)Li_2CO_3$ ceramics. All Li-doped $BaTiO_3$-based ceramics exhibit double hysteresis loops. Based on various measurements and the first-principles calculations, it is proposed that the interaction between Li, especially at B-site, and O-vacancy and the dipolar defect Li-OV and their clustering should play an important role in the electrical and piezoelectric properties.

Keywords: Lead-free, Piezoelectric, BaTiO3, Ceramics

Tuesday, September 5th, 2017 - Room3 - 10:50 - 11:15

Invited talk - RELAXORS I

Tu-S-O-01

(INVITED) Multiple length scales in relaxor ferroelectrics

Kenji Ohwada [1, 2], Jun'ichiro Mizuki [2, 1], Kazumichi Namikawa [3]

[1] *National Institutes for Quantum and Radiological Science and Technology, Sayo, Japan*
[2] *Kwansei Gakuin University, Sanda, Japan*
[3] *Tokyo Gakugei University, Koganei, Japan*

Relaxor ferroelectrics are characterized by a number of unique properties, many of which are strongly related to the scales inside. The elationship between the crystal coherence length and electrical response

of $Pb[(Mg_{1/3}Nb_{2/3})_{1-x}Ti_x]O_3$ near the morphotropic phase boundary have been precisely investigated using a single crystal with a Ti composition gradient at room temperature by synchrotron x-ray scattering. The crystal coherence length (ξ) determined from the widths of Bragg scattering varies by over two orders of magnitude in a 10 mol% range (ξ = 70 nm - > 10 μm) of the Ti composition. It is shown that there is a strong negative correlation between the low-frequency electrical response and the crystal coherence length at the sub-μm scale [1]. The study of $0.91Pb(Zn_{1/3}Nb_{2/3})O_3$-$0.09PbTiO_3$ near T_c = 455 K shows that the heterophase fluctuation with a size of $\xi \sim 200$ nm is expected to correlate to the low-frequency dielectric dispersion and contribute to the phase transition as a precursor phenomenon of the first-order phase transition [2]. Nanometer scale structures, a deviation from average structures discussed above, can contribute to the high-frequency response. The structures can be observed as a diffuse x-ray scattering around the Bragg position and the intensity shows similar temperature dependence to that of high-frequency dielectric response [2].

References

[1] D. Shimizu, K. O. *et al.*, Phys. Rev. B 92, 174121 (2015).

[2] K. Ohwada *et al.*, Phys. Rev. B 90, 104109 (2014), Phys. Rev. B 83, 224115 (2011).

Keywords: multiple length scale, synchrotron x-ray scattering, diffuse x-ray scattering

Tuesday, September 5th, 2017 - Room4 - 10:50 - 11:15

Invited talk - FERROICS/MULTIFERROICS I

Tu-S-O-01

(INVITED) Spin-lattice coupling in the potential multiferroic $SmFeO_3$

Mads Weber [1, 2, 3], Mael Guennou [1], Jens Kreisel [1, 2]

1 Luxembourg Institute of Science and Technology, Belvaux, Luxembourg
2 University of Luxembourg, Belvaux, Luxembourg
3 ETH Zürich, Zürich, Switzerland

Much current research is devoted to identify multiferroic materials that possess strongly coupled ferroic properties. So-called “type II" multiferroics attract interest for their magnetically-induced ferroelectricity providing direct coupling of both properties. Since recently, rare earth orthoferrites, RFeO3 have been considered as such type II multiferroics. Generally speaking, the rich magnetic landscape of rare-earth orthoferrites, including high Néel temperatures (600 K and 700 K), spin reorientations, ordering of the rare-earth sub-lattice and compensation of the two spin lattices, makes these materials potential candidates for magneto-electric coupling. In this work, we focus on SmFeO3, which has high magnetic transitions temperatures in comparison with other RFeO3. We have been particularly interested in investigating the coupling of different magnetic orders with the crystal lattice (spin lattice-coupling). For this, we have studied the structural evolution of SmFeO3 by optical

birefringence, Raman spectroscopy and Resonant Ultrasound Spectroscopy, over a wide range of temperature. Besides the well-known magnetic ordering at the Néel temperature and the spin reorientation, we have identified two new anomalies in the signature of spin-lattice coupling and two magnon excitations. Overall, our study illustrates a surprising rich landscape of lattice anomalies of different origin and coupling strength. These structural instabilities are triggered by different magnetic ordering processes and give rise to a multiplicity of possible coupling phenomena, some of which might lead to ferroelectricity.

Keywords: multiferroic, spin-lattice coupling, magnetic transitions

Tuesday, September 5th, 2017 - Room1 - 11:15 - 12:30

Oral presentation - THEORY I

Tu-S-O-01

First-principles study of (Ba,Ca)(Ti,Zr)O_3 solid solutions

Danila Amoroso [1, 2], Andres Cano [2], Philippe Ghosez [1]

[1] *Theoretical Materials Physics, Q-MAT, CESAM, University of Liege (B5), B-4000 Liege, Belgium, Liege, Belgium*
[2] *ICMCB, CNRS, University of Bordeaux, UPR 9048, F-33600 Pessac, France, Pessac, France*

By means of first-principles calculations different chemical compositions of (Ba,Ca)(Ti,Zr)O_3 solid solutions are investigated by focusing on the properties arising from the lattice dynamics. Our goal is to better understand the microscopic mechanisms involved in the appearence and competition of different phases and to rationalise the search of optimal compositions for large electrochemical response. We start by analyzing the four parents bulky compounds in order to clarify the dynamical properties and energetics at play between various phases. Then, a systematic characterization of the binary sistems $BaTiO_3$-$CaTiO_3$ and $BaTiO_3$-$BaZrO_3$ is carried out within both the Virtual Crystal Approximation (VCA) and standard Density Functional Theory (DFT) based on supercell calculations. It results that VCA is not appropriate to properly describe effects coming from both (Ba^{2+}-Ca^{2+}) and (Ti^{4+}-Zr^{4+}) substitutions. The failing of this approach is especially evident for Ba(Ti,Zr)O_3 system, where local correlations due to specific atomic and geometrical ordering give rise to unexpected polar activation of zirconium. A simple description of these mechanisms is achieved via a basic electrostatic model based on $BaZrO_3$/*m*$BaTiO_3$ supercells.

Keywords: First-principles, Pb-free solid solutions, lattice dynamics, structures

---

Tu-S-O-02

Fluctuations and topological defects in proper ferroelectrics

Sergei Prokhorenko [1, 2], Yousra Nahas [2], Laurent Bellaiche [2]

[1] *Université de Liège, Physique Théorique des Matériaux, Liège, Belgium*
[2] *Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, United States*

Topologically nontrivial dipolar patterns like vortices, hedgehogs (monopoles) and skyrmions are not commonly expected to appear in bulk ferroelectric materials. Indeed, unlike ferroelectric nanostructures or relaxors, bulk ferroelectrics exhibit neither depolarizing nor random local fields that can render topological defects energetically favorable. Furthermore, polar bulks also appear to fall short of alternative, "topological", defect stabilization mechanisms as a result of inherent discrete symmetries of these systems. In this study, we combine homotopy theory and first-principles-based effective Hamiltonian approach to explore stability of topological defects in bulk $BaTiO_3$. Our results show that, against all odds and theoretical expectations, this proper ferroelectric material can exhibit stable topological point defects in its tetragonal polar phase and stable topological line defects in its orthorhombic polar phase. The stability of such defects originates from a novel mechanism of topological protection related to finite-temperature fluctuations of local dipoles. Large-scale effective Hamiltonian Monte Carlo simulations are then conducted to confirm these theoretical predictions. The results of our work, hence, reveal a novel mechanism of topological protection that can be realized in proper ferroelectrics and provide a theoretical framework for investigations of topological defects in systems with finite underlying symmetries.

Keywords: proper ferroelectrics, BaTiO3, topological defects, fluctuations, local structure

---

Tu-S-O-03

Modelling the photostriction of ferroelectric materials from first-principles

Charles Paillard [1, 2], Bin Xu [1], Grégory Geneste [3], Brahim Dkhil [2], Laurent Bellaiche [1]

[1] *University of Arkansas, Fayetteville, United States*
[2] *Laboratoire SPMS, UMR CNRS/CentraleSupélec, Gif-sur-Yvette, France*
[3] *CEA DAM, Arpajon, France*

Photostriction is the non-thermal strain experienced by a material under illumination. Despite the intense scrutiny for its potential application in the control of magnetic layers through a ferroelectric substrate [1] or the generation of ultra-fast giant shear strain [2], it has so far been considered only very scarcely from a theoretical point of view. Here, we employ the first-principles ΔSCF method to model the photostriction phenomenon in various classical ferroelectric materials such as barium titanate, lead titanate, as well as the multiferroic bismuth ferrite [3]. This simple method reveals striking features common to all these ferroelectric, namely photostriction arises from the polarization relaxation caused by photo-induced carriers in the conduction and valence bands, resulting in a photo-induced strain mediated by the converse piezoelectric effect. Advances in the methodology, to take into account the polarization of light for instance, are also presented.

References

[1] Iurchuk, V., et al. Physical Review Letters 117, 107403 (2016).

[2] Lejman, M. et al., Nature Communications 5, 4301 (2014).

[3] C. Paillard, B. Xu, B. Dkhil, G. Geneste and L. Bellaiche, Physical Review Letters 116, 247401 (2016).

Keywords: Photostriction, first-principles

Tu-S-O-04

First-principle prediction of novel multiferroic phases in epitaxial (111) $BiFeO_3$ films

Changsong Xu [1], Hongjun Xiang [2], Laurent Bellaiche [1]

[1] *Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, United States*
[2] *Key Laboratory of Computational Physical Sciences (Ministry of Education), State Key Labora- tory of Surface Physics, and Department of Physics, Fudan University, Shanghai, China*

Multiferroic materials are currently attracting a lot of interest because of the cross-coupling between their electrical and magnetic properties, which has the potential to lead to novel devices. There is a relatively small number of multiferroics currently known to exist and, hence, plenty of researches are devoted to design materials and phases possessing both ordered electric and magnetic dipoles. Here, we perform first-principles calculations on epitaxial (111) $BiFeO_3$ films, and predict two novel stable multiferroic phases there. The first phase is the $YMnO_3$-type hexagonal $P6_3cm$ phase. It has an out-of-plane electrical polarization that anomalously increases when increasing the strength of the tensile epitaxial strain, and also possesses magnetic arrangements that are reminiscent of spin frustrations. The second phase adopts a $P1$ space group with a polarization having both out-of-plane and in-plane components, as well as, ferrimagnetism. These in-plane polarization and ferrimagnetism are both linked to a specific Fe-O bond, which is promising for inducing strong magnetoelectric coupling. The nature (i.e., improper *versus* proper) of the polarization in the $P6_3cm$ and $P1$ phases will also be discussed.

Keywords: BiFeO3, phases transitions, improper ferroelectricity, first-principles

---

Tu-S-O-05

Zone-boundary phonon instabilities investigated with neutron scattering combined with Anharmonic First-Principles simulations

Olivier Delaire [1, 2], Huibo Cao [2], Jiawang Hong [2, 3], Dipanshu Bansal [1, 2], Steven Hahn [2], Barry Winn [2], Songxue Chi [2], Georg Ehlers [2], Haidong Zhou [4], Lynn Boatner [2], Jiaqiang Yan [2, 4]

[1] *Duke University, Durham, NC, United States*
[2] *Oak Ridge National Laboratory, Oak Ridge, TN, United States*

[3] *Beijing Institute of Technology, Beijing, China*
[4] *University of Tennessee, Knoxville, TN, United States*

Zone-boundary soft-modes have long been of interest in antiferrodistortive (AFD) systems such as $SrTiO_3$, and more recently the antiferromagnetically-ordering $EuTiO_3$. Their coupling to polar modes are also central in novel hybrid-improper ferroelectric compounds, or the archetypal improper ferroelectric, $YMnO_3$. This presentation will illustrate how inelastic neutron scattering (INS) measurements resolve anharmonic lattice dynamics across the Brillouin zone, providing important constraints for theory. In addition, we will discuss our anharmonic first-principles simulations (DFT), of the temperature-dependent lattice dynamics, including in the paraelectric phase, and direct comparison to INS measurements. In $SrTiO_3$ and $EuTiO_3$, alternative tilts of oxygen octahedra are the dominant lattice instability and result in AFD transition from cubic perovskite to a tetragonal phase at Tc=105 K and 280 K, respectively. This transition involves the softening of the R_{25} phonon mode (R-point). The temperature dependence of this R_{25} mode -as well as the zone-center TO ferroelectric mode- are clearly seen in INS data, and quantitatively reproduced in our anharmonic DFT simulations, including the renormalization of phonon frequencies. In $EuTiO_3$, the low-temperature magnetic ordering and magnetic excitations were also investigated. In the hexagonal manganite $YMnO_3$, the (1260 K) improper ferroelectric transition is driven by a K-point lattice instability, coupled to a polar mode. We have successfully mapped the unstable phonon branch and its temperature dependence with INS, and also achieved realistic simulations of the high-temperature lattice dynamics.

Keywords: improper ferroelectrics, multiferroics, phase transition, soft-modes, phonon anharmonicity

Tuesday, September 5th, 2017 - Room2 - 11:15 - 12:30

Oral presentation - DIELECTRICS I

Tu-S-O-01

Structure, dielectric and ferroelectric properties of NBT- and KNN- based perovskite ceramics

Ekaterina Politova

L.Ya.Karpov Institute of Physical Chemistry, Moscow, Russia

Lead-free ferroelectric materials on the base of $(Na_{0.5}Bi_{0.5})TiO_3$ (NBT) and $(K_{0.5}Na_{0.5})NbO_3$ (KNN) are being intensively studied in order to replace widely used Pb-based ones. In this work, effects of modification of compositions by donor and acceptor dopants in the A- and B-sites of perovskite lattice and over stoichiometric additives on structure, dielectric and ferroelectric properties of ceramics in the $(K_{0.5}Na_{0.5})NbO_3$ (KNN), $(Na_{1/2}Bi_{1/2})TiO_3$ - $BaTiO_3$ (NBT-BT) and $(Na_{1/2}Bi_{1/2})TiO_3$ - $BaTiO_3$ - $Bi(Mg_{1/2}Ti_{1/2})O_3$ (NBT-BT-BMT) systems have been studied. Ceramic samples were prepared by the two-step solid-state reaction method at temperatures of 970–1470 K. The samples were characterized using the X-ray Diffraction, Scanning Electron Microscopy, Second Harmonic Generation (SHG), and Dielectric Spectroscopy methods. Ferroelectric phase transitions were revealed at ~ 350 - 400 K and at

~ 550 K (NBT-based) and at ~700 K (KNN) in the dielectric permittivity versus temperature curves. Phase transitions near 350-400 K revealed typical relaxor-type behavior attributed to the presence of polar nanoregions in a nonpolar matrix. Increase in the spontaneous polarization value was observed in modified ceramics using the SHG method. At the room temperature, non monotonous changes of the dielectric parameters were observed in modified compositions studied. The results obtained confirmed prospects of new lead-free materials development by modification of KNN- and NBT-based compositions close to the MPB by aliovalent cation substitutions.

Keywords: Perovskite structure, ferroelectric properties, NBT, KNN

Tu-S-O-02

In search for artificial MPBs: Dielectric spectroscopy of $BaTiO_3$-$KNbO_3$ composites

Maksim Ivanov [1], Sergejus Balčiūnas [1], Jūras Banys [1], Satoshi Wada [2]

[1] *Vilnius university, Vilnius, Lithuania*
[2] *Interdisciplinary Graduate School of Medical and Engineering, University of Yamanashi, Kofu, Japan*

High piezoelectric activity is of high demand for various applications. The desired properties are most often observed in solid solutions displaying the so-called Morphotropic Phase Boundary (MPB), when two different lattice structures are of similar energy, thus extrinsic stimulus leads to easy deformation. However, not all solid solutions exhibit the MPB. As a result artificial MPBs are of high interest, and they can be formed in ferroelectric composites. $BaTiO_3$ (BT) and $KNbO_3$ (KN) were selected as the starting members, as they are both lead-free ferroelectrics and have dissimilar lattice structures at room temperature. Creating epitaxial interfaces with KN inside BT structure creates stresses that increases domain wall count and, as a result, piezoelectric coefficient. Composites were prepared in two steps: cold-pressed BT particles were heated to 1000 °C for 2 h to create low-density ceramics, then KN were epitaxially deposited to BT structure. In this presentation dielectric properties of BT-KN with different KN molar ratios will be presented. It was found, that the piezoelectric effect gives a significant contribution to the total dielectric permittivity. Impact of KN on the piezoelectricity of the strained BT was obtained and compared.

Keywords: Dielectric spectroscopy, artificial MPB, composite, lead-free piezoelectric

---

Tu-S-O-03

Tuning optical responses with strain in multiferroelectrics and ferroelectrics

Yurong Yang [1], Daniel Sando [2], Lan Chen [4], Xiangkang Meng [4], Agnes barthelemy [2], Manuel Bibes [2], Eric Bousquet [3], Philippe Ghosez [3], Laurent Bellaiche [1]

[1] *University of Arkansas, Fayetteville, AR, United States*
[2] *Unité Mixte de Physique CNRS/Thales, Palaiseau Cedex, France*

[3] *Université de Liège, Sart Tilman, Belgium*
[4] *Nanjing University, Nanjing, China*

The control of optical fields is usually achieved through the electro-optic or acousto-optic effect in single-crystal ferroelectric or polar compounds such as $LiNbO_3$ or quartz. In recent years, tremendous progress has been made in ferroelectric oxide thin film technology, a field which is now a strong driving force in areas such as electronics, spintronics and photovoltaics. Here, we investigate, both from experiments and first-principle techniques, if and how epitaxial strain engineering can tune the optical response of $BiFeO_3$ and $PbTiO_3$ thin films [Nat. Commun. 7, 10718(2016); Phys. Rev. Lett. 115, 267602 (2015)]. We find a very large variation of the optical index with strain in $BiFeO_3$, corresponding to an effective elasto-optic coefficient larger than that of quartz. We also observe there a concomitant strain-driven variation in light absorption, which is reminiscent of piezochromism and which we show can be manipulated by an electric field. This constitutes an electrochromic effect that is reversible, remanent and not driven by defects. We also predict large elasto-optic coefficients in two strain-driven monoclinic phases (of *Pm* and *Cm* symmetries) in $PbTiO_3$ films being under small tensile epitaxial strain. The origin of such large conversion between elastic and optical properties is further elucidated. Our findings broaden the potential of multiferroics towards photonics and thin film acousto-optic devices, and suggest exciting device opportunities arising from the coupling of ferroic, piezoelectric and optical responses.

Keywords: elasto-optic effect, strain, ferroelectrics, multiferroics

---

Tu-S-O-04

Understanding the reason for large dielectric response in Pb-free (1-x)$Ba(Zr_{0.2}Ti_{0.8})O_3$-x$(Ba_{0.7}Ca_{0.3})TiO_3$ ferroelectric ceramics

Jinghui Gao [1], Xinghao Hu [1], Yan Wang [1], Yongbin Liu [1], Xiaobing Ren [2]

[1] *State Key Laboratory of Electrical Insulation and Power Equipment and Multi-disciplinary Materials Research Center, Frontier Institute of Science and Technology, Xi'an Jiaotong University, Xi'an, China*
[2] *Ferroic Physics Group, National Institute for Materials Science, Tsukuba, Japan*

(1-x)$Ba(Zr_{0.2}Ti_{0.8})O_3$-x$(Ba_{0.7}Ca_{0.3})TiO_3$ (BZT-*x*BCT) ceramics have been reported to exhibit large dielectric response in the vicinity of the multi-phase-coexisting point (i.e. triple point). However, the reason for large dielectric response in such a material system is still unclear and thus awaits explanation. In this paper, we investigate the reason for large dielectric response by studying the phase transition behavior around the triple point of BZT-*x*BCT ceramics. Rayleigh analysis indicates that strong dielectric response is due to large reversible contribution caused by phase transition. Moreover, TEM study shows a mottled domain structure with numerous nanodomains close to triple point. Further thermal analysis results suggest that the enthalpy nearly vanishes and the associated specific heat shows

discontinuity on the triple point, which suggest a nearly tricritical behavior, which maybe responsible for large dielectric permittivity in BZT-*x*BCT.

Keywords: Pb-free ferroelectric materials; dielectric property; domain structure; phase transition

---

Tu-S-O-05

(INVITED) Exploring $BiFeO_3$-based solid solutions and heterolayers for multifunctional applications

John Wang

Department of Materials Science and Engineering, National University of Singapore, Singapore, Singapore

$BiFeO_3$-based solid solutions, i.e., $BiFeO_3$-ABO_3, have been extensively studied for multiferroic behavior by manipulating the crystal structure and coupling between the ferroelectric order and magnetic order. Taking two different approaches, namely epitaxial straining and cation substitution (on either A-site or B-site or both sites), we have developed a series of BFO-based solid solutionsof perovskites structure as a class of important Pb-free electroceramics. Interestingly, several different crystal structures and therefore ferroelectric and piezoelectric behavior are realized. A particularly interesting structure is the super-tetragonal (T) phase, which can well be retained by chemical doping, such as Ga substitution for Fe in BFO, where $BiFe_{0.6}Ga_{0.4}O_3$is a good example. Investigations into the ferroelectric behavior, by both global property measurement, such as P-E, and local PFM studies, support a new type of microscopic origin of ferroelectric polarization from the ion displacement induced dipole moments. In addition to the multiferroic behavior, a newly emerging function of $BiFeO_3$-basedthin films is the photovoltaic behavior, which can well be tuned and much enhanced by both chemical doping and formation of proper heterolayers, examples of which are In_2O_3-SnO_2/ZnO/$BiFeO_3$/Pt and In_2O_3-SnO_2/$BiFe_{0.6}Sc_{0.4}O_3$/$LaNiO_3$. In this talk, we will report the latest development of $BiFeO_3$-based solid solutions for both multiferroic and photovoltaic applications.

Keywords: Ferroics, Photovoltaic

Tuesday, September 5th, 2017 - Room3 - 11:15 - 12:30

Oral presentation - RELAXORS I

Tu-S-O-01

The polar nano regions-to-relaxor transition in PMN and PSN [$Pb_{1-X}(Sc_{1/2}Nb_{1/2})O_{3-X}$], where X is the bulk concentration of nearest neighbor Pb-O divacancies

Benjamin Burton, Eric Cockayne

NIST, Gaithersburg, United States

In previous work, molecular dynamics simulations based on a first-principles-derived effective Hamiltonian for $Pb_{1-X}(Sc_{1/2}Nb_{1/2})O_{3-X}$ (PSN), with nearest-neighbor [Pb-O] divacancy pairs, was used to calculate X[Pb-O] vs. T, phase diagrams for PSN with: ideal rock-salt type chemical order; nanoscale chemical short-range order; and random chemical disorder. Here, we show that the phase diagrams should include additional regions in which a glassy relaxor-phase (or state) is predicted. Curves that locate the PNR-to-Relaxor transition are referred to as T*(X), where T* is a characteristic temperature at which a small but significant stiffining of polar nano-domains occurs; T* appears to be a weakly first-order transition, but these are numerical simulations, so order of transition, or crossover, can not be clearly established. With respect to phase diagram topology, these results strongly support the analogy between relaxors and magnetic spin-glass-systems. Similar calculations for PMN [$Pb(Mg_{1/3}Nb_{2/3})O_3$] evaluated the effects of various cation configurations on T* follow the same trends as those for PSN: increased cation order implies reduced random fields, and therefore higher T*-values. As in PSN, T* most often appears to be a weakly first-order transition, with the same caveat that numerical simulations can't unambiguously predict the order of a transition.

Keywords: relaxor, ferroelectric, T-star, phase diagram, PSN, PMN

Tu-S-O-02

Observation of positive and negative magnetodielectric effects in relaxor $PbCo_{1/3}Nb_{2/3}O_3$ ceramic

Adityanarayan H. Pandey [1, 2], Surya M. Gupta [1, 2], Anand M. Awasthi [3]

[1] *Homi Bhabha National Institute, Anushaktinagar, Mumbai, India*
[2] *Laser Materials Section, Raja Ramanna Centre for Advanced Technology, Indore, India*
[3] *cUGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore, India*

Lead cobalt niobate ($PbCo_{1/3}Nb_{2/3}O_3$: PCN) is a multifunctional relaxor electroceramic which are very popular due to their extraordinary properties and applications. To the best of our knowledge magnetoedielectric study of PCN ceramic has not been reported. We performed magnetodielectric measurement on PCN ceramic synthesized by two step columbite precursor method. Microstructure images revealed closely packed grains with grain size ~8-10 μm. Room temperature XRD pattern suggests single phase pseudo cubic crystal structure having *Pm*3*m* symmetry, where Co and Nb randomly sitting at B-site with lattice constant ~ 4.0496(2) Å. Rietveld refinement yields larger value of thermal parameters, implying Pb and O are disordered along *<111>* and *<110>* directions, respectively. The temperature dependent dielectric properties revealed re-entrant relaxor behaviour (T_m ~ 130 K and 210 K for 1 kHz) along with a high temperature diffused phase transition, T_c ~270 K. The low temperature frequency dependent dielectric maximum, $f(T_m)$ is analyzed using generalized glass model (also called critical slowing down model). The magnetodielectric effect (MDE(%) = (ε'(9T)-ε'(0T))/ε'(0T)*100) depicts positive and negative MDEs implying coupling between mangnetic and dielectric properties. Such positive and negative MDEs are also observed in disordred double perovskite Pr_2CoMnO_6 whereas single MDE peak is reported in B-site ordered phase. Therefore, it is believed that the re-entrant relaxor behaviour and multiple positive-negative megnetodielectric effects are associated

with the quenched disorder as well as multiple heterogeneities present in PCN ceramics and details will be discussed.

Keywords: Relaxor, magnetodielectric, lead cobalt niobate, reentrant phase

---

Tu-S-O-03

$BaZr_{0.5}Ti_{0.5}O_3$: lead-free relaxor ferroelectric or dipolar glass

Cene Filipic [1], Zdravko Kutnjak [1], Rasa Pirc [1], Giovanna Canu [2], Jan Petzelt [3]

[1] *Institute Jozef Stefan, Ljubljana, Slovenia*
[2] *Institute for Energetics and Interphases, Genoa, Italy*
[3] *3Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic*

Glassy freezing dynamics was investigated in $BaZr_{0.5}Ti_{0.5}O_3$ (BZT50) ceramic samples [1,2] by means of dielectric spectroscopy in the frequency range 0.001 Hz–1 MHz at temperatures $10 < T < 300$ K. From measurements of the quasistatic dielectric polarization in bias electric fields up to ∼28 kV/cm it has been found that a ferroelectric state cannot be induced, in contrast to the case of typical relaxors. This suggests that—at least for the above field amplitudes—BZT50 effectively behaves as a dipolar glass, which can be characterized by a negative value of the static third order nonlinear permittivity. The relaxation spectrum has been analyzed by means of the frequency-temperature plot, which shows that the longest relaxation time obeys the Vogel-Fulcher relation $\tau = \tau_0 \exp[E_0/(T - T_0)]$ with the freezing temperature of 48.1 K, whereas the corresponding value for the shortest relaxation time is ∼0 K, implying an Arrhenius type behavior. By applying a standard expression for the static linear permittivity of dipolar glasses and/or relaxors the value of the Edwards-Anderson order parameter q(T) has been evaluated. It is further shown that q(T) can be described by the spherical random bond-random field model of relaxors [3].

References

[1]. T. Maiti, R. Guo, and A. S. Bhalla, J. Appl. Phys. 100, 114109 (2006).

[2]. D. Wang, J. Hlinka, A. A. Bokov, Z.-G. Ye, P. Ondrejkovic, J. Petzelt, and L. Bellaiche, Nat. Commun. 5, 5100 (2014).

[3]. C. Filipic, Z. Kutnjak, R. Pirc, G. Canu, J. Petzelt, Phys. Rev. B 93, 224105 (2016).

Keywords: relaxors, dipolar glasses, BZT

Tu-S-O-04

Permittivity of relaxor $BNT_{0.925}BT_{0.075}x\%Mn$ ceramics found from impedance spectroscopy

V. Hugo Schmidt [1], Noah Archer [1], Chi-Shun Tu [2]

[1] *Montana State University, Bozeman, United States*
[2] *Department of Physics Fu Jen Catholic University, New Taipei City, Taiwan*

Bismuth sodium titanate $(Bi_{0.5}Na_{0.5})TiO_3$ (BNT) based ceramics which are near the morphotropic phase boundary (MPB) have piezoelectric properties comparable to those of lead-containing $Pb(Zr,Ti)O_3$ (PZT). However, the lower depolarization temperature Td for compositions near the MPB causes concern regarding thermal stability under long-time operation. In our previous study of $(Bi_{0.5}Na_{0.5})_{0.925}Ba_{0.075}(Ti_{1-x}Mn_x)O_3$ for x = 0, 0.2, 1.0, and 2.0 mol% ceramics we found that the depolarization temperature (Td) was enhanced remarkably to ~152 °C for the 0.2% Mn composition. We concluded that Mn doping can enhance structural thermal stability in BN7.5BT ceramics as temperature increases. Three ceramic disks of each composition, with 1 mm thickness and 8.3 mm diameter, were sintered for 2 hours at 1170 oC. The disks were coated with silver paste and placed inside a small home-built water-cooled oven and connected to a Solartron SI 1260 Impedance Gain-Phase Analyzer. Runs were made at 100 to 600 ºC in 50 ºC steps. The frequencies used were 0.1 Hz to 1 MHz in 71 logarithmically spaced steps. From the results for ac resistivity $\rho'+j\rho''$ we used the relations $\epsilon'= -\rho''/\omega\epsilon o(\rho'2+\rho''2)$ and $\epsilon''=-\rho'/\omega\epsilon o(\rho'2+\rho''2)$ to find the ac permittivity $\epsilon'+j\epsilon''$. The permittivity found using these relations showed intertwined dielectric and conductivity behavior, including effects of phase-shifted conductivity. The dielectric behavior is typical of relaxor ferroelectrics, obeying a power law relation above the dielectric peak and then the Curie-Weiss law above the Burns temperature.

Keywords: relaxor, perovskite, impedance spectroscopy, permittivity, bismuth sodium titanate

---

Tu-S-O-05

Improving the optical properties of poly(vinylidene fluoride) (PVDF) films by doping with Nd^{3+} compound: Synthesis and characterization

Laís Aguiar [1, 2], Cleiser Silva [2], Caires Anderson [3], Andrelson Rinaldi [2], Eriton Botero [1], Claudio Carvalho [1], Ruyan Guo [4], Evaristo Falcao [1], Amar Bhalla [4]

[1] *Federal University of Grande Dourados, Dourados, Brazil*
[2] *State University of Maringá, Maringá, Brazil*
[3] *Federal University of Mato Grosso do Sul, Campo Grande, Brazil*
[4] *University of Texas at San Antonio, San Antonio, United States*

In the last years ferroelectric polymers as PVDF has attracted the interest in the photonics area because of the possibility to be used as hosts for lanthanides photonics ions. However, few works can be found in the literature about the study of the optical properties of PVDF. In this work, PVDF samples were doped with a complex of 3,4-methylenedioxy cinnamic and neodymium (Nd-MCA) to verify the improvement in the optical fluorescence of the polymeric matrix. The measurements of FT-IR confirmed the incorporation of dopant in the polymeric host. From the optical measurements in

PVDF/Nd-MCA it was observed a broadening in absorption as well as the fluorescence spectra with the increase of the Nd-MCA content. In summary, the experimental results revealed that the PVDF/Nd-MCA is a potential candidate for optical and photonic applications.

We are grateful to the Brazilian Agencies, CAPES, CNPq (process 483683/2010-8 and 208232/2014-1), for the financial support of this work. E. A. Falcão also acknowledges UTSA and MeMDRL for hosting him under the NSF/INAMM and NSF ECCS 1002380 programs.

Keywords: PVDF, Neodymium Compound, Optical Properties,

Tuesday, September 5th, 2017 - Room4 - 11:15 - 12:30

Oral presentation - FERROICS/MULTIFERROICS I

Tu-S-O-01

Lattice dynamics, dielectric properties and phase transitions of $Ag_{1-x}Li_xNbO_3$ ceramics

Antoni Kania [1], Adrian Niewiadomski [1], Seweryn Miga [2], Godefroy Kugel [3], Mustapha Hafid [4], Jan Dec [2]

[1] *A. Che?kowski Institute of Physics, University of Silesia, Katowice, Poland*
[2] *Institute of Materials Sciemce, University of Silesia, Chorzow, Poland*
[3] *University of Metz, Supelec Metz, Metz, France*
[4] *Faculty of Science, Ibn Tofail University, Kenitra, Morocco*

Silver lithium niobates $Ag_{1-x}Li_xNbO_3$ (ALN) are promising lead-free piezoelectrics. X-ray and dielectric studies revealed that for $x \leq 0.05$ ALN solid solutions behave similarly to $AgNbO_3$ and undergo the same sequence of phase transitions between ferrielectric M_1, antiferroelectric M_2 and M_3, and paraelectric O_1, O_2, T and C phases. ALN with $x \geq 0.06$ exhibit normal ferroelectric state and undergo phase transitions between ferroelectric R, antiferroelectric M, and paraelectric T and C phases. Correlation between lattice dynamics and electric order appearance is a main aim of study. High quality $Ag_{1-x}Li_xNbO_3$ ($0 \leq x \leq 0.1$) ceramics were prepared by the conventional solid state reaction route. They were examined by linear and nonlinear dielectric response, Raman scattering and DSC investigations. Analysis of the low frequency Raman spectra showed that for $x \leq 0.05$ the relaxational frequency significantly slows down at freezing temperature T_f and at the ferrielectric M_1-M_2 phase transition, while maximum of central peak intensity corresponds to the M_2-M_3 maximum of permittivity. For $x \geq 0.06$ a significant softening of two low frequency modes is observed when approaching the ferroelectric-antiferroelectric (R-M) phase transition. These characteristic temperatures were confirmed by nonlinear dielectric response which is sensitive to instabilities in physical system. Raman and dielectric studies showed that Nb-ion dynamics plays a crucial role in appearance of specific properties of silver niobate based materials. The modified phase diagram of $Ag_{1-x}Li_xNbO_3$ is proposed.

Keywords: Ag1-xLixNbO3, Raman, nonlinear dielectric response

Tu-S-O-02

Large remnant polarization and enhanced magnetic properties in non-quenched $Bi(Fe,Ga)O_3$-$(Ba,Ca)(Zr,Ti)O_3$ multiferroic ceramics

Ruihong Liang

Shanghai Institute of Ceramics, Chinese Academy of Sciences, shanghai, China

It is a tough issue to unlock the underlying polarization and magnetization simultaneously in non-quenched BiFeO3 ceramics due to high conductivity, intensive domain wall clamping and long range spiral spin arrangement. Here, in this paper, $0.75BiFe_{0.98}Ga_{0.02}O_3$-$0.25(Ba_{0.85}Ca_{0.15})(Zr_{0.10}Ti_{0.90})O_3$ multiferroic ceramics was fabricated by conventional solid state reaction with non-quenched method. The crystalline structure analysis revealed that the ceramics was a single perovskite structure with coexistence of rhombohedral and pseudocubic phases. Complete domain switching was observed in the ceramics with high remnant polarization (44 $\mu C/cm^2$), which was superior to other reported $BiFeO_3$ based lead-free ceramics. Moreover, enhanced ferromagnetism with remnant magnetization (0.20emu/g) was also obtained. We believe that this excellent ferroelectric and ferromagnetic performance demonstrates this non-quenched BiFeO3 based ceramics as quite promising candidate for practical applications.

Keywords: multiferroic ceramics, BiFeO3, polarization , magnetic properties

---

Tu-S-O-03

Structure-property relationships in multiferroic compounds

Luiz F, Cotica [1], Guilherme M. Santos [1], Igor B. Catelani [1], Gustavo S. Dias [1], Ivair A. Santos [1], Jose E. Padilha [2], Ruyan Guo [3], Amar Bhalla [3]

[1] *Department of Physics - State University of Maringa, Maringa - PR, Brazil*
[2] *Federal University of Parana at Jandaia do Sul, Jandaia do Sul - PR, Brazil*
[3] *Department of Electrical and Computer Engineering - University of Texas at San Antonio, San Antonio - TX, Brazil*

Multiferroic magnetoelectric compounds are highly promising candidates for technological applications. Also, these compounds present a rich base for fundamental studies. In this work, we have studied $BiFeO_3$-$XTiO_3$ (X = Ba or Pb) solid solutions, rare-earth A-site substitutions ($Bi_{1-y}Nd_yFeO_3$) and lead free compositions ($AlFeO_3$ and $TbMnO_3$). The samples were processed by a high-energy ball-milling route. Their structural characteristics were carefully investigated by the conventional X-ray diffraction, synchrotron radiation X-ray diffraction and neutron diffraction. Structural refinements were performed by the Rietveld method in order to obtain crystal structure properties and allow electron density calculations (maximum entropy method). Density functional calculations were also used to

study the structural and electronic structures. Ferroic properties were studied by using the dielectric, ferroelectric, magnetic and magnetoelectric measurements.

Keywords: multiferroics, structure-property, electronic structure

---

Tu-S-O-04

Neutron diffraction studies of multiferroic $BiCoO_3$

Keith Taddei [1], Santosh KC [2], Alexei Belik [3], Clarina dela Cruz [1], Valentino Cooper [2]

1 Quantum Condensed Matter Division Oak Ridge National Laboratory, Oak Ridge, United States
2 Materials Science and Technology Division Oak Ridge National Laboratory, Oak Ridge, United States
3 International Center for Materials Nanoarchitectonics National Institute for Materials Science, Namiki Tsukuba, Japan

Room temperature multiferroics have long been a goal of the condensed matter community. A material which exhibits coupled (anti)ferroelectricity and (anti)ferromagnetism with reasonably high ordering temperatures would have imminently practical and widely spanning technological applications. However, to date very few such materials have been discovered ostensibly due to the normally adversarial conditions needed to stabilize either polarization or magnetism. BiFeO3, with *TC* ~ 1100 K, *TN* ~ 650 K and polarization *P* ~ 80 μC/cm2, has proven the most promising of these materials and so provides a natural starting point in the search for new compounds. Here we report the results of neutron diffraction studies on the related BiCoO3 material which exhibits a promisingly high *TN* of ~ 470 K and has been predicted from DFT calculations to exhibit a large spin-driven ferroelectric polarization of ~160 μC/cm2. We comment on the coupling between the stabilization of long range magnetic order and the deformation of the CoO6 octahedra.

Keywords: Muliferroics, Neutron powder diffraction, Magnetism

---

Tu-S-O-05

On the microstructure in the charge-glass state of $Pb_{1-x}Sr_xCrO_3$

Kousuke Kurushima [1, 3], Hirofumi Tsukasaki [1], Yui Ishii [1], Shigeo Mori [1], S Ogata [2], Masaki Azuma [2]

1 Osaka Prefecture University, Sakai Osaka, Japan
2 Tokyo Institute of Technology, Yokohama, Japan
3 Toray Research Center, Shiga, Japan

In this work, we investigated local structures of perovskite PbCrO3, which shows a metal-to-insulator transition and ~ 10% volume collapse, by electron diffraction, high-resolution TEM, HAADF-STEM and EDX mapping experiments. It is revealed that the charge glass state is characterized as the coexisting state of the crystalline state with the cubic structure and the non-crystalline state. The crystalline state in the charge-glass state has characteristic nanodomains consisting of the modulated structure with

3ap×3 ap×3 ap in average, which gives rise to the unique diffuse scattering around the fundamental spots. Furthermore, we investigated variations of nanoscaled local structures of Pb1-xSrxCrO3 by partial substitution of Sr2+ for Pb2+ by electron diffraction and high-resolution scanning TEM experiments. It is found that Pb1-xSrxCrO3 for x = 0.2 shows the coexisting state of charge glass state and five-hold superstructure.

References

[1] M. Wu et al., J. Phys. Chem. C 118, 23274 (2014).

[2] A. M. Arevalo-Lopez et al., J. Solid State Chemistry 180, 3271 (2007).

[3] R. Yu et al., J. Am. Chem. Soc. 137, 12719 (2015).

Keywords: Metal-insulator transition, electron diffraction, mulitiferroic

Tuesday, September 5th, 2017 - Room1 - 13:50 - 14:20

keynote speaker - DOMAINS I

Tu-S-O-01

(INVITED) Domain wall engineering: concept, challenges

Jiri Hlinka

Institute of Physics, Czech Acad. Sci., Prague, Czech Republic

Domain engineering is generally understood as a discipline aimed to modify macroscopic material properties by inducing a desirable domain structure. Recently, however, lots of attention is payed to the properties of individual ferroelectric domain walls. Experimental and theoretical tools allowing to determine local, nanoscale properties become available. Here we would like to consider circumstances under which the properties of ferroelectric domain walls themselves may have an important influence on the overall macroscopic material properties.

Keywords: ferroelectric domain walls

Tuesday, September 5th, 2017 - Room2 - 13:50 - 14:20

keynote speaker - DESIGN & SIMULATION I

Tu-S-O-01

(INVITED) Accelerated discovery and design of ferroelectrics through statistical learning methods

KRISHNA RAJAN

Department of Materials Design and Innovation- University at Buffalo- the State University of New York, Buffalo, United States

This presentation will provide an overview of computational strategies that harness statistical learning methods to selection and design of crystal chemistry for ferroelectrics and related classes of materials. We show how data driven methods can identify new parameters and correlations that augment theoretical and/or experimentally derived data. A particular emphasis of our discussion will be on the challenges to deal with the high dimensional nature of the data governing structure-chemistry-property relationships. Examples are provided in how one may use these methods to permit significant acceleration of materials discovery and design.

Keywords: crystal chemistry, informatics, data

Tuesday, September 5th, 2017 - Room3 - 13:50 - 14:20

keynote speaker - GROWTH & MATERIALS I

Tu-S-O-01

(INVITED) Processing and properties of next generation textured piezoelectric ceramics

Gary Messing [1], Yunfei Chang [1], Beecher Watson [1], Elizabeth Kupp [1], Mark Fanton [2], Richard Meyer [1, 2]

[1] *Department of Materials Science and Engineering, Pennsylvania State University, University Park, United States*

[2] *Applied Research Lab Pennsylvania State University, University Park, United States*

Highly $[001]_c$ oriented Pb $(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PIN-PMN-PT) relaxor ferroelectric ceramics with texture fraction ~98 % have been successfully textured by templated grain growth using $BaTiO_3$ (BT) platelets. The effects of dopants and template amounts on the densification behavior, texture evolution, microstructure development, and dielectric, piezoelectric and ferroelectric properties were investigated. The results show that the addition of CuO sintering aid was very effective in achieving highly oriented and dense PIN-PMN-PT ceramics at much lower texturing temperatures with shorter holding time. With maintaining the same texture quality, lowering BT concentration reduced the adverse effect of heterogeneous template on the property of textured ceramics. A significant enhancement in the magnitude of piezoelectric response (d_{33} ~1013 pC/N) was obtained in the textured ceramics, which is about 2.4 times higher than that of randomly oriented ceramics. The domain structure of the textures ceramics was characterized by piezoelectric force microscopy, and domain contribution to the enhanced piezoelectric response in the textured PIN-PMN-PT ceramics was

analyzed. The high quality textured ternary ceramics are very promising for new-generation electromechanical devices with high performance and wide temperature usage range.

Keywords: piezoelectric, texture, bulk ceramics

Tuesday, September 5th, 2017 - Room4 - 13:50 - 14:20

keynote speaker - ELECTROCALORICS I

Tu-S-O-01

(INVITED) Multicaloric effects in multiferroics

Antoni Planes [1], Teresa Castán [1], Lluís Mañosa [1], Avadh Saxena [2]

[1] *Departament de Física de la Matèria Condensada. Universitat de Barcelona, Barcelona, Spain*
[2] *Los Alamos National Laboratory, Los Alamos, United States*

Ferroic and multiferoic materials thermally respond to externally driven changes of ferroic properties. Usually these changes are induced either by application or removal of the field thermodynamically conjugated to a given property. The corresponding isothermal change of entropy and adiabatic change of temperature are commonly used to quantify the caloric response of the studied material. From this perspective we provide a general thermodynamic framework to investigate multicaloric effects in multiferroic materials. This is applied to the study of both magnetostructural and magnetoelectric multiferroics. Mesoscopic Landau models with appropriate interplay between the corresponding ferroic properties (i.e. order parameters such as polarization, magnetization and strain) are proposed for specific materials and multicaloric effects are obtained as a function of the two relevant applied fields. It is further shown that these effects comprise the contributions from each ferroic property as well as the cross-contribution arising from the interplay between these properties. The obtained results will be compared with available experimental data.

Keywords: Multiferrics; Caloric effects; multicaloric effects; Landau modeling

Tuesday, September 5th, 2017 - Room1 - 14:20 - 14:45

Invited talk - DOMAINS I

Tu-S-O-01

(INVITED) Towards ferroelectric domain wall electronics

Marty Gregg

Queens University Belfast, Belfast, United Kingdom

For many decades, electrical hardware has been realised by configuring fixed electronic components using fixed hard-wired connections. There has, however, been a recognition that an alternative could be useful, in which electrical connections could be actively reconfigured as part of the operation of the electronic system itself. “Adaptive circuitry” of this kind is already in existence and the concept seems likely to gain ground in applications over the coming years. Extending this idea to the point where entire devices could be controllably created, moved and destroyed dynamically is, however, completely new and could lead to a revolutionary alternative paradigm in electronics. Ferroelectric domain walls may offer the first opportunity to explore this paradigm shift. It is now well established that some domain walls show much larger conductivity than the domains that they enclose and that active carriers can be both p and n type. Domain wall intersections can therefore, in principle, create 1D p-n junctions that are innately nanoscale. Moreover, because domain walls can be created, moved and annihilated, the opportunity for "now-you-see-it-now-you-don't" device deployment is real.□ This talk will explore recent progress in developing conducting domain walls with specific carrier types [1], controlling the motion and injection of these domain walls [2,3] and creating and investigating p-n junctions formed at domain wall intersections.□

References

[1] M. P. Campbell *et al.* Nature Commun. 7, 13764 (2016).

[2] J. R. Whyte and J. M. Gregg, Nature Commun. 6, 7361 (2015).

[3] R. G. P. McQuaid *et al.* Nature Commun. (2017). No prelo.

Keywords: domain walls, domains, domain wall conduction

Tuesday, September 5th, 2017 - Room2 - 14:20 - 14:45

Invited talk - DESIGN & SIMULATION I

Tu-S-O-01

(INVITED) Simulation of topological domains in hexagonal $RMnO_3$ patterns and kinetics of domain walls

Jun-Ming Liu

Nanjing University, Nanjing, China

The real-space topological domain structure has been receiving increasing interests recent years and its dynamics remains to be explored if any potential application becomes possible. We have investigated carefully the real-space topological domain structures of hexagonal $RMnO_3$ manganites from various aspects, based on the phenomenological Ginzburg-Landau theory. First, the in-plane and out-of-plane

stiffness anisotropies have been revealed to play a substantial role in controlling the domain structure. Second, we disclose in details of the dynamic response of the domain structure on external electric field. The present work provides a comprehensive understanding of the topological domain pattern evolution in hexagonal manganites, addressing the significance of the vortex-antivortex topology and proposing possible modulation of the domain structure by strain engineering and field stimuli.

Keywords: hexagonal manganites, vortex-antivortex, topological domain structure

Tuesday, September 5th, 2017 - Room3 - 14:20 - 14:45

Invited talk - GROWTH & MATERIALS I

Tu-S-O-01

(INVITED) Optical and electrooptical properties of rare earth doped transparent ferroelectric ceramics

Ducinei Garcia [1], Flavio Milton [1], Eriton Botero [2], Fernando Londono [3], Jose Antonio Eiras [1]

[1] *Federal University of Sao Carlos, Sao Carlos, Brazil*
[2] *Federal University of Grande Dourados, Dourados, Brazil*
[3] *University of Antioquia, Medellin, Colombia*

In the processing of PMN-PT ceramics, as in the case of the well-known lanthanum doped PZT ceramics, the La-doping can promote high densification and homogeneous microstructure, allowing low light scattering by pores and grain boundaries and high optical transmittance from visible to near infrared. This work will present the overcome of processing challenges and the optical/electro-optical characterization of these ferroelectric transparent ceramic systems, particularly when other rare earth ions are added as modifiers. From Kerr and Pockels electrooptical responses over a broad temperature range and X-ray diffraction analysis, as well as from basic rules of structural stability and ion occupancy, we will discuss how the addition of a rare earth ion can reduce the optical transmittance even for pore-free lanthanum doped PZT (or PMN-PT) ceramics.

Keywords: transparent ferroelectric ceramics, PLZT, PMN-PT, rare earth, doping

Tuesday, September 5th, 2017 - Room4 - 14:20 - 14:45

Invited talk - ELECTROCALORICS I

Tu-S-O-01

(INVITED) Some guidelines for improving caloric responses using ferroelectrics

Brahim Dkhil

Laboratoire Structures, Propriétés et Modélisation des Solides, CentraleSupélec, CNRS-UMR8580, Université Paris-Saclay, 92290 Châtenay-Malabry, France on behalf of many authors, Chatenay-Malabry, France

The search for alternative solid-state refrigeration materials to hazardous gases in conventional and cryogenic cooling devices is a very active field of condensed matter [1,2]. The use of phase transitions is a powerful tool to achieve giant caloric effects in ferroic materials in which magnetization, polarization, strain and/or volume can be strongly tuned under a moderate external stimulus. Here, we explored various strategies to reveal ferroelectric potentialities as solid state coolers such as multiphase points composition, elasto- and baro-caloric responses, negative electrocaloric effect in antiferroelectrics as well as the use of dual-stimuli by taking advantage of multicaloric effects combining stress and electric field in ferroelectrics or magnetic and electric fields in multicalorics [3-7].

B.D. acknowledge Fonds National de la Recherche (FNR) du Luxembourg through the InterMobility project 16/1159210 "MULTICALOR"

[1] X. Moya, S. Kar-Narayan, N. D. Mathur, Nat. Mater. 13, 439 (2014).

[2] T. Correia and Q. Zhang (Eds.). Electrocaloric Materials, Springer: Berlin (2014).

[3] Y. Liu, J.F. Scott, B. Dkhil, APL Materials 4, 064109 (2016).

[4] Y. Liu, B. Dkhil, E. Defay, ACS Energy Lett. 1, 521 (2016).

[5] Y. Liu, L. C. Phillips, M. Bibes, A. Barthélémy, B. Dkhil, Nat. Comm. 7, 11614 (2016).

[6] Y. Liu, J.F. Scott, B. Dkhil, Appl. Phys. Reviews 3, 031102 (2016).

[7] Y. Liu, G. Zhang, Q. Li, L. Bellaiche, J.F. Scott, B. Dkhil, Q. Wang, Phys. Rev. B 94, 214113 (2016).

Keywords: electrocalorics, multicalorics

Tuesday, September 5th, 2017 - Room1 - 14:45 - 16:20

Oral presentation - DOMAINS I

Tu-S-O-01

First-principles theory of domain wall dynamics in improper ferroelectric hexagonal manganites

Sergey Artyukhin [1], Urko Petralanda [1], Sang-Wook Cheong [2], Keji Lai [3]

[1] *Italian Institute of Technology, Genova, Italy*
[2] *Rutgers University, Piscataway NJ, United States*
[3] *UT Austin, Austin TX, United States*

Electric field-driven dynamics of ferroelectrics and multiferroics is at the heart of their applications. While loss at GHz frequencies was seen in bulk ferroelectrics, the unambigous assignment of its origin was problematic until the recent spatially resolved measurements pinpointed that the loss is localized at domain walls [1]. We use phenomenological theory and first-principles calculations to model domainwall localized excitations and interpret recent scanning impedance microscopy measurements in hexagonal manganites and proper ferroelectrics as excitation of these localized vibrations.

References

[1] Xiaoyu Wu, Urko Petralanda, Lu Zheng, Yuan Ren, Rongwei Hu, Sang-Wook Cheong, Sergey Artyukhin, Keji Lai, Science Advances (accepted), arxiv:1702.06205

Keywords: domain wall conductance, phonons

Tu-S-O-02

(INVITED) Ultrafast and high-resolution imaging of polarization switching in ferroelectrics

Suhas Somnath [1, 2], Sergei Kalinin [1, 2], Stephen Jesse [1, 2]

[1] *The Institute of Functional Imaging of Materials, Oak Ridge National Laboratory, Oak Ridge, United States*
[2] *The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, United States*

Polarization switching in ferroelectric and multiferroic materials forms the basis for the next generation of electronic devices such as race-track memories, field effect transistors, and tunneling devices. The switching mechanisms in these materials are highly sensitive to the local defects and structural imperfections at the nanometer scale which in-turn have undesirable effects on ferroelectric domains. These considerations necessitated the development of Piezoresponse Force Microscopy (PFM) techniques to measure and manipulate local polarization states. However, the current state-of-art PFM spectroscopy techniques suffer from serious compromises in the measurement speed, voltage and spatial resolutions since they typically combine a slow (~1 sec) switching signal with a fast (~1 – 10 msec) measurement signal. Moreover, transients in the cantilever response at higher vibrational modes and harmonics are lost since the signal from only a single, or a narrow band of frequencies is typically acquired. We report on a fundamentally new approach that combines the complete acquisition of the cantilever response signal with data-driven signal filtering techniques to directly measure material strain in response to the probing bias. Our technique, called General mode Voltage Spectroscopy (G-VS),

enables precise spectroscopic imaging of the polarization switching phenomena 3,500 times faster than currently reported methods. Rapid acquisition of large numbers of hysteretic loops on very dense grids will enable significant insight into nanoscale polarization dynamics and phenomena such as polarization fatigue and local wall displacements that remain difficult to study at the desired spatial and temporal scales, which are crucial for developing future electronic devices.

Keywords: Scanning probe microscopy, Piezoresponse force microscopy, signal processing, big data

---

Tu-S-O-03

Roles of electronic orbital hybridizations in rare-earth-substituted $BiFeO_3$ in the vicinity of morphotropic phase boundary

Chi-Shun Tu [1], Cheng-Sao Chen [2], Pin-Yi Chen [3]

[1] *Department of Physics, Fu Jen Catholic University, New Taipei City, Taiwan*
[2] *Department of Mechanical Engineering, Hwa Hsia University of Technology, New Taipei City, Taiwan*
[3] *Department of Mechanical Engineering, Ming Chi University of Technology, New Taipei City, Taiwan*

The field-induced polarization and electromechanical strain near the morphotropic phase boundary (MPB) are critical phenomena in ferroelectrics. However, the phase evolution, domain, and electronic state in multiferroics still lack consistent understanding near the MPB. We report phase revolution, domain structure, magnetization, ferroelectric polarization, strain, magnetization, phonon vibration, oxidation, and electronic hybridization in multiferroic $(Bi_{1-x}RE_x)FeO_3$ ceramics (*RE*=Nd and Sm) across the MPB. The Rietveld refinements reveal reductions of bismuth and oxygen vacancies with increasing rare earth. The local ferroelectric polarization and electromechanical strain hysteresis loops were observed by the piezoresponse force microscope (PFM) due to the reduced leaky conductivity. The Fe K- and $L_{2,3}$-edges synchrotron X-ray absorptions suggest a mixture of Fe^{3+} and Fe^{4+} valences and reduction of the FeO_6 octahedral distortion by the Nd substitution. The Fe L edge does not indicate valence shift by the Sm substitution. A sequential composition-driven transition from the ferroelectric rhombohedral *R*3*c* to nonpolar orthorhombic *Pbam* and then orthorhombic *Pnma* phases were revealed in $(Bi_{1-x}Sm_x)FeO_3$ near the MPB. A coexistence of rhombohedral *R*3*c* and $PbZrO_3$-like orthorhombic *Pbam* symmetries was identified by the *1/2*(*ooo*) and *1/4*(*ooo*) superlattice diffractions for x=0.10-0.16. This study highlights the importance of the O 2*p*–Fe 3*d* and the O 2*p*–Bi 6*sp* orbital hybridizations, which play critical roles in the FeO_6 octahedral distortion and phase evolution.

Keywords: Rare-earth-substituted BiFeO3; O 2p-Fe 3d orbital hybridization; O 2p-Bi 6sp orbital hybridization; Piezoresponse hysteresis loops; Synchrotron X-ray absorption

---

Tu-S-O-04

Impact of flexoelectricity and surface charges on the formation and properties of domain structures in thin ferroelectric films

Ivan Vorotiahin [1, 2], Eugene Eliseev [3], Qian Li [4], Sergei Kalinin [4], Yuri Genenko [1], Anna Morozovska [2]

[1] *Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany*
[2] *Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine*
[3] *Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Kyiv, Ukraine*
[4] *The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, United States*

Flexoelectric effect, or flexocoupling, is a basic property of virtually all solid-state materials. Direct flexoeffect couples polarization and mechanical strain via their gradients, effectively describing a poling of the bulk material when it is subjected to the inhomogeneous stress, an inverse effect exists too. The effect itself is weak and only becomes remarkable in thin films and nanostructures, however, it may influence their macroscopic properties. In this work, the effect of flexoelectricity on domain structures in thin ferroelectric films is studied using Landau-Ginzburg-Devonshire theory. Properties of the structures, including phase transitions, domain and domain wall shapes, domain sizes and periodicity, are found to be impacted to a different extent by the flexocoupling. Surface screening is another film property that affects domain structures. The screening can be caused by metallic electrodes, as well as by charges adsorbed from the ambience on the free surface of the film. Modification of the surface charge results in adjustment of domain shapes and the structure type, forcing transitions between stripe domains, closure domains and the single-domain state. This work investigates competition between the two above mentioned mechanisms always present in real films. At larger surface charge compensation, classical stripe domains are formed, while at smaller surface charge compensation, closure domain structures appear which effectively suppress bound polarization charges at the free film surface. Flexoeffect leads to formation of enhanced stress regions at the clamped bottom surface of the film and to appearance of metastable nanodomains in the bulk of films of higher thicknesses.

Keywords: Flexoelectric effect, domain structures, surface charge

---

Tu-S-O-05

Structural characterizations of hardening in A-site non-stoichiometric (1-*x*)$Bi_{0.5}Na_{0.5}TiO_3$-*x*$BaTiO_3$ lead free piezoelectric ceramics

Sasiporn Prasertpalichat [1], Noppadon Nuntawong [2], David Cann [3]

[1] *Department of Physics, Faculty of Science, Naresuan University, Phitsanulok, Thailand*
[2] *National Electronics and Computer Technology Center, Pathum Thani, Thailand*
[3] *Materials Science, School of Mechanical Industrial and Manufacturing Engineering Oregon State University, Corvallis, United States*

Lead-free piezoelectric ceramics 1-*x*($Bi_{0.5}Na_{0.5}TiO_3$)-*x*$BaTiO_3$ where $x = 0.055$, 0.06 and 0.07 (i.e., near the morphotropic phase boundary) were prepared with modified A-site cation stoichiometry to induce acceptor (excess Na) and donor (excess Bi) doping. Donor doping had no effects on the crystal structure while acceptor doping promoted rhombohedral distortions. A significant improvement in the dielectric properties was observed in all donor-doped while a deterioration in dielectric properties was observed in all acceptor-doped compositions. Compared to the stoichiometric composition, acceptor-doped compositions exhibited all of the expected "hardening" characteristics, including a decrease in d_{33}, and tanδ , as well as an increase in mechanical quality factor (Q_m) and coercive field (E_c). The measured

increase in E_c and decrease in remanent polarization (P_r) were confirmed by remanent *P-E* hysteresis and PUND measurements. Rietveld refinement and raman spectroscopic studies were also done in order to gain more insight on the effect of structure and symmetry on the observed hardening characteristics. The possible defect chemistry conditions responsible for the observed hardening characteristics will also be discussed.

Keywords: Lead free piezoelectric ceramics, Bi0.5Na0.5TiO3-BaTiO3, Hardening, Rietveld refinement, Raman Spectroscopic

---

Tu-S-O-06

(INVITED) Science and technology of interface-engineered biocompatible piezoelectric oxide/ultrananocrystalline diamond (UNCD^{TM}) films for a new generation of multifunctional/biomedical MEMS/NEMS devices

Orlando Auciello

University of Texas-Dallas, Departments of Materials Science and Engineering and Bio-engineering, Richardson, United States

A new paradigm for piezoelectrically actuated MEMS/NEMS biosensors and energy harvesting devices, impacting quality of life, is based on the integration of dissimilar biocompatible piezoelectric oxide and nanocarbon-based materials. This talk reviews recent R&D performed to integrate lead-free piezoelectric $BiFeO_3/SrTiO_3$/BFO nanolaminate structures, with superior properties to BFO films, with novel ultananocrystalline diamond (UNCD) films, to develop a new generation of multifunctional MEMS/NEMS actuators and sensors for medical applications. BFO may provide biocompatibility as opposed to lead-based PZT. BFO exhibit remnant polarization P_r and piezoelectric coefficient d_{33} of comparable to Ti-rich PZT films. However, BFO films exhibit large coercive fields/leakage current, the latter not properly reduced via atomic doping. One part of this talk will focus on reviewing the R&D recently performed on a novel approach to reduce leakage current and increase piezoelectric response of BFO films by producing structured BFO/STO/BFO nanolaminates involving an insulating $SrTiO_3$ layer. The BFO/STO/BFO nanolaminates exhibit strain-engineered BFO/STO interfaces, providing the mechanism for high piezoelectric deflection/low leakage current ($\sim 10^{-8}$ A/cm^2 -1 V), revealed by systematic HRTEM/PFM studies. The talk will review also R&D that produced new biocompatible UNCD film based MEMS/NEMS structures integrated with piezoelectric films, demonstrating the feasibility of oxide piezoelectric/UNCD integrated MEMS biosensor and energy harvesting devices, the latter via mechanical motion triggered by biting mice heart cells grown on the UNCD film. The integrated biocompatible piezoelectric BFO/STO/BFO nanolaminates/UNCD films provide the bases for a new generation of multifunctional MEMS/NEMS devices for biomedical applications.

Keywords: Piezoelectric, BiFeO3/SrTiO3/BiFeO3 nanolaminates, ultrananocrystalline diamond films, biomedical MEMS/NEMS.

Tuesday, September 5th, 2017 - Room2 - 14:45 - 16:20

Tu-S-O-01

Microscopic origins of the large piezoelectricity of lead-free (Ba,Ca)(Zr,Ti)O_3

Yousra Nahas [1], Alireza Akbarzadeh [1], Sergei Prokhorenko [1], Sergey Prosandeev [1, 2], Raymond Walter [1], Igor Kornev [3], Jorge Iniguez [4], Laurent Bellaiche [1]

1 Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, United States
2 Institute of Physics, South Federal University, Rostov on Don, Russia
3 Laboratoire Structures, Propriétés et Modélisation des Solides, Université Paris-Saclay, CentraleSupélec, CNRS-UMR8580, Châtenay-Malabry, France
4 Materials Research and Technology Department, Luxembourg Institute of Science and Technology, (LIST), Esch/Alzette, Luxembourg

In light of directives around the world to eliminate toxic materials in various technologies, finding lead-free materials with high piezoelectric responses is an important current scientific quest.As such, the recent discovery of a large electromechanical conversion near room temperature in (1-x)Ba(Zr0.2Ti0.8)O3-x(Ba0.7Ca0.3)TiO3 compounds has attracted a lot of attention. Strikingly, the origin of such a strongly desired response is not conclusively understood, with various explanatory mechanisms having been proposed. Here, we report the development of a large-scale atomistic scheme providing a microscopic insight into this technologically-promising material. The use of such a scheme reveals that high piezoelectricity in (1-x)Ba(Zr0.2Ti0.8)O3-x(Ba0.7Ca0.3)TiO3 originates from the existence of large fluctuations of the polarization in the orthorhombic state arising from the combination of flat free-energy surfaces, a fragmented local structure reflected in the relative small strength of the so-called percolating cluster, and the narrow temperature window around room temperature at which this orthorhombic phase is the equilibrium state. In addition to deepening the current knowledge on piezoelectricity, these findings have the potential to guide the design of other novel lead-free materials with large electromechanical responses.

Keywords: first-principles-based simulations, effective Hamiltonian, lead-free ferroelectric, local order, piezoelectricity

---

Tu-S-O-02

Correlations in polarization switching kinetics in polycrystalline ferroelectrics

Ruben Khachaturyan [1], Yuri Genenko [2]

[1] 1, Darmstadt, Germany
[2] 2, Darmstadt, Germany

The switching time distribution plays a crucial role in polarization reversal of polycrystalline ferroelectric materials. As the switching time is strongly field dependent, the field distribution has a great impact on the time-dependent ferroelectric poling. The current work is dedicated to investigation

of switching kinetics in ferroelectric ceramics. The main kinetic equation to describe the local polarization reversal is derived from the Kolmogorov-Avrami-Ishibashi equation for 180° switching. Using the finite element method the field values in the granular matrix are evaluated and then the kinetic equation is iteratively solved using the average field values inside the grains updated at each iteration step. Iteractions are repeated until the total saturation polarization is reached. Simulations are performed for a matrix containing 400 grains of random form and size (with average size of 1 μm) under applied field values 3 V/μm, 4 V/μm, and 5 V/μm. The obtained polarization-time curves, and polarization and electric field maps are presented. The case of 3 V/μm is exemplarily investigated in detail disclosing statistical polarization and electric field distributions and their spatial correlations. We found that the field distribution is continuously broadening during the poling of an anisotropic material. However, for isotropic permittivity the width of the field distribution is proportional to an absolute value of the polarization and thus changes non-monotonically. An analytical explanation of these effects is given in terms of the dielectric tensor and the bound charge distributions. We have also established that short-range correlations of polarization components and field components are present. However, no cross-correlations between the polarization and field components are observed.

Keywords: Polarization kinetics, field distribution, spacial correlations

---

Tu-S-O-03

Pressure induced switching in ferroelectrics: on the junction between physics and electrochemistry

Ye Cao [1, 2], Anna Morozovska [3], Sergei Kalinin [2]

[1] *University of Texas at Arlington, Arlington, United States*
[2] *The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, United States*
[3] *Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine*

Pressure-induced polarization switching in ferroelectric thin films has emerged as a powerful method for domain patterning, allowing to create predefined domain patterns on free surfaces and under thin conductive top electrodes. However, the mechanisms for pressure induced polarization switching in ferroelectrics remain highly controversial, with flexoelectricity, polarization rotation and suppression, and bulk and surface electrochemical processes all being potentially relevant. Here we classify possible pressure induced switching mechanisms, perform elementary estimates, and study in depth using phase-field modeling. We show that magnitudes of these effects are remarkably close, and give rise to complex switching diagrams as a function of pressure and film thickness with non-trivial topology or switchable and non-switchable regions.

Keywords: Ferroelectrics, electrochemistry, dielectrics

Tu-S-O-04

Designing lead-free antiferroelectrics for energy storage

Bin Xu [1], Jorge Íñiguez [2], Laurent Bellaiche [1]

[1] *University of Arkansas, Fyetteville, United States*
[2] *Luxembourg Institute of Science and Technology (LIST), Esch/Alzette, Luxembourg*

Dielectric capacitors, although presenting faster charging/discharging rates and better stability compared with supercapacitors or batteries, are limited in applications due to their low energy density. Antiferroelectric compounds, however, show great promise due to their atypical polarization-versus-electric field curves. Here we report our first-principles-based theoretical predictions that $Bi_{1-x}R_xFeO_3$ systems (R being a lanthanide, Nd in this work) can potentially allow high energy densities (100–150 $J.cm^{-3}$) and efficiencies (80–88%) for electric fields that may be within the range of feasibility upon experimental advances (2–3 $MV.cm^{-1}$). Additionally, a simple model is derived to describe the energy density and efficiency of a general antiferroelectric material, providing a framework to assess the effect on the storage properties of variations in doping, electric field magnitude and direction, epitaxial strain, temperature, etc., which can facilitate future search of antiferroelectric materials for energy storage.

Keywords: Antiferroelectrics, Energy Storage, Effective Hamiltonian, Monte Carlo Simulations

---

Tu-S-O-05

Coupling effect in relaxor-ferroelectric layered composite – phase field simulation and analytical solution

Shuai Wang [1, 2], Bai-Xiang Xu [1]

[1] *Mechanics of Functional Materials, Materials Science Department, Technical University of Darmstadt, Darmstadt, Germany*
[2] *Graduate School of Computational Engineering, Technical University of Darmstadt, Darmstadt, Germany*

Layered Relaxor-Ferroelectric composite has been shown experimentally to be able to enhance large-signal response d_{33} in lead-free ceramics, for instance by Zhang et al.. [1] The enhancement of the d_{33} is found at some specific ratio of each component. The underlying mechanism of the abnormal behavior in the layered structure is elucidated as the strain coupling effect accompanied with polarization coupling effect between the layers. In this presentation, two approaches are established to investigate the coupling effect of the Relaxor-Ferroelectric layered structure. In the analytical approach, two criteria are given independently for the serial layered model, i.e., polarization equality condition by which only the polarization coupling effect is included, and strain equality condition by which only the strain coupling effect is included. The typical hysteresis loops, such as P-E loops and S-E loops of the composite can be calculated by the hysteresis loops of each component. In the phase-field approach, the detailed polarization and strain distribution in relaxor layer and ferroelectric layer can be calculated by our previous random field model. [2] Both polarization and strain coupling effect are intrinsically included in the model. Two lead-free material systems are used, and the enhancement of the d_{33} is observed.

The work of Shuai Wang is supported by the 'Excellence Initiative' of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt.

References

[1] H. Zhang, C. Groh, Q. Zhang, et al. Advanced Electronic Materials, 1-6 (2015).

[2] S. Wang, M. Yi and B.-X. Xu, International Journal of Solids and Structures, 83, 142-153 (2016).

Keywords: relaxor ferroelectrics, phase field, finite element method, composite, large signal response

---

Tu-S-O-06

Machine learning guided computational search for Ruddlesden-Popper oxides without inversion symmetry

Prasanna V. Balachandran [1], Joshua Young [4], Turab Lookman [1], James M. Rondinelli [3]

[1] *Los Alamos National Laboratory, Los Alamos, United States*
[3] *Northwestern University, Evanston, United States*
[4] *Naval Research Laboratory, Washington, United States*

I will discuss a machine learning guided density functional theory (DFT) approach to accelerate the search for noncentrosymmetric (NCS) materials in the layered n = 1 Ruddlesden-Popper (RP) oxides. Our approach is built on the foundations of applied group theory, machine learning and DFT to uncover quantitative symmetry-chemistry guidelines for rapidly predicting novel compositions with NCS ground state. Group theory identifies how configurations of oxygen octahedral rotation patterns, ordered cation arrangements and their interplay break inversion symmetry, while machine learning tools allow us to learn from available data to predict candidate compositions that fulfil the group theoretical postulates. Finally, we validate the machine learning predictions using DFT phonon calculations and identify novel compositions (e.g. stannates, ruthenates etc) that show potential for NCS ground state. Our approach enables rational design of new materials with targeted crystal symmetries and functionalities.

Keywords: Machine Learning, Ruddlesden-Popper, Informatics, Rational Design, Functional Materials

Tuesday, September 5th, 2017 - Room3 - 14:45 - 16:20

Oral presentation - GROWTH & MATERIALS I

Tu-S-O-01

Simulation , Growth and Properties Characterization of Large Size $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ Single Crystal

Zhuo Xu, Kexin Song, Yao Liu, Zhenrong Li, Shiji Fan, Haisheng Guo, Ming Ma, Fei Li

Xi'an Jiaotong University, Xi'an, China

Relaxor based ferroelectric single crystals $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$(PIN-PMN-PT) with composition near morphotropic phase boundary exhibit extraordinary piezoelectric properties. In order to make large crystal growth more efficient, the characteristics of heat and mass transport in the growth process of PIN-PMN-PT single crystal were also simulated by changing macro parameters, such as furnace structure, temperature distribution, and interface shape. It is found that the suitable conditions would reduce the save time and improve crystal quality. Large bulk single crystal with 108 mm in diameter and 170 mm in length was successfully grown by modified Bridgman method. Dielectric, piezoelectric and ferroelectric properties of the [001] samples along single crystal growth direction were systematically measured. The excellent properties (d_{33} - 2700 pC/N, k_{33} - 0.94, d_{15} - 4500 pC/N, k_{15} - 0.91, E_C - 4 kV/cm, T_C - 180 °C, T_{RT} - 100 °C) were found near morphotropic phase boundary. However, due to composition segregation, morphotropic phase boundary is narrow region in the as-grown crystal boule. It is found that the uniform composition with relatively high properties was appeared in the rhombohedral phase near MPB which take up 70% length of crystal boule. In this region, piezoelectric constant d_{33}, T_{RT} and Curie temperature are about 1500-1800 pC/N, 110 °C and 160-180 °C, respectively. In the same range of boule, PIN, PMN and PT content was around 24 mol%, 44 mol% and 32 mol%.

Keywords: Pb(In1/2Nb1/2)O3-Pb(Mg1/3Nb2/3)O3-PbTiO3, Single crystal growth, Bridgman technique, Piezoelectric materials

---

Tu-S-O-02

Texture engineering: A convenient method to enhance the performance of piezoelectric ceramics

Li Peng, Jiwei Zhai

School of Materials Science and Engineering, Tongji University, Shanghai, China

Crystallographic texturing of polycrystalline piezoelectric ceramics offers a convenient means of achieving significant enhancement in the electromechanical properties. Textured ceramics are usually prepared by template grain growth (TGG) or reactive template grain growth (RTGG) utilizing preferred orientation seed crystal. The synthesis mechanism confirmed that the texture process is driven by the difference in the surface free energies between the template crystal plane and the matrix grains. A series of results reported by our group suggested that texture engineering was an efficient means of enhancing piezoelectric performance not only in BNT-based system but also in KNN- and BCZT-based materials. In the case of <001>-textured BNT-BKT ceramics, a high field-induced strain coefficient of 710 pm/V was obtained under a relatively low driving field of 45 kV/cm. Furthermore, the <001>-textured KNN-based ceramics exhibited a 60%-70% improvement in the longitudinal piezoelectric coefficient as

compared to its randomly oriented counterpart. Improvement in piezoresponse by the texture process can be attributed to the intrinsic anisotropy of crystallography and the domain switching difference.

Keywords: Lead-free piezoelectric ceramics, KNN, Texturing, Property.

Tu-S-O-03

Giant piezoelectric voltage coefficient in grain-oriented modified-$PbTiO_3$ material

Yongke Yan [1, 2], Jie E. Zhou [3], Deepam Maurya [1], Shashank Priya [1, 2]

[1] *Center for Energy Harvesting Materials and Systems (CEHMS), Virginia Tech, Blacksburg, United States*
[2] *Institute for Critical Technology and Applied Science (ICTAS), Virginia Tech, Blacksburg, United States*
[3] *Department of Materials Science and Engineering, Michigan Tech, Houghton, United States*

εA rapid surge in the research on piezoelectric sensors is occurring with the arrival of the Internet of Things (IoTs). Single-phase oxide piezoelectric materials with giant piezoelectric voltage coefficient (g, induced voltage under applied stress) and high Curie temperature (Tc) are crucial towards providing desired performance for sensing, especially, under harsh environmental conditions. Here, we provide rational design criterion for such piezoelectric sensing material by incorporating (a) anisotropy/composition/phase structure, (b) microstructure and (c) domain engineering. Using this criterion we report a grain-oriented (with 95% <001> texture) modified-$PbTiO_3$ material that has a high Tc (~364 ºC) and an extremely large g_{33} (115 $\times 10^{-3}$ Vm/N) in comparison to other known single phase oxide materials. Diffraction and scanning probe microscopy studies reveal that self-polarization due to grain orientation along the spontaneous polarization direction plays an important role in achieving large piezoelectric response in a domain-motion-confined material. Domain-level mechanisms were verified quantitatively by simulations using phase field model. The simulations confirm that the large piezoelectric voltage coefficient g_{33} originates from maximized piezoelectric strain coefficient d_{33} and minimized dielectric permittivity ε_{33} in [001]-textured $PbTiO_3$ ceramics where domain wall motions are absent.

Keywords: piezoelectric, ferroelectric, textured, ceramic, piezoelectric voltage coefficient

---

Tu-S-O-04

Understanding processing-structure-property relationships in textured lead-free materials

Deepam Maurya, Shashank Priya

Bio-inspired Materials and Devices Laboratory (BMDL), Center for Energy Harvesting Materials and Systems (CEHMS), Virginia Tech, Blacksburg, United States

Lead-free piezoelectric materials have attracted great attention in recent past. However, despite worldwide research, the properties of these materials are still inferior to that of lead-based piezoelectric

materials. Out of various techniques, dopant engineering has been very effective in improving the functional response of the lead-based piezoelectric ceramics. Though, the dopant engineering was not very fruitful in improving the piezoelectric response in lead-free piezoelectric ceramics. However, the anisotropy in piezoelectric properties provides opportunity to achieve enhanced piezoelectric response in oriented single crystals. But, the synthesis of single crystals is expensive and cannot be used for mass scale applications. The textured (grain–oriented) piezoelectric ceramics has been considered as an effective solution to this challenge. Here, we present a novel and cost-effective method for the synthesis of high performance textured $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) based piezoelectric materials. The synthesis of $[001]_{pc}$ (*pc*: pseudo cubic) grain oriented NBT-based ceramics was performed using NBT as seed template. The driving force for the growth of textured ceramics was found to be originated from the difference in the surface energy and the chemical potential gradient between the stable NBT seeds and the metastable liquid phase. The piezoelectric response was found to increase significantly with the increase in the degree of texturing. The optimized textured system was found to provide 2x enhancement in the magnitude of the piezoelectric coefficient as compared to its randomly oriented form. The NBT-based textured lead-free piezoelectric materials further exhibited giant electric field induced strain (~ 0.48%) with ultra low hysteresis (~ 5%).

Keywords: Piezoelectric, lead-free, ferroelectric domains

Tu-S-O-05

A novel high Curie temperature piezo-ferroelectric solid solution of $Bi(Zn_{2/3}Ta_{1/3})O_3$-$PbTiO_3$

Yi Yuan

1Department of Chemistry and 4D LABS, Simon Fraser University, Burnaby, British Columbia, V5A 1S6, Canada, Coquitlam, Canada
2Electronic Materials Research, Key Laboratory of the Ministry of Education & International Center for Dielectric Research, Xi'an Jiaotong University, Xi'an, 710049, China, Xi'an, China

Ferro-/piezoelectric materials which can function at high temperatures and high electric fields are highly desired for transducers, sensor and actuators. The current high-performance lead-based materials like PMN-PT are not suitable for many of those applications due to their relatively low Curie temperatures (T_C < 160 °C) and low coercive fields (E_C < 5 kV/cm). Additionally, their high lead content presents a big concern due to lead toxicity to human health and environment. In this work, a novel lead-reduced binary solid solution system $xBi(Zn_{2/3}Ta_{1/3})O_3$-$(1-x)PbTiO_3$ (x = 0 to 1) was synthesized by solid state reaction method and systematically characterized in terms of crystal structure and electrical properties by various techniques. Powder X-ray diffraction indicated the formation of a solid solution with x = 0 to 0.27, which crystallize in a tetragonal phase symmetry of perovskite structure. A very high tetragonality (a/c > 1.06) was observed in this system indicating a large crystal distortion and high polarization. Dielectric measurements showed that the solid solution has high Curie temperatures (T_C > 400°C). Ferroelectric characterization indicated a high coercive field (E_C > 20 kV /cm) for this system. The materials also exhibit good piezoelectric properties. These electrical properties were explained from the crystal chemistry aspects. The high-TC and high-EC features signify that the $Bi(Zn_{2/3}Ta_{1/3})O_3$-

$PbTiO_3$ system is a promising and more environmental friendly candidate for electromechanical transductions applications that can operate in a wider temperature range and higher electric field range.

Keywords: High Tc, Piezo-/ferroelectric, Perovskite, Tetragonality

---

Tu-S-O-06

(INVITED) Electromechanical characterization of high-coupling textured PMN-PT and PMN-PZT ceramics

John Blottman [1], Richard Pérez-Moyet [2], Daniel Sherman [1], Adam Heitmann [1]

[1] *Naval Undersea Warfare Center, Division Newport, Newport, United States*
[2] *American Society of Engineering Education, Newport, United States*

Relaxor ferroelectrics remain essential for high power transduction applications due to their exceptional electromechanical response. In single crystal form at near-morphotropic compositions, high-coupling modes are stable under typical naval operating conditions. Over the past two decades, the Navy has interfaced directly with single crystal manufacturers worldwide in a collaborative effort to achieve the required stability and electromechanical performance. While ideal electromechanical performance is realized in single crystal form due to full microstructural alignment, the lack of a complex grain structure is disadvantageous to stable operation under large field drive and/or tensile loading. Crystallographic texturing of a polycrystalline ceramic affords a means to achieve enhanced electromechanical performance without sacrificing mechanical robustness. Adhering to the same methodology put forth during the development of relaxor single crystals, the Navy has begun to invest in the realm of textured ceramic materials. In this work, [001] oriented and poled $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) and $Pb(Mg_{1/3}Nb_{2/3})O_3$-$Pb(Zr,Ti)O_3$ (PMN-PZT) textured ceramics are evaluated and compared with their single crystal counterparts. Electromechanical response under large drive fields (E ~ 1.5 MV/m) and uniaxial compression is investigated as a function of temperature. For PMN-PT, the role of dopants on the losses during operation is examined, while for PMN-PZT the mechanical strength and fracture toughness under bending is explored. In total, lessons learned during the development of relaxor single crystals are being actively applied to textured ceramics to minimize development time and address known shortcomings of relaxor ferroelectrics.

Keywords: Relaxor ferroelectrics, Textured Ceramic, Electromechanical Response, High Power

Tuesday, September 5th, 2017 - Room4 - 14:45 - 16:20

Oral presentation - ELECTROCALORICS I

Tu-S-O-01

Antiferroelectric and lead-free ferroelectric materials as electrocaloric coolants

Brigita Rozic [1], Bouchra Asbani [3], Hana Ursic [1], Mimoun El Marssi [3], Rasa Pirc [1], Jurij Koruza [1, 2], Barbara Malic [1], Zdravko Kutnjak [1]

[1] *Jožef Stefan Institute, Jamova cesta 39,, Ljubljana, Slovenia*
[2] *Technische Universität Darmstadt, Alarich-Weiss-Str. 2, Darmstadt, Germany*
[3] *LPMC, University of Picardie Jules Verne, 33 rue Saint-Leu, Amiens, France*

The electrocaloric (EC) effect has recently attracted significant interest for developing new heat-management devices that have the potential to replace the existing technologies [1,2]. In this contribution the direct measurements of the large EC effect in antiferroelectric and lead-free ferroelectric materials [3,4] will be presented. Specifically, the negative EC effect in antiferroelectric n/95/5 PLZT and PBZ ceramics will be investigated by direct experiments. Here, it is demonstrated that both negative and positive EC response can be arbitrarily invoked in antiferroelectric materials by properly controlling the electric field and temperature. In addition, the large positive EC response observed by direct experiments in lead-free BCTZ-based ferroelectric materials will be reviewed.

References

[1] Z. Kutnjak., B. Rožič, R. Pirc., Wiley Encyclopedia of Electrical and Electronics Engineering, p. 1-19 (2015).

[2] A. S. Mischenko et al., Science 311, 1270 (2006).

[3] R. Pirc, B. Rožič, J. Koruza, G. Cordoyiannis, B. Malič, Z. Kutnjak, J. Phys.:Condens.Matter 27, 455902 (2015).

[4] B. Asbani, J.-L. Dellis, A. Lahmar, M. Courty, M. Amjoud, Y. Gagou, K. Djellab, D. Mezzane, Z. Kutnjak, M. El Marssi, Appl. Phys. Lett. 106, 042902 (2015).

Keywords: antiferroelectrics, lead-free materials, negative ECE, large positive ECE, phase transition

---

Tu-S-O-02

Effect of Mn-addition on electrocaloric and dielectric properties of $0.9Pb(Mg_{1/3}Nb_{2/3})O_3$-$0.1PbTiO_3$ ceramics

Marko Vrabelj [1], Ringailė Katiliūtė [2], Maksim Ivanov [2], Lovro Fulanović [1, 3], Andraž Bradeško [1, 3], Zdravko Kutnjak [1, 3], Jūras Banys [2], Barbara Malič [1, 3]

[1] *Jožef Stefan Institute, Ljubljana, Slovenia*
[2] *Faculty of Physics, Vilnius University, Vilnius, Lithuania*
[3] *Jožef Stefan International Postgraduate School, Ljubljana, Slovenia*

The electrocaloric (EC) effect is defined as the change in entropy and, consequently, in the temperature of a dielectric material due to the electric-field-induced changes in the polar states. The $0.9Pb(Mg_{1/3}Nb_{2/3})O_3$–$0.1PbTiO_3$ (PMN-10PT) relaxor ceramic is one of the candidate EC materials due to its excellent dielectric properties, such as high dielectric permittivity, large change of polarization

with temperature and low hysteresis losses. The EC temperature changes ΔT_{EC} which are large enough for possible applications are achieved at electric field amplitudes well exceeding the coercive field, typically above 100 kV/cm, so the EC materials should possess also high dielectric breakdown strength. It has been shown that Mn-doping of lead-based perovskites significantly reduces their dielectric losses and electrical conductivity, so we expect that such materials could withstand high electric fields. We studied the influence of Mn-doping on dielectric and EC properties of PMN-10PT ceramics. The PMN-10PT ceramic samples with addition of MnO_2 (0.5 and 1.0 mol%) were prepared by the mechanochemical synthesis and sintering at 1200 °C for 2 h. The samples were single-phase perovskites with a relative density above 95 % and grain sizes in the 3-5 micron range. The Mn-addition significantly decreases the dielectric permittivity and losses. Furthermore, doped samples exhibit pinched polarization-electric field loops, indicating that Mn acts as an acceptor dopant. However, doping does not importantly influence the EC temperature change at comparable fields. In the contribution we also discuss the effect of Mn-addition on the dielectric breakdown strength of PMN-10PT ceramics.

Keywords: PMN-PT, Electrocaloric, Dielectric spectroscopy, Mn-doping, relaxor ferroelectric

---

Tu-S-O-03

Understanding the true electrothermal response of ferroelectric thin films

Brendan Hanrahan [1], Yomery Espinal [1, 3], Cameron Neville [1], Andrew Smith [2], S. Pamir Alpay [3]

[1] *U.S. Army Research Laboratory, Adelphi, United States*
[2] *U.S. Naval Academy, Annapolis, United States*
[3] *University of Connecticut, Storrs, United States*

Ferroelectric thin films have been the focus of significant research on understanding and improving their pyroelectric/electrocaloric performance. The standard characterization method for these materials is the isothermal hysteresis loop, from which the pyroelectric coefficient can be extracted. The electrothermal conversion performance is subsequently calculated using Maxwell's relations. Using direct measurement of the pyroelectric response, we find the isothermal hysteresis loop to incorrectly predict the response of three ferroelectric materials systems: a standard ferroelectric lead zirconate titanate (PZT) thin film, an antiferroelectric (AFE) PZT thin film, and a PZT thin film with an interposed hafnia buffer layer. The pyroelectric coefficient is extracted by measuring the current response to pulsed laser heating at a frequency of 1 kHz superimposed over an applied triangle wave electrical bias at 1 Hz, creating a pyroelectric hysteresis loop. When this technique is applied to a standard PZT thin film, we find that the pyroelectric response to electric field is underestimated by the coefficient calculated from isothermal hysteresis loops. In the case of the AFE film, the inverse pyroelectric response at low fields is dramatically over-estimated by the isothermal method. These results are confirmed by energy conversion experiments at different fields. Finally, films with an interposed buffer layer have a unique charging method, which masks the real pyroelectric response of these films. We will discuss the implications of this work on electrothermal conversion performance and techniques for measuring the pyroelectric response moving forward.

Keywords: pyroelectric energy conversion, PZT, thin films

Tu-S-O-04

Electrocaloric effect, dielectric, ferroelectric and piezoelectric properties in normal and relaxor phases of La-doped PZT(65/35)

Shibnath Samanta, V Sankaranarayanan, K Sethupathi

Department of Physics, Indian Institute of Technology Madras, Chennai, India

In recent years, an important fact which has drawn much attention in the field of ferroelectrics is electrocaloric effect (ECE). In this study, we report the change in electrocaloric effect due to the change in doping concentration of La in PZT. In order to do this, PZT (65/35) with La 6, 7, 8 and 9 % are prepared using alkoxide route of sol-gel synthesis, followed by heat treatment at 700 °C. Samples are sintered using a specially designed double atmospheric layer protected sintering method to protect lead loss at high temperatures. The morphological study and phase confirmation are carried out using scanning electron microscopy and X-ray diffraction respectively. The dielectric measurements are done in the frequency range from 100 Hz to 10 MHz at different temperatures from -50 °C to 300 °C. Polarization (P) vs. electric field (E) measurements are carried out in the required temperature range to calculate the ECE. The relation between strain and relative permittivity with electric field are analyzed from P-E measurements. The piezoelectric properties are also studied at room temperature. High value of ECE in the vicinity of room temperature is desirable for practical applications. For a material, ECE is highest around its Curie temperature. The Curie temperature of the PZT (65/35) is found to decrease with increasing La concentration, which in turn makes the material more suitable for refrigeration and other applications near room temperature.

Keywords: Ferroelectric, Electrocaloric effect, Dielectric, Piezoelectric

---

Tu-S-O-05

Molten salt synthetic method for making perovskite nanoparticles

Yuanbing Mao

University of Texas Rio Grande Valley, Edinburg, United States

The molten-salt synthesis (MSS) method is one of the simplest, most versatile, and cost-effective approaches available for obtaining crystalline, chemically purified, single phase powders at lower temperatures and often in overall shorter reaction times with little residual impurities as compared with conventional solid-state reactions. While bulk materials have long been prepared using the MSS method, the preparation of uniform nanostructures using this technique has only arisen relatively recently, that is, within the current century. Over the years, our laboratory has applied this generalized methodology to the fabrication of complex transition-metal oxide nanostructures. In this presentation, various examples will be demonstrated, including barium titanate $BaTiO_3$, strontium titanate $SrTiO_3$, calcium doped strontium titanate $Ca_xSr_{1-x}TiO_3$, barium zirconate $BaZrO_3$, and double perovskite oxides La_2BMnO_6 (B = Ni and Co), along relevant growth mechanism studies and the property measurements of these synthesized nanoparticles. Therefore, it is expected that this MSS method will be widely

disseminated and broadly adopted as a facile, reliable, scalable and cost-effective approach in synthetic nanochemistry.

Keywords: Synthesis; perovskite; nanoparticles

Tuesday, September 5th, 2017 - Poster Room - 16:30 - 18:30

Poster session - Poster Session 1

Tu-S-P-01

Electrochemical and structural characterization of *polyacrylonitrile* (PAN) based gel polymer electrolytes blended with tetrabutylamonium iodide for dye-sensitized solar cells

Faisal Chowdhury

Department of Chemistry, University of Chittagong, Bangladesh, Chittagong, Bangladesh
Center for Ionics University Malaya (CIUM), Department of Physics, University of Malaya, 50603 Kuala Lumpur, Malaysia, Kuala Lumpur, Malaysia

P*olyacrylonitrile* (PAN) based gel polymer electrolytes (GPEs) consisting of Plasticizers: ethylene carbonate (EC) and propylene carbonate (PC) and different compositions of tetrabutylammonium iodide (TBAI) salt were investigated, aiming to apply in dye-sensitized solar cells (DSSC). The interactions between the polymer and EC/PC were analyzed by EIS, FTIR, XRD and DSC techniques. EIS study shows that the GPE containing 20% TBAI has lowest bulk impedance and highest ionic conductivity (2.4×10^{-3} S.cm^{-1}) as well as a diffusion coefficient of 1.9×10^{-7} cm^2.s^{-1}. The interactions between nitrile (-CN) groups in the polymer and the ether oxygen (-O-) groups in the EC/PC were observed. The GPEs are applied to fabricate dye sensitized solar cell (DSSC) for photovoltaic studies. The DSSC with GPE containing 20% TBAI has highest efficiency of 4.2% with short circuit current density of 16.85 mA/cm^2, open circuit voltage of 549 mV and fill factor 0.45.

Keywords: Polyacrylonitrile; Gel polymer electrolytes (GPEs); Dye-sensitized solar cells (DSSC); Ionic conductivity

---

Tu-S-P-02

Effects of La^{3+} ions on the physical properties of $(Bi_{0.5}Na_{0.5})_{0.92}Ba_{0.08-3x/2}La_xTiO_3$ lead-free ceramics

Yanela Méndez-González [1], Aimé Peláiz-Barranco [1], José de los Santos Guerra [2], Pierre Saint-Grégoire [3], Arbelio Pentón-Madrigal [1]

[1] *Facultad de Física-Instituto de Ciencia y Tecnología de Materiales, Universidad de La Habana, La Habana, Cuba*

[2] *Grupo de Ferroelétricos e Materiais Multifuncionais, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Brazil*
[3] *MIPA Laboratory, University of Nîmes, Nîmes, France*

The $(Bi_{1/2}Na_{1/2})TiO_3$-$BaTiO_3$ system (BNT-BT) is a promising lead-free material, which has been extensively studied concerning its piezoelectric properties. It exhibits complex dielectric behaviors, including the transformation from ferroelectric to antiferroelectric phase on heating. The present paper shows the structural, dielectric and ferroelectric hysteresis analysis on $(Bi_{0.5}Na_{0.5})_{0.92}Ba_{0.08-3x/2}La_xTiO_3$ (x = 0, 1, 2 and 3 at%) ceramics. Both antiferroelectric-tetragonal (*P*4*bm*) and ferroelectric-rhombohedral (*R*3*c*) phases co-exist at room temperature. Scanning Electronic Microscopy (SEM) micrographs and energy dispersive spectroscopy analysis suggest that a homogenous solid solution has been formed and that the La^{3+} ions have been incorporated into the BNT-BT lattice. The dielectric behavior shows two phase transitions, one of seems to exhibit typical relaxor characteristics. The La^{3+} ions content shows an important influence on the dielectric parameters. The electric field dependence of the polarization (P-E, hysteresis loops) is also influenced by the lanthanum concentration. For x = 0.01, P-E curve exhibits double-like hysteresis loops suggesting a higher stability of the antiferroelectric phase (AFE). For the other ceramics, squareness-like P-E curves have suggested a higher ferroelectric phase (FE) stability. Antiferroelectric loops are obtained on heating for all compositions.

Keywords: ferroelectrics, antiferroelectrics, lead-free, dielectrics, phase transitions

---

Tu-S-P-03

Dielectric and structural analysis of three-layered ferroelectric perovskites

Yuslin González-Abreu [1], Aimé Peláiz-Barranco [1], Pierre Saint-Grégoire [2], Yaovi Gagou [3], José de los Santos Guerra [4]

[1] *Facultad de Física - Instituto de Ciencia y Tecnología de Materiales, Universidad de La Habana, La Habana, Cuba*
[2] *MIPA Laboratory, University of Nîmes, Nîmes, France*
[3] *University of Picardie Jules Verne, Amiens, France*
[4] *Grupo de Ferroelétricos e Materiais Multifuncionais, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Brazil*

The Aurivillius systems with high Curie temperature or fatigue-free are possible candidates for applications in high temperature piezoelectric devices or non-volatile ferroelectric random access memories. The structure of these materials is represented by the equation Am-1Bi2BmO3m+3 where m is the number of perovskite blocks between $[Bi_2O_2]^{2+}$ layers. The $SrBaBi_2Nb_2TiO_{12}$ ferroelectric material belongs to the Aurivillius family with m = 3. A previous structural study on this system, by using X-ray diffraction, has shown a tetragonal structure with space group *I*4*/mmm* at room temperature [1]. A cation sites mixing have been reported between A sites and bismuth sites into the $[Bi_2O_2]^{2+}$ layered structure [1]. The present work shows the dielectric analysis for this material in a wide range of frequencies and temperatures. Two anomalies are observed in the temperature dependence of the real dielectric permittivity, one near room temperature and the other one at high temperature. By using X-ray diffraction and Raman spectroscopy, in a wide temperature range, both anomalies are studied in

order to evaluate phase transitions or another cause for the observed behaviors, especially at room temperature.

References

[1] Haluska MS and Misture ST, J Solid State Chem. 177, 1965–1975 (2004).

Keywords: Aurivillius, ferroelectrics, phase transitions

Tu-S-P-04

Electromagnetic pulse protection circuits design of piezoelectric vibration acceleration sensor

Cui Hao, Denghua Li

Electronic Information and Control Experimental Teaching Center, Beijing Information Science and Technology University, Beijing, China

As signal acquisition part of equipment, piezoelectric vibration acceleration sensor is used widely in the practical engineering. There are lots of precision circuits in the sensor. So, if there is a big electromagnetic pulse in the environment, the electromagnetic pulse will be coupled into the circuits in the sensor through power cords and data cords. It's important to protect the sensor from the damage of electromagnetic pulse. The electromagnetic pulse protection circuits of power cords and data cords are researched in this paper. The piezoresistor and TVs are used as transient components in the protection circuits. Through optimization grouping, the optimized protection circuit is found. The simulation and experimental results show that the protection circuits proposed in this paper can protect the sensor very well. The protection circuits' design method can be referenced in the engineering practice.

Keywords: piezoelectric vibration acceleration sensor; electromagnetic pulse; protection circuit; transient component; power cord

---

Tu-S-P-05

Piezoelectric stack transducer evaluation and comparison for optimized energy harvesting

Bryan Gamboa, Ruyan Guo, Amar Bhalla

University of Texas at San Antonio, San Antonio, United States

The primary focus of this research is on the application and optimization of direct piezoelectric effect in energy harvesting from low frequency mechanical vibration. The specific research aim is to evaluate the stacked PZT transducers in their mechanisms and performance on effective electromechanical energy conversion. Piezoelectric power output has been determined based on understanding of the fundamental concepts in composites (1:3 bi-phasic) and stack transducers. Several property structure

relations are evaluated by various experimental methods including the utilization of electrodynamic test systems. Power evaluation is compared among several samples in order to understand the most efficient configuration utilizing PZT ceramics. Power density as function of applied mechanical force and pressure, are calculated and compared with the experimental results which yield good agreement. Three types of stack PZT transducers were compared and systemically tested for their electromechanical power conversion performance. The 1:3 composite stack PZT transducer was found to be the best performer in term of power density per unit active volume, the specially designed and fabricated stacked PZT transducers (UTSA stack sample) were found to have the highest power density per transducer volume, 0.615 mW/mm^3, measured at 965 kN/m^2 (140 PSI), among the three types studied (1:3 composite stack sample, assembled stack sample and the commercially available stack sample).

Keywords: Piezoelectric, Stack PZT, Energy Harvesting, Power Density

---

Tu-S-P-06

An Interpretation of relaxor behavior by the Weiss field approach

Andreas Leschhorn, Herbert Kliem

Saarland University, Germany, Saarbruecken, Germany

The so called relaxor materials are characterized by high permittivities in a broad temperature range. In the Arrhenius plot, the relaxation times follow a nonlinear curve, often described as a Vogel-Fulcher law, instead of a straight line. Cooling down from high temperatures relaxors exhibit no spontaneous polarization without applied field. Only in sufficiently high external fields a polarization appears. We present a model which derives typical relaxor characteristics from simple and plausible microscopic assumptions. The model is based on interacting charges which fluctuate thermally activated in double well potentials. The relaxor behavior can be achieved if the double wells have intrinsic asymmetries. Such intrinsic asymmetries are caused by disorder in the system. The electrostatic interaction between the charges is considered via a mean field approach according to Pierre Weiss. The interaction evokes an additional field which is proportional to the polarization. This field modifies the local fields at the double wells and in that way the transition rates of the charges which determine the polarization. So we get a feedback loop for the polarization. This model yields the typical relaxor features: we find high susceptibilities in a broad temperature range with dynamics following the Vogel-Fulcher law. In the framework of the model no spontaneous polarization arises at cooling without strong external field in accordance to experimental findings for relaxors. Furthermore the model yields hysteresis loops of the polarization which become more and more thin and deformed with increasing temperature.

Keywords: Simulation of relaxors, dipolar coupling by Weiss field approach, Vogel-Fulcher empirical law, susceptibility frequency and temperature behavior, asymmetric double well potentials

---

Tu-S-P-07

Phase transition and ferroelectric properties of Aurivillius Bi_4Ti_2 $Nb_{0.5}Fe_{0.5}O_{12}$

Cristian Lavado, Marcelo Stachiotti

Instituto de Fisica Rosario, Universidad Nacional de Rosario, Rosario, Argentina

Bi4Ti2 Nb0.5Fe0.5O12 (BTNF) ceramics were synthesized via the conventional solid-state reaction route to evaluate the effect caused by the addition of Fe3+ and Nb5+ ions on the electrical properties of Bi4Ti3O12 (BIT). The XRD pattern obtained for BTFN is the characteristic of a layered structure belonging to the n = 3 member of the Aurivillius family. The dielectric behavior of the material was studied in a wide frequency and temperature range. The results at room-temperature indicate that BTFN has a dielectric constant of ~115, negligible frequency dispersion, and a dissipation factor less than 0.01. The relationship between dielectric constant and temperature showed a single peak with a transition temperature ~40oC lower than BIT. The electric-field-induced polarization switching behavior at 50 Hz exhibited hysteresis loops indicating ferroelectric character.

Keywords: Aurivillius, multiferroics.

Tu-S-P-08

Fabrication and characterization of (Fe+Nb)-doped PZT thin films

Lucia Imhoff, Sebastian Barolin, Nora Pellegri, Marcelo Stachiotti

Instituto de Física Rosario, Universidad Nacional de Rosario., Rosario, Argentina

We report the synthesis of $[PbFe_{0.5}Nb_{0.5}O_3]_x$ $[PbZr_{0.52}Ti_{0.48}O_3]_{1-x}$ (PZTFNx) thin films by a Chemical Solution Deposition (CSD) technique to evaluate the effect caused by the addition of Fe^{3+} and Nb^{5+} ions on the structural and electrical properties of lead zirconate titanate thin films. The PZTFNx films ($0 < x < 0.5$) were prepared by spin□coating on Pt/TiOx/SiO2/Si substrates. The films were thermally treated between 600 and 700 °C by rapid thermal annealing. Structural and morphological characterizations were performed by XRD and AFM. The effect of Fe+Nb doping on the dielectric and ferroelectrical properties were tested.

Keywords: Thin films, multiferroics.

Tu-S-P-09

Structural and electrical properties of $Mg_{0.05}Ba_{0.95}Zr_{0.1}Ti_{0.9}O_3$ ceramics

Ariel Di Loreto [1, 2], Agustín Frattini [1, 2], Rodrigo Machado [2], Marcelo Stachiotti [2]

[1] *Área Física, Facultad de Ciencias Bioquímicas y Farmacéuticas, Universidad Nacional de Rosario., Rosario, Argentina*
[2] *Instituto de Física Rosario, Universidad Nacional de Rosario., Rosario, Argentina*

Pure and 5% Mg-doped $BaZr_{0.1}Ti_{0.9}O_3$ (BZT) ceramics have been prepared by the conventional solid-state route. Microstructure, dielectric properties, and ferroelectric behaviour of samples sintered at different temperatures were investigated. The results indicate that Mg^{+2} ions facilitates the formation of the perovskite phase during the calcination process, lowering the sintering temperature of the ceramics. We show that Mg-doped ceramics sintered at 1250 ºC display better dielectric and ferroelectric properties than pure BZT. The addition of 5% of magnesium leads to the decrease of the Curie temperature by ~ 75 ºC.

Keywords: Lead-free ceramics.

Tu-S-P-10

Polarised-light and electron microscopy of the static domain structure of ferroic $Fe_3B_7O_{13}I$ boracite at room temperature

Guillermo Castellanos-Guzman [1], O. Jimenez [1], Carmen Miramontes-Corona [2], D. Mendoza [2], Oziel R.Camacho [2], Alan Y.Vargas-Aguilera [2]

[1] *Universidad de Guadalajara Centro de investigacion en Materiales DIP Cucei, Guadalajara, Mexico*
[2] *Universidad de Guadalajara Posgrado en Ciencias de Materiales, Guadalajara, Mexico*

The static domain structure of ferroic $Fe_3B_7O_{13}I$, abbreviated in what follows as Fe-I, synthetic boracite crystals has been analysed by polarised-light microscopy (PLM) [1.2] and by field emission scanning electron microscopy (FE-SEM) [3,4] at room temperature. As for most boracites, Fe-I possess dielectric, elastic, magnetic and optical properties of unusual interest. Upon cooling, Fe-I botacite shows a sequence of structural phase transitions from the cubic 43m1´to the orthorhombic mm21´, the monoclinic m1´and the trigonal 3m1´phases [5] Fe-I boracite single crystals were grown by the chemical-vapour transport technique [6]. At room temperature, the Fe-I crystals present an orthorhombic domain structure which consists of six fully ferroelectric/fully ferroelastic domains are totally coupled [5]. The usefulness and possibilities of combining PLM and FE-SEM for the studying and visualizing the domain structure of ferroic boracites will be shown

The authors would like to thank Coordinacióbn General Académica and Cucei from Universidad de Guadalajara for financial support.

References

[1] Schmid H., Ferroelectric Ceramics Ed. By N. Setter. Monte Veritá (1992) Birkhaussen Verlag.Basel.

[2] Forsbergh P.W. Jr. Phys. Rev. 76, 1187-1201 (1949).

[3] Le Bihan R. Ferroelectrics 97, 67-70 (1989).

[4] Castellanos-Guzmán A.G:, and O. Jiiméne Ferroelectrics 482, 46-53 (2015).

[5] Ye Z-G, A- Janner and H. Schmid. J,. Phys: Conden. Matter 9, 2607-2621 (1997).

[6] Schmid H. J. Phys. Chem. Solids 26 (1965) 26, 973-982 (1965).

Keywords: Boracites, ferroic domains. polarised light microscopy, Fe Scanning electron microscopy, phase transitions

---

Tu-S-P-11

$BiFeO_3$-$SrTiO_3$ thin film as new lead-free relaxor-ferroelectric capacitor with ultrahigh energy storage performance

Hao Pan, Yi Zeng, Yang Shen, Yuan-Hua Lin, Jing Ma, Liangliang Li, Ce-Wen Nan

State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science and Engineering, Tsinghua University, Beijing, China

Capacitors with high electrostatic energy density, long-term stability, and environmental friendliness are strongly demanded in modern electrical and electronic systems. Here, we obtained a new lead-free relaxor-ferroelectric Mn-doped $0.4BiFeO_3$-$0.6SrTiO_3$ (BFSTO) thin film capacitor with an ultrahigh energy density of ~ 51 J/cm^3, which is superior to other lead-free systems and comparable with the best lead-based films. The breakdown strength of the BFSTO film reached ~ 3.6 MV/cm. Besides, the thin film capacitor showed strong fatigue endurance after 2×10^7 cycles and possessed good thermal stability of energy storage performance in a wide temperature range (-40 ~ 140 ^oC). These excellent features should be ascribed to the good epitaxial quality, strong relaxor behavior, and suppressed leakage current of the film. The results prove the great potential of the BFSTO film for electrostatic energy storage. More importantly, our findings could motivate the design and fabrication of a series of $BiFeO_3$-based dielectrics with suppressed leakage currents and high breakdown strengths to develop a new kind of lead-free dielectrics with ultrahigh energy storage performance.

Keywords: BiFeO3-SrTiO3; thin film; energy storage; fatigue; thermal stability

---

Tu-S-P-12

Ab-Initio study on the electronic properties of perovskite structure-based ferroelectrics

Abrahan Pablo Aslla-Quispe [1, 2], Roberto Hiroki Miwa [3], José de los Santos Guerra [1]

[1] *Grupo de Ferroelétricos e Materiais Multifuncionais, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Brazil*
[2] *Universidad Nacional Tecnológica de Lima Sur, Lima, Peru*
[3] *Grupo de Propriedades Eletrônicas e Magnéticas de Moléculas e Sólidos, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Brazil*

During the last decades, increasing progresses have been made on the theoretical study of ferroelectric materials since the discovery of the barium titanate system ($BaTiO_3$). Such advances are mainly due to the development of new theoretical approaches based on quantum mechanics, which have been complemented by the implementation of new, and more efficient, software and the rapid advance in the development of more powerful hardware. The ab-initio methods are approximations based on the Schrodinger's equation of quantum mechanics, which takes into account only fundamental physical constants, one of them being the Density Functional Theory (DFT). The DFT is a method, which allows to solve, in a self-consistent way, the well known Kohn-Sham equation by using an exchange and correlation potential. This work aims the study of the electronics properties of the perovskite oxide based on $BaTiO_3$, considering the inclusion of rare-earth ions as impurities into the structure. By using first-principles calculations and the DFT method, the presence of defects such as vacancies and dopants, as well as their influence on the physical properties, will be investigated.

The authors would like to thank to FAPEMIG, CAPES and CNPq Brazilian agencies for financial support. A. P. Aslla-Quispe also thanks to PAEC-OEA/GCUB nº 001/2015 for the financial support.

Keywords: Ab-initio, First-principles calculations, Density Functional Theory, Ferroelectrics

---

Tu-S-P-13

Chrome influence on the physical properties of $Bi_{0.90}Ba_{0.10}Fe_{0.90}Ti_{0.10}O_3$ multiferroic ceramic system

Yalina García-Puente [1], Osmany García-Zaldívar [1], Aimé Peláiz-Barranco [1], Martin A. Hernández-Landaverde [2], Francisco Calderón Piñar [1], Sergio Díaz-Castañón [3], José de los Santos Guerra [4], Marcos A. Oliveira [4]

[1] *Facultad de Física-Instituto de Ciencia y Tecnología de Materiales, Universidad de La Habana, La Habana, Cuba*
[2] *CINVESTAV-Unidad Querétaro, IPN, Querétaro, Mexico*
[3] *División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tecnológica, San Luis Potosí, Mexico*
[4] *Grupo de Ferroelétricos e Materiais Multifuncionais, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Brazil*

$Bi_{0.90}Ba_{0.10}Fe_{0.90}Ti_{0.10}O_3$ and $Bi_{0.90}Ba_{0.10}Fe_{0.88}Cr_{0.02}Ti_{0.10}O_3$ multiferroic ceramic systems were prepared, by using conventional solid-state reaction method from oxides and carbonates, in order to evaluate the chrome influence on physical properties of the Ba^{2+} and Ti^{4+} co-doped $BiFeO_3$ (BFO). The structural analysis was carried out by using X-ray diffraction and Scanning Electronic Microscopy at room

temperature. A rombohedral perovskite structure has been evaluated for both compositions. The dielectric analysis was carried out in a wide temperature and frequency ranges. The results have showed a clear magneto-electric coupling; the Cr^{3+} ions play also an important role decreasing the electrical conductivity of the studied multiferroic compositions. The doping element has also showed an important influence on the characteristic magnetic hysteresis, which has been evaluated at room temperature.

Keywords: multiferroics, ceramics

Tu-S-P-14

Study of the crystallization kinetics of ferroelectric nanocrystals into TeO_2-based glass system

Renato Cruvinel de Oliveira [1, 2, 3], Anielle Christine Almeida Silva [4], Noélio Oliveira Dantas [4], José de los Santos Guerra [1]

[1] *Grupo de Ferroelétricos e Materiais Multifuncionais, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia – MG, Brazil*
[2] *Departamento de Física e Química, Universidade Estadual Paulista, Campus de Ilha Solteira, Ilha Solteira – SP, Brazil*
[3] *Instituto Federal Goiano, IF Goiano - Campus Rio Verde, Rio Verde – GO, Brazil*
[4] *Laboratório de Novos Materiais Isolantes e Semicondutores, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia – MG, Brazil*

Tellurite-based (TeO_2) glass systems are known to have relatively high chemical and thermal stability, high transmittance in the infrared region as well as low light dispersion. They also stand out for being excellent host-matrix for rare-earth ions in order to improve the high optical linearity. On the other hand, additional applications involve their use as acoustic-optical materials and photochromic glasses. Parallel to the investigations of the optical properties of TeO_2-based glasses, there is a growing interest in the manufacture of transparent oxides containing specific nanocrystals in the glass-matrix, thus promoting the formation of glass-ceramic materials. These new class of materials are very interesting for new optical-glasses applications. In this case, I would be possible, for instance, the investigation of the effect of second-harmonic generation from the incorporation of ferroelectric nanocrystals (NCs) in the glass-matrix. The objective of the present work is to investigate the synthesis and formation of ferroelectric nanocrystals in tellurite glasses-matrix. The samples will be obtained by the quenching method and crystallization kinetics will be studied by using the differential thermal analysis (DTA), Raman spectroscopy and x-ray diffraction (XRD) techniques.

The authors would like to thank to FAPEMIG, FAPEG and CNPq Brazilian agencies for financial support. R. C. Oliveira also thanks the Materials Science Post-Graduation Program (PPGCM), UNESP, Ilha Solteira – SP, Brazil.

Keywords: Tellurite glasses, Nanocrystals, Ferroelectrics

Tu-S-P-15

Li, La doped KNNT ceramics obtained by RTGG

Jorge Portelles [1], Juan Fuentes [1], Jose Juan Gervacio [2], Oscar Raymond [2], Jesus M Siqueiros [2], Jesus Heiras [2], Ma. de la Paz Cruz [2], Norma Palmero [1], Carlos Ostos [3]

[1] *Facultad de Física, Universidad de La Habana, San Lázaro y L, La Habana 10400, Cuba., La Habana, Cuba*
[2] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, AP 14, Ensenada, B.C, México, 22860, Ensenada, Mexico*
[3] *Universidad de Antioquia, Instituto de Química, Facultad de Ciencias Exactas y Naturales, A.A. 12-26, Medellín, Colombia., Medellin, Colombia*

The results obtained in the study of $(K_{0.44}\ Na_{0.52}\ Li_{0.04})_{0.97}\ La_{0.01}Nb_{0.9}Ta_{0.1}0_3$ ceramics obtained by solid state sintering from the precursor $NaNbO_3$ synthetized by the reactive templated grain growth (RTGG) technique are presented. X-ray diffraction studies show the coexistence of two crystal phases, orthorhombic and tetragonal, the last one being the more abundant. Dielectric measurements evince the effect of La doping through a decrease in the transition temperatures with respect to those reported for undoped KNN (tetragonal-cubic T_{T-C}= 264 ^{o} C and orthorhombic -tetragonal T_{O-T} = 90 ^{o}C, in our case). The maximum value for the dielectric permittivity is surprisingly high at 6800 at room temperature and 1 kHz. Ferroelectric hysteresis measurements performed at room temperature give P_r = 20 μC/cm^2 for the remnant polarization and Ec = 9 kV/cm for the coercive field. Piezoforce microscopy (PFM) shows domain switching areas in response to the applied electric field but also non-switching zones where the polarization is either perpendicular to the applied field or non-existent. The hysteresis loop obtained by PFM gives a piezoelectric coefficient d_{31} = 164 pC.N^{-1} comparable to the best published values of PZT and KNN ceramics.

Financial support from CoNaCyT, Grants No. 282778 and 280309 and PAPIIT-DGAPA-UNAM Grants No. IN105307 and IN110315 is acknowledged. Technical support from I. García, I .Gradilla, E. Aparicio, E. Murillo, is greatly appreciated.

Keywords: KNN, PFM, Hysteresis, dielectric permittivity

Tu-S-P-16

Microwave dielectric properties of $Bi_2(Zn_{1/3}Nb_{2/3})_2O_7$ thin films by microwave sintering

Siyuan Dong [1, 2], Meng Li [2], Ruyan Guo [2], Amar Bhalla [2], Xiaoli Wang [1]

[1] *XI'AN JIAOTONG UNIVERSITY, Xi'an, China*
[2] *University of Texas in San Antonio, San Antonio, United States*

Zirconolite $Bi_2(Zn_{1/3}Nb_{2/3})_2O_7$ multi-layer thin films were fabricated on high resistivity (HR)-Si substrates by sol-gel method. The thin films were synthesized either by conventional sintering at 700 oC for 1 hour or by microwave sintering at 2400W for short time. The microwave dielectric properties

of $Bi_2(Zn_{1/3}Nb_{2/3})_2O_7$ thin films were measured using the cavity perturbation technique. Experimental results showed that the BZN film synthesized by microwave sintering has a lower dielectric loss than the one synthesized by conventional sintering. With the increasing microwave sintering time, the dielectric loss of BZN thin films decreased from 0.04 to 0.005 while the permittivity remained stable. The temperature dependence of microwave dielectric permittivity and dielectric loss of BZN thin films by conventional sintering and microwave sintering was also investigate. High permittivity, low dielectric loss make the $Bi_2(Zn_{1/3}Nb_{2/3})_2O_7$ thin films are competitive candidates for the applications of microwave device.

Keywords: thin film, microwave sintering, dielectric

Tu-S-P-17

Magnetoelectricity at nanoscale

Soutik Betal [1], Eduardo Ortega [2], Moumita Dutta [1], Amar Bhalla [1], Ruyan Guo [1]

[1] *Department of Electrical and Computer Engineering, University of Texas at San Antonio, San Antonio, United States*
[2] *Department of Physics and Astronomy, University of Texas at San Antonio, San Antonio, United States*

Magnetoelectric composite nanoparticles of $BaTiO_3$:$CoFe_2O_4$ have been synthesized and characterized. Microstructure analysis and electromagnetic behaviour of the spinel core (cobalt ferrite) and perovskites shell (barium titanate) of the core-shell magnetoelectric nanoparticles using transmission electron microscopy, off-axis electron holography and piezo-response force microscopy has been investigated. The result shows the coating layer of $BaTiO_3$ is highly uniform in composition and thickness around the core. Such a uniform deposition of perovskites on spinel with expected high lattice mismatch is unique. Also, the optoacoustic measurements and MENR-cellular interactions proves the magnetoelectricity behaviour of the nanostructure via stress transfer from core to shell in the presence of applied magnetic field. The results are discussed in details.

Keywords: Nanoscale magnetolectricity, off-axis electron holography, multiferroics

---

Tu-S-P-18

Effect of oxygen flow rate on optical and electrical properties of flexible SnO_2/Ag/SnO_2 multilayer thin films on PET substrate

Guneik JANG, Taekeun Kim

Chungbuk National University, Cheongju, Korea, Republic of (South)

We investigated effect of oxygen flow rate on structural, optical, and electrical properties of SnO_2/Ag/SnO_2 multilayer thin films that were deposited by sequential using RF/DC magnetron sputtering at room temperature on PET substrate. As the oxygen flow rate increases from 0 to 0.5 sccm,

the transmittances of SnO_2 (35 nm)/Ag (13 nm)/SnO_2 (35 nm) varied from 81.2 to 87.1 % at 550 nm wavelength and the sheet resistance remained around 7 Ω/□. The highest value of figure of merit φTC was 35.3 10-3Ω-1 for the film with oxygen flow rate of 0.4 sccm, while the transmittance was 87.1 % at 550 nm wavelength and the sheet resistance was 7.14 Ω/□.

Keywords: transmittance, sheet resistance , figure of merit, oxygen flow rate

---

Tu-S-P-19

Dielectric and dilatometric studies of Rb_2ZnI_4 and its mixed systems

Toshihisa Yamaguchi, Masaaki Takashige

Meisei University, Hino, Tokyo, Japan

Rb_2ZnI_4 is a crystal having monoclinic structure with $P2_1/m$ at room temperature. On cooling, it undergoes a phase transition to an incommensurate phase below 62 K [1], where the *b*-axis dielectric constant ε_b forms a λ-type peak. On further cooling, ε_b again increases and forms a broad peak at around 5 K, however, it shows no ferroelectricity at any temperatures. To elucidate such properties, we performed dielectric measurements for Rb_2ZnI_4 and mixed systems such as $(Rb_{1-x}K_x)_2ZnI_4$ and $Rb_2Zn_{1-x}Cd_xI_4$ and revealed that the system shows a ferroelectric transition of the first order for $x > 0.13 \sim 0.14$, and with increase of x, ferroelectric Curie point moves high temperature [2-4]. On the other hand, Mashiyama [5] theoretically derived a phase diagram which reproduces an aspect of our results. In this presentation, we shall report the latest data of thermal expansion measurements for both $(Rb_{1-x}K_x)_2ZnI_4$ and $Rb_2Zn_{1-x}Cd_xI_4$.

References

[1] J. Puragahn: Doctor Thesis, Karlsruhe University (1998).

[2] M. Takashige *et al*: J. Phys. Soc. Jpn. 81, 045001-2 (2012).

[3] T. Yamaguchi *et al*: Ferroelectrics 462, 104-109 (2014).

[4] R. Shibata *et al*: J. Korean Phys. Soc. 66, 1367-1370 (2015).

[5] H. Mashiyama: J. Phys. Soc. Jpn. 84, 104712 (2015).

Keywords: Rb2ZnI4, K2ZnI4, Rb2CdI4, Sr2GeS4 structure, Thermal expansion

---

Tu-S-P-20

Micro-Raman scattering, dielectric and DSC investigations of phase transitions behavior in the $PbHf_{1-x}Sn_xO_3$ single crystal

Irena Jankowska-Sumara [1], Maria Podgórna [1], Jae-Hyeon Ko [2], Andrzej Majchrowski [3]

[1] *Institute of Physics, Pedagogical University of Cracow, Kraków, Poland*
[2] *Department of Physics, Hallym University, Chuncheon, Korea, Republic of (South)*
[3] *Institute of Applied Physics, Military University of Technology, Warszawa, Poland*

Using Raman scattering spectroscopy, the sequence of phase transitions in antiferroelectric $PbHfO_3$ modified with Sn ions was investigated in the temperature range from 80-830K. The frequencies of the Raman lines were analyzed and discussed in terms of the sequence of structural phase transitions. The modifications of the Raman spectra were observed in details in the vicinity of structural phase transitions: *AFE1-AFE2-IM-PE* phase transition. The Raman measurements were supplemented by dielectric and DSC measurements. Light scattering and dielectric investigations were concentrated in PHS in order to explain the nature and sequence of the phase transition, as well as the large dielectric permittivity values measured at the phase transition, by searching for the soft-phonon-mode behavior. In the scenario developed recently for analogous antiferroelectric-$PbZrO_3$-there exists at once three relevant, strongly softening lattice modes however direct observation of the soft optic mode by Raman spectroscopy failed in pure $PbZrO_3$. In $PbZr_{0.72}Sn_{0.28}O_3$ enhanced polar fluctuations above Tc lead to the appearance of two soft optic modes that were experimentally observed in paraelectric phase. Here we tested the influence of Sn ions on the dynamics of phase transitions in $PbHfO_3$. It is demonstrated that the structural phase transformations in $PbHf_{1-x}Sn_xO_3$ can also be considered as the result of softening of many modes, not only the ferroelectric one.

Keywords: antiferroelectrics, Raman Spectroscopy, phase transitions, soft modes

---

Tu-S-P-21

Negative diploar heat capacity in relaxor ferroelectrics and dipolar glasses

Zdravko Kutnjak, Rasa Pirc

Institute Jozef Stefan, Ljubljana, Slovenia

The temperature and electric field dependence of the specific heat of relaxor ferroelectrics and dipolar glasses is investigated by means of a Landau-type theoretical model. It is shown that the dipolar specific heat, which is due to the randomly interacting polar nanoregions in relaxors and electric dipoles in dipolar glasses, is negative in a temperature region below the permittivity maximum and its magnitude can be tuned by the external electric field. Also, it follows that for sufficiently low values of the field, where the induced polarization shows a quasi linear field dependence, the dipolar specific heat is proportional to the second temperature derivative of the dielectric polarization. This quantity can be extracted from the experimental temperature profile of the polarization, thus enabling an indirect experimental estimate of the negative specific heat, which is demonstrated for a set of representative relaxor and dipolar glass systems [1].

References

[1] Z. Kutnjak, R. Pirc, J. Appl. Phys. 121, in press (2017).

Keywords: relaxor ferroelectrics, dipolar glasses, heat capacity

---

Tu-S-P-22

Perovskite relaxor multiferroics in novel dielectric cooling designs

Brigita Rozic [1], Andraz Bradesko [1], Marko Vrabelj [1], Hana Ursic [1], Lovro Furlanovic [1], Uroš Plaznik [2], Barbara Malic [1], Tadej Rojac [1], Qiming Zhang [3], Andrej Kitanovski [2], Zdravko Kutnjak [1]

[1] *Jozef Stefan Institute, Jamova 39, Ljubljana, Slovenia*
[2] *University of Ljubljana, Faculty of Mechanical Engineering, Askerceva 6, Ljubljana, Slovenia*
[3] *Materials Research Institute, The Pennsylvania State University, University Park, Penn State, United States*

The interest in electrocaloric (EC) effect has been recently revived due to great potential for developing new cooling technologies [1]. Recently, PMN-10PT ceramics have been successfully utilized in a prototype of an electrocaloric cooling device [2]. The recent advances in development of new perovskite relaxor multiferroics with large caloric effects and their use in different solid-state cooling designs will be presented [3]. The effect of electric-energy recovery, the heat regeneration, and the polarization hysteresis losses on the energy efficiency of the system is analyzed. Testing of the cooling device demonstrates the efficient regeneration and establishment of the significant temperature span across the regenerator, exceeding several times the EC temperature change within a single electrocaloric element. The influence of the material's fatigue will also be tested and discussed.

References

[1] A. S. Mischenko et al., Science 311, 1270 (2006).

[2] U. Plaznik et al., Appl. Phys. Lett. 106, 043903 (2015).

[3] A. Bradesko, D. Juricic, M. Santo Zarnik, B. Malic, Z. Kutnjak, T. Rojac, Appl. Phys. Lett. 109, 143508 (2016).

Keywords: prototype of EC device, large caloric effect, heat-regeneration, energy efficiency, fatigue

---

Tu-S-P-23

Piezoelectric properties and local structure analysis of $(1-x)(Na_{0.50}K_{0.45}Li_{0.05})NbO_3$-$(x)Ca(Zr_{0.50}Ti_{0.50})O_3$ solid solutions produced by malic acid complex solution method

Masafumi Kobune [1], Haruka Nagai [1], Takeyuki Kikuchi [1], Yasuhiro Yoneda [2]

[1] *University of Hyogo, Himeji, Japan*
[2] *Japan Atomic Energy Agency, Kouto, Japan*

(1-x)($Na_{0.50}K_{0.45}Li_{0.05}$)$NbO_3$-(x)Ca($Zr_{0.50}Ti_{0.50}$)$O_3$ (NKLN-CZT, x = 0-0.08) powders were synthesized by the malic acid complex solution method, and NKLN-CZT solid solutions were then fabricated using a conventional solid-state reaction technique. The piezoelectric properties of the resulting materials were measured, and the x = 0.02 sample was found to exhibit the maximum longitudinal-length-mode piezoelectric coefficient and radial-mode electromechanical coupling factor values of 238 pC/N and 35%, respectively. On the basis of both the results for piezoelectric properties and for the local structural analysis using high-energy X-ray diffraction (HEXRD), measuring the degree of distortion of NbO_6 octahedra using HEXRD can be an effective method for the development of high-performance piezoelectric materials.

Keywords: Lead-free piezoelectric, alkali niobate, NKLN-CZT, local structure analysis, HEXRD

Tu-S-P-24

Phase transitions in dense perovskite formate frameworks: EPR and dielectric study

Mantas Simenas [1], Sergejus Balciunas [1], Monika Trzebiatowska-Gusowska [2], Miroslaw Maczka [2], Georg Völkel [3], Andreas Pöppl [3], Juras Banys [1]

[1] *Faculty of Physics, Vilnius University, Sauletekio 9, Vilnius, Lithuania*
[2] *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box-1410, Wroclaw, Poland*
[3] *Faculty of Physics and Earth Sciences, Universität Leipzig, Linnestrasse 5,, Leipzig, Germany*

Lately, novel porous materials called metal-organic frameworks (MOFs) emerged and immediately attracted attention of the scientific community. These crystalline compounds are unique due to the high degree of porosity which can be utilized for gas adsorption related applications. Additionally, many MOFs containing paramagnetic transition-metal ions exhibit peculiar magnetic properties. The organic part in several of such compounds consists of polar molecules which below a certain phase transition temperature order into a ferroelectric-type phase, making these materials single-phase hybrid multiferroics. We use EPR, ENDOR and dielectric spectroscopic techniques to investigate and characterize the ferroelectric-like phase transitions in manganese and copper doped dense [A][$Zn(HCOO)_3$] MOFs based on the perovskite architecture. Here A^+ is $NH_2NH_2CH_3^+$ or $(CH_3)_2NH_2^+$) molecular cations. The temperature dependent continuous-wave EPR spectra reveal that the local paramagnetic ion-probes are indeed sensitive to the local structural changes occurring at the phase transitions. Spectral simulations are used to obtain the ***g***, hyperfine ***A*** and fine structure ***D*** tensors at different temperatures. This allows us to probe the temperature dependence of the local order parameter and to characterize the observed phase transitions. Pulse EPR and ENDOR measurements are performed to study structure of the framework, lattice dynamics and motion of the molecular cations in the low temperature phases. The magnetic resonance methods are complemented by the dielectric spectroscopy

of MOF single crystal samples providing information about the nature of the phase transitions and dynamics of the molecular cations.

Keywords: Metal-organic framework, phase transition, EPR, perovskite architecture

---

Tu-S-P-25

Preparation of $BiFeO_3$ thin films by MOCVD

Masaru Shimizu, Nao Yoshimura, Hironori Fujisawa, Seiji Nakashima

Graduate School of Engineering, University of Hyogo, Himeji, Japan

$BiFeO_3$ is one of the most important candidates for realization of functional devices due to its good ferroelecricity, piezoelectricity and multiferroelectricity. $BiFeO_3$ thin films have generally been prepared using sputtering, PLD (Pulsed Laser Deposition) and CSD (Chemical Solution Deposition) techniques. However, in these films, it was quite difficult to control stoichiometric composition and oxygen deficiencies in films which cause the high leakage. In order to obtain $BiFeO_3$ thin films with low leakage current densities for an application to 3D-FeRAMs with nanowire capacitors, in our study, MOCVD (Metalorganic Chemical Vapor Deposition) process was used. In our MOCVD, $Bi(C_6H_5)_3$ and $Fe(thd)_3$ were used as an source precursor and O_2 containg O_3 as an oxidizing gas. $BiFeO_3(001)$ epitaxial thin films were successfully grown on $SrRuO_3/SrTiO_3(100)$ at 620 ^oC. Process window in Bi/(Bi+Fe) was observed by changing Bi supply ratio. $BiFeO_3$ thin films obtained showed good ferroelectric P-E hysteresis loops (Pr ~ 60μ C/cm^2, Ec ~ 300 kV/cm). $BiFeO_3$ thin films gown by MOCVD showed lower (10_2-10^4 order) leakage currrent densities ($\sim 10^{-6}$ A/cm^2 at 3 V) comparing with those of the sputtered $BiFeO_3$ thin films. These experimental results indicate that the film growth under high oxygen pressure and precise film composition control in MOCVD process are indispensable for obtaining high quality $BiFeO_3$ thin films with low leakage.

Keywords: BiFeO3 thin film, MOCVD, epitaxial thin film

Tu-S-P-26

Phase transition studies on the multiferroic (1-x)$BiFeO_3$-(x)$BaTiO_3$ solid solutions below room temperature

ARUN KUMAR, Dhananjai Pandey

School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005, India

The practical applications of Magnetoelectric (ME) materials essentially require a strong linear coupling between the magnetization (M) and ferroelectric polarization (P) at room temperature. $BiFeO_3$ is unique

amongst various magnetoelectric multiferroics, as its ferroelectric and magnetic transition temperatures (T_C~1103 K, T_N~ 643 K) are well above the room temperature. In recent years, (1-x)$BiFeO_3$-(x)$BaTiO_3$ (BF-xBT) solid solutions have received considerable attention due to large ferroelectric polarization, large remnant magnetization, linear magnetoelectric coupling and highest depolarization temperature (T_d) for piezoelectric applications. However, the ground state of neither $BiFeO_3$ nor BF-xBT is still not clear. We present here results of Rietveld analysis of x-ray and neutron powder diffraction data in conjunction with results of magnetization, AC susceptibility and specific heat measurements. Our results reveal presence of two spin glass (SG) phases below room temperature both of which coexist with the long range ordered (LRO) antiferromagnetic (AFM) phase formed well above room temperature at the Neel transition temperature. It is shown that both the spin glass transitions are accompanied with decrease in the ordered magnetic moment and strong magnetoelastic coupling suggesting that the LRO-AFM and SG transitions occur on the same magnetic sublattice in agreement with theoretical predictions for Heisenberg systems. We also present a magnetic phase diagram of the BF-xBT system.

Keywords: Multiferroics, BiFeO3, Solid solutions, Spin glass, Phase transitions

---

Tu-S-P-27

Synthesis and characteristics of high dielectric constant material: $BaCu_3Ti_4O_{12}$

Kalpana Parida, RNP Choudhary
Department of Physics,Siksha O Anusandhan University , Odisha, India, Bhubaneswar, India

Now-a-days, there is a rapid development of high-low dielectric constant materials for microelectronics industry. More emphasis is given on reduction of volumetric size of the material for electronic devices such as capacitors, filters, resonators and memory devices by using the high dielectric constant materials. Although the high permittivity materials are helpful for diminishing the size of the components in microelectronic systems, their applications are still very limited due to many inherent problems of the materials including high dielectric losses. Several attempts have been made to solve the problems. In this attempt, we have carried out extensive studies on capacitive and resistive characteristics of BaCu3Ti4O12 (family member of giant dielectric constant material CaCu3Ti4O12). In this presentation we report crystal structure, dielectric, impedance spectroscopy of chemically prepared sample. X-ray diffraction study exhibits the formation of single-phase compound at 900 oC. Dielectric and impedance spectroscopy study of this ceramic compound has been characterized in a wide frequency (1 kHz-1 MHz) and temperature (25 oC-500 oC) ranges. In the impedance analysis, Nyquist plots discuss the presence and contributions of grain, grain boundary and electrode effect. The bulk resistance of the material decreases with increasing temperature showing negative temperature showing a typical semiconducting property, i.e. negative temperature coefficient of resistance (NTCR) behavior.

Keywords: chemical reaction method, XRD, SEM, giant dielectric constant.

Tu-S-P-28

The defect and dielectric relaxation of Nb and Mn Co-doping $BaTiO_3$ ceramics

Yang Xiaojing [1], Liu Xiaobing [2], Ding Shihua [3]

[1] *School of Bioengineering, Xihua University, Chengdu, China*
[2] *Key Laboratory of Fluid and Power Machinery, Ministry of Education of China, Xihua University, Chengdu, China*
[3] *School of Materials Science and Engineering, Xihua University, Chengdu, China*

$BaTiO_3$ based ceramics were prepared by solid state reaction. Mn and Nb were co-doped in the B site of $BaTiO_3$ based ceramics. The effect of donor and acceptor (Nb and Mn) on the dielectric properties of $BaTiO_3$ based ceramics was investigated. The Mn = 1.6% mol and Nb = 0, 0.18%, 1.0%, 1.1%, and 2.0% mol respectively. When the content of Nb is less than 1.0% mol (Mn is fixed at 1.6% mol), the temperature dependence of the dielectric constant appeared a diffuse phase transition(DFT) characteristics, and a normal-like ferroelectric characteristics was observed as the content of Nb is 1.0% mol. When the content of Nb increases further, up to 1.1% mol, it showed a dielectric relaxation. Atomic computer simulation has been used to predict the binding energy for different defect associations [$2Nb_{Ti}^{\cdot}+V_{Ba}^{''}$] and [$2V_{O}^{\cdot\cdot}+Mn_{Ti}^{''}$] which leads to random electrical fields and polar nanoregions (PNRs). The change from DFT ferroelectrics to relaxors could be related to the size of PNRs.

Keywords: BaTiO3 ceramics, dielectric relaxation, polar nanoregions

---

Tu-S-P-29

Defects and dielectric properties of BCZT ceramics doped with Nd

Ding Shihua, Peng Yong, Song Tianxiu

School of Materials Science & Engineering, Xihua University, Chengdu, China

$(Ba_{0.92-x}Ca_{0.08}Nd_x)(Ti_{0.82}Zr_{0.18})O_3$ ($0\leq x\leq 0.02$) Ferroelectric ceramics samples were prepared by conventional solid-state reaction methods. The structure and dielectric properties of the samples were investigated by XRD, LCR and other techniques. The results revealed that when the doping amount is 0.015, the second phase occurred. The structure of defects, charge compensation and configuration of [$4Nd_{Ba}^{\cdot}+V_{Ti}^{''''}$] defect cluster were discussed in BCZT ceramics doped with Nd^{3+} using the general utility lattice program (GULP). With Nd^{3+} content increasing, both dielectric constant and dielectric loss declined, the dielectric peak temperature shifted to low temperature and the dielectric peak broadened. With increasing Nd^{3+} content, the dielectric relaxation characteristics were obtained, which were attributed to the random field induced by off-center Nd^{3+} ions and defect dipoles [$4Nd_{Ba}^{\cdot}+V_{Ti}^{''''}$].

Keywords: (Ba0.92-xCa0.08Ndx)(Ti0.82Zr0.18)O3 ceramics, defects, solution energy, dielectric properties

---

Tu-S-P-30

Double hysteresis loops in $Pb(Zn_{1/3}Nb_{2/3})O_3$-$PbTiO_3$

Makoto Iwata [1], Yasutaka Kaiden [1], Yoshihiro Ishibashi [2]

1 Nagoya Institute of Technology, Nagoya, Japan
2 Nagoya University, Nagoya, Japan

(1-*x*)Pb(Zn1/3Nb2/3)O3-*x*PbTiO3 (PZN-*x*PT), regarded as relaxor ferroelectrics, is one of the most important materials in applications because of their high electro-mechanical coupling coefficient near the morphotropic phase boundary (MPB) located at x = 9%. Such relaxors are known to undergo the diffuse phase transition with a broad peak in the dielectric permittivity as a function of temperature owing to heterogeneity such as polar nanoregions (PNRs). However, the physical mechanism for the appearance of relaxor properties seems to be still controversial. On the other hand, the critical endpoint (CEP) has been found in (1-*x*)Pb(Mg1/3Nb2/3)O3-*x*PbTiO3 being isomorphous compound of PZN-*x*PT [1]. In a series of our studies, we have investigated the temperature dependence of the permittivity under the dc biasing field in PZN-*x*PT, and have found that the broad peak in the permittivity changes to the sharp peak under the dc biasing field, suggesting the existence of CEP on the temperature-field phase diagram [2]. In the present study, to reinforce our previous conclusion that the CEP certainly exists, we have observed double hysteresis loops in PZN-9%PT showing the field induced transition just above the first-order transition temperature. It has been found that the hysteresis of the double loops disappears at CEP located at 190oC and 1.2 kV/cm.

References

[1] Z. Kutnjak et al.: Nature 441, 956 (2006).

[2] M. Iwata et al.: Phase Transitions 88, 306 (2015).

Keywords: PZN, hysteresis loop, phase transition, critical endpoint

---

Tu-S-P-31

Domain kinetics in KTP single crystals for periodical poling applications

Vladimir Shur [1], Andrey Akhmatkhanov [1], Elena Pelegova [1], Ekaterina Vaskina [1], Maria Chuvakova [1], Ekaterina Gachegova [1], Maxim Ivanov [2], Andrei Kholkin [2]

[1] School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg, Russia
[2] Department of Physics and CICECO-Aveiro Institute of Materials, Aveiro, Portugal

The domain structure evolution during polarization reversal in uniform electric field has been studied in potassium titanyl phosphate (KTiOPO4, KTP) single crystals using various complementary experimental methods. The studied KTP samples representing 2-mm-thick plates cut perpendicular to polar axis were grown by top-seeded solution method. The optical microscopy without selective chemical etching has been used for in situ visualization of domain structure evolution with high temporal

resolution. The obtained contrast was attributed to local change of the refractive index in the vicinity of the domain wall caused by residual depolarization field. The in situ visualization allowed revealing two elongated domain shapes: stripe and rhombus, oriented along Y direction. Two types of the moving domain walls were distinguished: (a) the walls of the rhombus domains deviated from Y-direction for the angle below 10 degrees (Y+ walls) and (b) the walls deviated from X-direction for about 30 degrees (X+30 walls). It was shown that the X+30 walls were essentially faster than the Y+ ones. The jump-like domain wall motion caused by domain merging was revealed. The domain shape stability effect representing the fast restoration of the rhombus shape just after merging of small isolated rhombus was demonstrated. The dependence of the wall motion velocity on its orientation has been measured. The model of domain growth by generation of elementary steps and kink motion was presented. The revealed polarization reversal induced by chemical etching was attributed to action of the residual depolarization field appeared after partial removing of the screening charge layer.

Keywords: domain structure evolution, domain kinetics, potassium titanyl phosphate, KTP

Tu-S-P-32

Formation of self-assembled domain structure at non-polar surfaces of $LiNbO_3$ by tip scanning without application of external field

Vladimir Shur, Anton Turygin, Denis Alikin, Jury Alikin

School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg, Russia

The investigation of the domain evolution under local electric field produced by conductive tip of the scanning probe microscope on polar surface is one of the most informative. Recently the investigation by this method of the domain growth on non-polar surfaces allowed to reveal the detail information about forward domain growth. We provide the results of experimental study of the formation of quasi-regular structure of spike-like domains during scanning by grounded tip of scanning probe microscope without application of external electric field in the vicinity of the spike-like domain switched by rectangular field pulse. The effect was revealed at the non-polar X and Y cuts of congruent lithium niobate single crystals. The domains were visualized by piezoresponse force microscopy and the spatial distribution of the surface potential was measured by Kelvin probe force microscopy. The key role of the charges injected during pulse application was demonstrated. The multiplication of the domain structure period (doubling and tripling) has been observed. The formation of domain structure was attributed to: (1) action of the field created by localized injected charges, (2) screening of depolarization field by current in the external circuit, (3) electrostatic interaction of the isolated domains. We demonstrated non-uniformity and unipolarity of the charge injection and showed their influence on the parameters of domain structure. It was shown that during application of the switching pulse the injected charge propagated over the distance about tens of microns from the tip. The measured relaxation time of the injected charge is about several hours.

Keywords: Lithium niobate, scanning probe microscopy, self-assembled structures, non-polar cut.

Tu-S-P-33

Dynamics of ferroelectric polarization simulated by a second-order Landau model

Michael Richman, Paul Rulis, Anthony Caruso

Department of Physics and Astronomy, University of Missouri-Kansas City, Kansas City, Missouri, United States

By using a second-order time-dependent Ginzburg–Landau model, we simulate the dynamic polarization hysteresis behavior of a ferroelectric system subjected to a sinusoidal electric field. We examine polarization hysteresis loop structure as a function of field amplitude and field frequency. The relationship between these parameters and hysteresis loop structure is quantified by considering the Fourier transform spectrum of the time series of polarization. This spectrum is used to determine a deforming factor that measures the amplitude- and frequency-dependent distortion of polarization hysteresis loops from ellipticity. Our results indicate that the considered model produces results in agreement with experimental observations.

Keywords: Time-dependent Ginzburg–Landau theory, hysteresis dispersion

---

Tu-S-P-34

Multi-shell nanowires including ferroelectrics

Hironori Fujisawa, Yohei Takeuchi, Masaru Shimizu, Seiji Nakashima

University of Hyogo, Himeji, Japan

Recently, one-dimensional nanostructures of functional materials have been attracted much attention from the viewpoint of practical applications and as well as for studying their basic physics. Among nanowires (NWs) of various materials, NWs including ferroelectrics can be used as capacitors and transistors in very high density non-volatile memories, and as piezoelectric transducers in vibration energy harvesters. We have developed fabrication technique of ferroelectric NWs/nanotubes using ZnO NWs as a template via MOCVD. In this study, we report introduction of HfO_2-based ferroelectrics, which is more suitable for nanowire capacitors than conventional perovskite typed ferroelectrics because of its excellent ferroelectric properties in thin films below 10nm, into NW capacitors and their electrical properties. ZnO NW templates were grown on Pt-covered SiO_2/Si substrate by MOCVD using $Zn(C_2H_5)_2$ and O_2 as the precursor and oxidizing gas, respectively. Amorpous $(Hf,Zr)O_2$ layer was prepared on ZnO NW template at 200 ^oC by MOCVD, and crystallized to ferroelectric orthorhombic phase by high temperature annealing at 800 ^oC and 60-300 s in N_2. Finally, $(Hf,Zr)O_2$/ZnO NWs are covered with ZnO top layer by MOCVD at low temperature of 300 ^oC. ZnO/$(Hf,Zr)O_2$/ZnO Multi-shell structure was clearly confirmed by back scattering electron microscopy which can contrast a difference in atomic numbers. XRD analysis revealed that $(Hf,Zr)O_2$ was successfully crystallized to orthorhombic phase which can show ferroelectricity after annealing. In the conference, ZnO/$(Hf,Zr)O_2$/ZnO NW capacitors will be discussed.

Keywords: HfO2, nanowires, capacitors, ZnO

Tu-S-P-35

Effect of electric field on 180° domain switching in uniaxial $Ca_{0.30}Ba_{0.70}Nb_2O_6$ crystals studied by Brillouin Scattering

Md Aftabuzzaman [1], Md Al Helal [1], Jan Dec [2], Wolfgang Kleemann [3], Seiji Kojima [1]

[1] *Graduate School of Pure and Applied Sciences, University of Tsukuba, 305-8573, Tsukuba, Japan*
[2] *Institute of Materials Science, University of Silesia, PL-40-007, Katowice, Poland*
[3] *Angewandte Physik, Universität Duisburg-Essen, D-47048, Duisburg, Germany*

The elastic properties of uniaxial relaxor $Ca_xBa_{1-x}Nb_2O_6$ (x = 0.30, CBN30) c-plate single crystals were studied under a dc electric field using broadband Brillouin scattering spectroscopy. Below the Curie temperature, T_C = 231 °C, a sizable change of the longitudinal acoustic (LA) velocity (v_{LA}) was observed near the coercive field when switching the electric field direction from [001] (+E) to [00-1] (-E). Internal random fields (RFs) restrict the growth into macrodomains by stabilizing the nanodomain state, while the external +E suppresses RFs and, as a result, a gradual increase of polarization was observed. After complete switching of polarization and just before the growth of nanodomain into a macrodomain state, +E was gradually removed and -E was applied. By increasing –E, a sharp increase of v_{LA} was observed which indicates a complete switching of the nanodomain into the macrodomain state with opposite polarity along -E. After removing –E and gradually reapplying +E, LA mode splitting was observed, which indicates a state consisting of coexisting macrodomains induced by -E and +E, respectively. The lower-frequency LA mode corresponds to the macrodomain state due to -E, while the higher-frequency LA mode corresponds to the macrodomain state due to +E. The v_{LA} of the macrodomain state induced by +E is higher than that of the macrodomain state induced by –E. This proves that the macrodomain state triggered by +E is more stable. Field cooling processes under +E and –E were also investigated.

Keywords: Uniaxial relaxor, Domain Switching, Nanodomain, Macrodomain, Brillouin scattering

Tu-S-P-36

Temperature dependent local structure of MFe_2O_4 (M = Ni and Mn) determined by *in-situ* X-ray absorption fine structure (EXAFS)

PINIT KIDKHUNTHOD

Synchrotron Light Research Institute, Muang, Nakhon Ratchasima, Thailand

The magnetic spinel ferrites, MFe_2O_4 (M = Ni, and Mn), have been widely studied for their novel magnetic and electronic properties. In this work, MFe_2O_4 were prepared by solid state reaction and co-precipitation method. The synthesis parameter and the phase formation behavior were investigated in details via several techniques, including thermal analysis, X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS). A change in local structure was investigated using in-situ extended X-ray absorption fine structure (EXAFS). The temperature ranged

between 50 °C and 300 °C with air condition was applied for this study. The results will be presented and discussed in details.

Keywords: The magnetic spinel ferrites; X-ray absorption fine structure.

Tu-S-P-37

Aging in relaxor ferroelectric systems

Jan Dec [1], Wolfgang Kleemann [2]

[1] *Institute of Materials Sciences, University of Silesia, PL-40-007 Katowice, Poland*
[2] *Angewandte Physik, Universität Duisburg-Essen, D-47048 Duisburg, Germany*

The polar correlations in relaxor ferroelectrics (REFs) are usually considered as being promoted by quenched random electric fields (RFs). Within this approach the local polarization of individual PNR is controlled by the fluctuations of the RFs and thus precludes macroscopic ferroelectric symmetry breaking, even if uniformly charged chemically ordered regions counteract as observed in the heterogeneous relaxor-like lead magnesium niobate, $PbMg_{1/3}Nb_{2/3}O_3$ (PMN). These PNR interact dipolarly and consequently, on cooling, a cluster-glassy ground state sets in at T_g [1]. On the other hand, below T_g the observed unusual dielectric response of REFs originates from the side-wall motion of mesoscopic domains [1]. Actually the glassy state concept versus a microdomain model is still puzzling [2]. One of the experimental possibilities for distinguishing between these two models is to study effects of aging. While the domain-like growth typically displays cumulative aging, the aging in glassy systems includes characteristic rejuvenation and memory effects. The goal of this contribution is to report results of our systematic studies of the aging processes in the canonical PMN and the uniaxial strontium-barium niobate (SBN) realaxor systems in the vicinity of their glass temperatures. The experimental results confirm the superdipolar glassy scenario of relaxors as their dominant ground state.

References

[1] W. Kleemann and J. Dec, Phys. Rev. B 94, 174203 (2016)

[2] Y. Uesu, H. Tazawa, K. Fujishiro, and Y. Yamada, J. Kor. Phys. Soc. 29, S703 (1996).

Keywords: Ferroelectric relaxors, ferroic superglass, aging

Tu-S-P-38

Large electro-mechanical energy conversion in PZT-PNN ceramics

Muangjai Unruan [1, 2], Sujitra Unruan [3], Yutthapong Inkong [1, 2], Rattikorn Yimnirun [4]

[1] *Department of Applied Physics, Faculty of Sciences and Liberal Arts, Rajamangala University of Technology Isan, Nakhon Ratchasima, Thailand*

[2] *Department of Materials Science and Innovation, Faculty of Sciences and Liberal Arts, Rajamangala University of Technology Isan, Nakhon Ratchasima, Thailand*
[3] *Department of Material Engineering, Faculty of Engineering and Architecture, Rajamangala University of Technology Isan, Nakhon Ratchasima, Thailand*
[4] *School of Physics, Faculty of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand*

This paper reports on an indirect measurement of energy density of PZT-PNN ceramics utilizing mechanical stress. The method use Olsen like cycle and allows for a large amount of electro-mechanical energy conversion. A maximum energy density was achieved under 0-100 MPa and 1-15 kV/cm of applied mechanical stress and electric field, respectively. The obtained result is substantially higher than the results reported in previous studies in many piezoelectric materials utilizing direct piezoelectric effect.

Keywords: Energy conversion, Energy harvesting, Olsen cycle, mechanical stress

---

Tu-S-P-39

Effect of $BaZr_{0.4}Ti_{0.6}O_3$ addition on electrical and magnetic properties of Multiferroic (1-x)$BiFeO_3$-x$BaTiO_3$ ceramics

Sujitra Unruan [1], Rattikorn Yimnirun [2], Rungnapa Tipakontithikun [3], Muangjai Unruan [4]

[1] *Department of Materials Engineering and Smart Materials and Innovation Research Unit, Faculty of Engineering and Architecture, Rajamangala University of Technology Isan, Nakhon Ratchasima, Thailand*
[2] *School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand*
[3] *Department of Physics, Faculty of Science, Ubon ratchathani University, Ubon ratchathani, Thailand*
[4] *Department of Applied Physics, Faculty of Sciences and Liberal Arts, Rajamangala University of Technology Isan, Nakhon Ratchasima, Thailand*

In this study, high purity (1-x)$BiFeO_3$-x$BaTiO_3$ powders at x = 0.23, 0.24, 0.25, 0.26 and 0.27 were mixed with high purity $BaZr_{0.4}Ti_{0.6}O_3$ powder in the ratio of 1:3 respectively. The mixed powders were pressed as pallet and then sintered at 1150 oC. Attention has been focused on dielectric, ferroelectric and magnetic properties of the sintered ceramics. It was found that $BaZr_{0.4}Ti_{0.6}O_3$ addition affected significantly to increasing of dielectric, ferroelectric and magnetic properties of (1-x)$BiFeO_3$-x$BaTiO_3$ ceramics.

Keywords: Multiferroics, Perovskite, BFO-BTO-BZT

Tu-S-P-40

Influence of humidity on electrophysical properties of pure silicon dioxide

Milovidova SD [1], Nguyen Hoai Thuong [2], Rogazinskaya OV [1], Sidorkin AS [1], Zolotukhina MA [1]

[1] *Voronezh State University, Voronezh, Russia*
[2] *Industrial University of Ho Chi Minh City, Ho Chi Minh, Vietnam*

Ferroelectric nanocomposite materials have emerged as a modern research object for studying advanced properties suitable for nanotechnology applications due to the possibility of regulating their properties caused by the size effects. In this context, the development of nanotechnology led to the production of nano-sized silica SiO_2, which is widely used as a filler in these composites. With the high absorption ability of nanoparticles SiO_2 relating to moisture due to the presence of -OH groups on their surface, the study of influence of humidity on electrophysical properties of SiO_2 can be considered as an urgent task and as a necessary step to understand properties of nanocomposite materials with the component of SiO_2 nanoparticles. The present work devoted to the study of influence of humidity on electrophysical properties of SiO_2 in a weak electric field (1 V/cm) at low frequencies in a temperature range from 15 °C to 112 °C. Samples SiO_2 were prepared from silica hydrosol with nanodispersed particles of ~ 6 nm by using the evaporation method. The obtained experimental results for SiO_2 samples in high-moistened regime showed high values of dielectric constant (up to 240 000) and a sharp increase in the values of dielectric loss with decreasing frequency at infra-low frequencies. The indicated anomalies can be associated to the reorientation of dipole moments of water molecules in nanochannels as well as the accumulation of volume charges at boundaries between SiO_2 nanoparticles due to Maxwell-Vagner polarization.

Keywords: nano-sized silica, nanocomposite, dielectric properties

---

Tu-S-P-41

Local piezo-ferroelectric properties of highly textured $(K_{0.5}Na_{0.5})_{0.985}La_{0.005}NbO_3$ thin films

H´Linh H´Mok [1, 2], Espiridión Martínez Aguilar [1, 2], Jose Juan Gervacio Arciniega [2], Xavier Vendrell [3], Jesús M. Siqueiros [2], Oscar Raymond Herrera [2]

[1] *Posgrado en Física de Materiales, Centro de Investigación Científica y de Educación Superior de Ensenada, Carretera Tijuana-Ensenada No. 3918, Ensenada, 22860, Baja California, Mexico*
[2] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México AP 14, Ensenada, 22860, Baja California, Mexico*
[3] *Departament de Química Inorgánica, Universitat de Barcelona, 08028, Barcelona, Spain*

High quality thin films of the lead-free $(K_{0.5}Na_{0.5})_{0.985}La_{0.005}NbO_3$ (KNNLa) compound were successfully deposited on Nb-doped $SrTiO_3$ substrates with orientation [100] (NSTO100) and [110] (NSTO110) by rf-sputtering. Highly textured thin films, 200 nm thick, grew conditioned by the substrate surface. The KNNLa films on NSTO100 are characterized by the coexistence, at room temperature, of a commensurate [001]-oriented tetragonal phase and two incommensurate [010]-oriented monoclinic phases; while on NSTO110 the KNNLa films grew only in an incommensurate [101]-oriented monoclinic phase. Local ferroelectric and piezoelectric properties were evaluated by piezoresponse force microscopy. Both samples show excellent and homogenous out-of-plane polarization switching patterns of up and down ferroelectric domains corresponding with 180° domains walls. For the KNNLa/NSTO100 sample, asymmetric switching voltages of -30 V and +15 V were required because the KNNLa film grew with net polarization pointing down, with high coercivity depending on the

spontaneous polarization direction in each of the coexisting phases. For the KNNLa/NSTO110 sample, lower symmetric switching voltages of +5 V and -5 V were required since the KNNLa film grew with polarization pointing up along the [110] direction (~45° away from the out-of-plane direction). The KNNLa/NSTO100 film exhibits the higher piezoelectric constant, d_{33} = 29 pm/V and global electromechanical resonance response at ~396 kHz.

This work was supported by PAPIIT-DGAPA-UNAM (Grants IN110315 and IN105317) and CONACYT (Grants Fronteras-2026, 282778 and 280309). Two of the authors, H.-H. and E. M-A. thank CoNaCyT for their scholarships. The authors acknowledge E. Aparicio, E.A. Murillo, and P. Casillas for their technical assistance.

Keywords: KNN thin films, ferroelectric domains, commensurate and incommensurate growths, sputtering, piezoreponse force microscopy

---

Tu-S-P-42

Dielectric properties of $BaTiO_3$ based composites

Sergejus Balčiūnas [1], Maksim Ivanov [1], Satoshi Wada [2], Jūras Banys [1]

[1] *Faculty of Physics, Vilnius University, Vilnius, Lithuania*
[2] *Interdisciplinary Graduate School of Medical and Engineering, University of Yamanashi, Yamanashi, Japan*

For the past 40-50 years, lead based perovskite $Pb(Zr_xTi_{1-x})O_3$ (PZT) piezoelectric ceramics have dominated the commercial market of piezoelectric devices due to their remarkable dielectric and piezoelectric properties and ability to operate in wide temperature range. But due to environmental concerns the use of PZT in the European Union was limited. In our presentation broadband dielectric properties of $BaTiO_3$ (BT) based composites with core-shell superstructure in temperature range of 100 to 500 K will be presented. The composites were prepared in two steps. BT, $BiFeO_3$ (BF), $BaTiO_3$-$Bi(Mg_{0.5},Ti_{0.5})O_3$ (BT-BMT) and $BaTiO_3$-$Bi(Mg_{0.5},Ti_{0.5})O_3$-$BiFeO_3$ (BT-BMT-BF) nanoparticles were compressed into low density pellets and head treated to create a necking structure. Then using solvothermal reaction method the epitaxial layer of BT was deposited around BT, BF, BT-BMT and BT-BMT-BF particles. In such systems cores are stressed by barium titanate shell creating similar conditions as in morphotropic phase boundary (MPB), thus increasing dielectric and piezoelectric constants. We have investigated 4 different composite systems where core is a good dielectric, a relaxor, a ferroelectric and a non-ferroelectric material.

Keywords: KNBT, morphotropic phase boundary, barium titanate, potassium niobate, lead free

---

Tu-S-P-43

Thermophysical properties of multiferroic bismuth ferrite with rare-earth elements

Suleiman Kallaev [1], Abumuslim Bakmaev [1], Zairbek Omarov [1], Alikber Bilalov [1], Larisa Reznichenko [2], Sedik Hazbulatov [2]

[1] *Institute of Physics, Dagestan Scientific Center, Russian Academy of Sciences, Makhachkala, 367003 Dagestan, Russia, Makhachkala, Russia*
[2] *Research Institute of Physics, Southern Federal University, Rostov-on-Don, Russia., Rostov-on-Don, Russia*

Thermal diffusion, thermal conductivity, and heat capacity of $Bi_{1-x}Re_xFeO_3$ multiferroics (Re – rare-earth element; x = 0 - 0.20) are investigated in the temperature interval of 130 K to 1200 K. The rare earth substitution leads to a change in the temperature anomalies of the thermal diffusion and conductivity and in antiferromagnetic phase transition region, the increase of the heat capacity in a wide temperature range, and the temperature displacement of the antiferromagnetic transition. It is established that the temperature dependence of the excess heat capacity is associated with the Schottky effect for three states of the level resulting from structure distortions in the rare-earth-doped compositions. The analysis of the results along with structural and acoustic data indicates that local distortions of the crystal lattice, which are caused by the distortions of oxygen octahedra of FeO_6 and polar shifts of Bi^{3+} and Fe^{3+} ions from their initial positions, constitute the main mechanism of the scattering of phonons in $BiFeO_3$ and $Bi_{1-x}Re_xFeO_3$ multiferroics. It is found that Re doping leads to a significant change in the temperature anomalies of the thermal diffusion and thermal conductivity near phase transitions, namely, to the smearing of the ferroelectric transition T_c and the appearance of a minimum in the region of the antiferromagnetic transition T_N. The dominant mechanisms of phonon heat transfer in the region of ferroelectric and antiferromagnetic phase transitions are revealed. The temperature dependence of the mean free path of phonons is determined.

Keywords: Thermophysica, multiferroic, thermal diffusion, thermal conductivity, heat capacity

---

Tu-S-P-44

Effects of morphology and surface potential shift of mechanosynthesized $BiFeO_3$ nanoparticles on the visible-light catalysis for decontamination of organic dyes

Eduardo Volnistem, Raquel Bini, Gustavo Dias, Luiz Cótica, Ivair Santos

State University of Maringá, Maringá, Brazil

In the last years, photocatalytic materials has achieved an important role in several applications as water splitting, nitrogen fixation and degradation of organic pollutants for waste water decontamination. Among this class of materials, perovskite-based materials presents a great potential for catalysis under visible light. Bismuth Ferrite ($BiFeO_3$) is a multiferroic magnetoelectric material with rhombohedral distorted perovskite structure (ABO_3) showing ferroelectricity and antiferromagnetism at room temperature. Recently, $BiFeO_3$ has been successfully applied as a catalyst for discoloration of some organic dyes in waste water due to their band gap (~2.3 eV) and controllable electron-hole separation owing the ferroelectric properties. However, the synthesis of $BiFeO_3$ for the use as catalyst are focoused mainly in wet-chemical routes such as PVA and co-preciptation techniques. In this sense, $BiFeO_3$ was synthesized by milling techniques and used as catalyst in the decontamination of Methylene Blue. The

particles surface potential was measured by photo-assisted kelvin force microscopy (PKFM) in the dark and under visible light and the results were correlated with the morphology and the catalysis results.

Keywords: Bismuth Ferrite, Photocatalysis, Kelvin Force Microscopy, Surface potencial

---

Tu-S-P-45

Computational design of new semiconductor ferroelectric perovskite oxides

Ilya Grinberg [1], Jing Yang [2], Andrew Rappe [2]

[1] *Department of Chemistry, Bar Ilan University, Ramat Gan, Israel*
[2] *Department of Chemistry, University of Pennsylvania, Philadephia, United States*

Ferroelectric materials exhibit spontaneous inversion symmetry breaking and polarization that can be exploited for excited carrier separation in photovoltaic devices. The wide band gaps of traditional ferroelectric oxide materials limit their utility for use in photovoltaic and optoelectronic devices, motivating the search for ferroelectric oxide semiconductors with band gaps in the visible range. We use density functional calculations for a variety of ferroelectric oxide solid solutions to examine the effects of compositional and local structure changes on the electronic structure of these materials. We find that W- and Mo-containing solid solutions exhibit high absorption coefficients and visible-range band gaps, making these materials promising for use as solar absorbers in photovoltaic devices.

Keywords: photovoltaics, semiconductors

Tu-S-P-46

Dielectric, piezoelectric and optical properties of a $PbZr_{1-x}Ti_xO_3$ single crystal

Iwona Lazar [1], Krystian Roleder [1], Andrzej Majchrowski [2], Dariusz Kajewski [1], Andrzej Soszyński [1], Janusz Koperski [1]

[1] *Institute of Physics, Department of Ferroelectric Physics, University of Silesia ul. Uniwersytecka 4, 40-007 Katowice, Poland, Katowice, Poland*
[2] *Institute of Applied Physics, Military University of Technology ul. Kaliskiego 2, 00-908 Warsaw, Poland, Warsaw, Poland*

Although the $PbZr_{1-x}Ti_xO_3$ (PZT) materials have been studied for many years, there are still many questions concerning their phase diagram. Recently a new diagram has been proposed [1]. However, it is worth mentioning that the most of studies, also those presented in [1], were carried out on ceramics due to difficulties in obtaining PZT single crystals of good quality. Recently transparent PZT single

crystal with x = 0.13, and with homogenous Ti concentration, has been successfully grown by means of top-seeded solution growth method [2]. Composition of this crystal was determined by EDS technique. It was also confirmed that distribution of the Pb and Zr ions was homogenous. From diagram reported in [1] it appears that the crystal with such Ti concentration reveals a coexistence of phases of different symmetries. In $PbZr_{0.87}Ti_{0.13}O_3$ single crystal the dielectric, piezoelectric and optical properties confirm this mixture of phases, and distinct anomalies of permittivity near 284 ºC and 115 ºC correspond to two main transitions known as P_C ($m3m$)-$F_{R(HT)}$ ($R3c$) and $F_{R(HT)}$($R3c$)-$F_{R(LT)}$ (R3m). However, another anomaly around 250 ºC inside the $F_{R(HT)}$ phase was also observed. The details of this anomaly will be presented and discussed.

References

[1] Zhang N. et al. Nature Comm. 5, 5231 (2014).

[2] Lazar I. et al. Ferroelectrics, 500, 67–75 (2016).

Keywords: PZT single crystals, piezoelectricity, dielectric and optical properties,

---

Tu-S-P-47

Resistivity of relaxor $BNT_{0.925}BT_{0.075}$x%Mn ceramics found from impedance spectroscopy

Noah Archer [1], Hugo Schmidt [1], Chi-Shun Tu [2]

[1] *Department of Physics, Montana State University, Bozeman, United States*
[2] *Department of Physics, Fu Jen Catholic University, New Taipei City, Taiwan*

Bismuth sodium titanate $(Bi_{0.5}Na_{0.5})TiO_3$ (BNT) based ceramics which are near the morphotropic phase boundary (MPB) have piezoelectric properties comparable to those of lead-containing $Pb(Zr,Ti)O_3$ (PZT) but concerns arise regarding thermal stability during long term operation due to lower depolarization temperatures. A previous study showed that T_d was remarkably improved to ~152 °C for the 0.2% Mn composition, demonstrating that Mn doping improves structural thermal stability in BNT7.5BT at increased temperatures. Ceramic disks of each composition were prepared and sintered for 2 hours at 1170ºC. Disks coated with silver paste were placed in an oven and connected to an impedance gain-phase analyzer. Runs from 100 ºC to 600 ºC in 50 ºC steps were made at frequencies from 0.1 Hz to 1 MHz in 71 logarithmic steps. Two samples were run for each Mn concentration, the first to 500 ºC and the second to 600 ºC. The 0% Mn samples had activation energies near 0.75 eV. The 0.2% Mn samples showed high E_a near 1.64 eV indicative of electronic conductivity. The 1% Mn samples showed low E_a near 0.71 eV characteristic of ionic conductivity, and had the lowest resistivity of all the samples. The first 2% Mn sample showed a low E_a indicating ionic conductivity to 400 ºC. The second sample had similar results to 400 ºC showing ionic conductivity at lower temperatures, but additional data points to 600 ºC revealed a curved semi-log plot ending in straight lines showing electronic conductivity dominating at higher temperatures.

Keywords: Resistivity, Piezoelectric, Conductivity, Activation Energy, Impedance Spectroscopy

---

Tu-S-P-48

Tailoring the properties of $BiFeO_3$ for applications through first-principles calculations

Espiridion Martinez Aguilar [1], H'Linh H'Mok [1], Maria Guadalupe Moreno Armenta [2], Jesus Maria Siqueiros Beltrones [2]

[1] *Centro de Investigación Científica y de Educación Superior de Ensenada Carretera Tijuana-Ensenada No. 3918, Zona Playitas, C.P. 22860., Ensenada, Baja California, Mexico*
[2] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México AP 14, C.P. 22860, Ensenada, Baja California, Mexico*

Presently, current solar energy conversion devices are still limited by high cost and low efficiency. The use of non-centrosymmetric materials, ferroelectrics in particular, is a new approach that is being tested for boosting conversion efficiency. Ferroelectric materials show phenomena such as the bulk photovoltaic effect and the anomalous photovoltaic effect as consequence of being non-centro-symmetric.

To improve on this line of work, the electronic and optical properties of Bismuth ferrite ($BiFeO_3$) are theoretically investigated when doped with transition metals (TM) up to 10 %, using the density functional theory within the generalized gradient approximation (GGA) and a simple Hubbard correction (GGA + U). To determine the Band Gap of BiFeO3(BFO):TM calculations were performed using PBEsol pseudopotential with energy cutoffs of 70 Ry. We used the Berry phase formalism of electric polarization to calculate the electric and ionic polarization in BFO:MT. By incorporating dopants in the cationic site, the most favorable results show an increase of the Fermi energy, generating a displacement, that turns out favorable for photovoltaic properties by reducing the the band gap. According to our results, these materials seem to be promising candidates for solar-to-electric energy conversion through the bulk and/or anomalous photovoltaic effects.

Financial support from CoNaCyT, Grants No. 282778 and 280309 and PAPIIT-DGAPA-UNAM Grants No. IN105307 and IN110315 is acknowledged. Two of the authors, E. M-A. and H.-H. thank CoNaCyT for their scholarships.

Keywords: BiFeO3, Photovoltaic effect, DFT

Tu-S-P-49

Study of the multiferroic ordering in $BiFeO_3(012)/La_{0.67}Sr_{0.33}MnO_3(012)$ heterostructures by first principles calculations

H´Linh H´Mok [1, 2], Espiridión Martínez Aguilar [1, 2], Jordi Ribas Ariño [3], Jesús M. Siqueiros Beltrones [2], Oscar Raymond Herrera [2]

[1] *Posgrado en Física de Materiales, Centro de Investigación Científica y de Educación Superior de Ensenada, Carretera Tijuana-Ensenada 3918, Zona Playitas, Ensenada, Baja California, Mexico*
[2] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México AP 14, Ensenada*

22850, Baja California, Mexico
[3] Departament de Ciencia de Materials i Química Física, Universitat de Barcelona, Barcelona, Spain

During the last few years, multiferroic materials as $BiFeO_3$ (BFO) have received a great deal of attention due to their potential applications for magnetoelectric devices. At room temperature, the BFO is a single-phase magnetoelectric multiferroic with antiferromagnetic and ferroelectric ordering that exhibits a large spontaneous electric polarization. However, a novel ferromagnetic state coexisting with ferroelectric ordering at room temperature in (012)-oriented and strained BFO thin films grown using a sputtering technique on $La_{0.7}Sr_{0.3}MnO_3/SiO_2/Si(100)$ has been reported, recently, by M.C. Ramírez-Camacho et. al. (Acta Materialia 128, 2017, 451-454). The aim of this theoretical work is to study the existence and stability of such ferromagnetic state in BFO when it grows epitaxial on (012)-oriented $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) substrate. The role of the structural parameters and the magnetic ordering of the LSMO constraining the new ferromagnetic configuration in the BFO structure and coexisting with the characteristic ferroelectric order, is evaluated. The calculations of the electronic, structural, optical, and magnetic properties of (012)-oriented LSMO and BFO films, and BFO/LSMO interface have been carried out within the Density Functional Theory + Hubbard U (DFT+U) formalism using the Quantum Espresso package. The spontaneous polarization of the BFO phase has been computed by means of the Modern Theory of Polarization. A comparative analysis with the experimental evidence is presented.

This work was partially supported by PAPIIT-DGAPA-UNAM Grants IN110315, IN105317 and CoNaCyT Grants Fronteras 2026, and Projs. 282778 and 280309. Thanks are due to A. G. Rodriguez for his technical assistance.

Keywords: Multiferroics, heterostructures, ferromagnetism and ferroelectricity, first principles calculations, Quantum Espresso

---

Tu-S-P-50

AC conductivity of multiferroic $BiFeO_3$ nanocrystalline ceramics

Sadyk Sadykov, Nariman Alikhanov
Dagestan State University, Department Physics, Makhachkala, Russia

Electrical conductivity results for of $BiFeO_3$ ceramics obtained by spark plasma sintering and synthesized by the organic nitrate precursors combustion are presented.. The average size of particle estimated from the diffractograms are ~ 50 nm. The ac - conductivity measurements were conducted in 1 kHz - 10 MHz frequency range over a temperature range of 25 - 500 °C. It is shown that $\sigma_{ac}(\omega)$ obeys a power law of ω^s, where $s < 1$. At temperatures > 350 °C and frequencies of > 1 MHz conductivity passes through a maximum, and with increasing frequency the conductivity maximum temperature is shifted to lower temperatures. The conductivity has the thermally activated character. In the investigated temperature range the three overlapping processes are involved in the relaxation conductivity: i) in the temperature range 25 - 150 °C with E_a = 0.46 - 0.042 eV; ii) in a temperature range of 150 - 350 °C with E_a = 0,65-0,11 eV and iii) at temperatures > 350 °C with E_a = 0,96 - 0,76 eV. The activation energy E_a decreases with increasing frequency. The low-frequency conductivity is identified with the dc conductivity. At frequencies > 100 kHz conductivity behavior can be interpreted in the representation

of the model correlated barrier hopping (CBH) charge carriers. It is assumed that the hopping mechanism implemented in ceramic grains between the ions Fe^{2+} and Fe^{3+}. The role of oxygen vacancies in the conductivity is also discussed.

Keywords: multiferroic, ceramic, conductivity, frequency, temperature

---

Tu-S-P-51

Phase transformation induced bloating behavior in diopside glass-ceramics used for microwave dielectric materials

Kuei Chih Feng [1], Pin-Yi Chen [1], Cheng-Sao Chen [2], Chi-Shun Tu [3]

[1] *Department of Mechanical Engineering, Ming Chi University of Technology, New Taipei City, Taiwan*
[2] *Department of Mechanical Engineering, Hwa Hsia University of Technology, New Taipei City, Taiwan*
[3] *Department of Physics, Fu Jen Catholic University, New Taipei City, Taiwan*

Phase transformation and bloating behavior of novel $CaMgSi_2O_6$ glass-ceramics with ZrO_2 nucleating agents, prepared using two-stage heat treatment; were investigated and evaluated as microwave dielectric materials. Experiments show that specimens annealed below critical nucleation temperature (T_{cn}) and sintered at 950°C reveal significant bloating phenomena. Kinetic study of CaO-MgO-SiO_2-ZrO_2 (CMSZ) glass annealed below T_{cn} reveals high activation energy of crystallization for ZrO_2 nucleation, and zirconia dissolved into CMSZ glass and formation of fleeing oxygen can be attributed to sluggish crystallization of ZrO_2 agents. On the other hand, specimens of CMSZ glass annealed above T_{cn}, microstructural features exhibit that zirconia precipitated significantly in the CMSZ glass at beginning, and then are accompanied by the rapid growth of $CaMgSi_2O_6$ phase around the ZrO_2 crystallites, indicating enhanced crystallization of nuclei due to growth over the critical size of nuclei at an annealing temperature above T_{cn}. In addition, specimens using two-stage heat treatment and annealed above T_{cn} reveal much higher densification properties as microwave dielectric materials.

Keywords: diopside, glass-ceramic, nucleating agent, activation energy

---

Tu-S-P-52

Structural characteristics and large electric-field-induced strains in strontium and manganese Co-doped 92.5%($Bi_{0.5}Na_{0.5}$)TiO_3 - 7.5%$BaTiO_3$ crystals

Cheng-Sao Chen [1], Pin-Yi Chen [2], Yi-Ping Syu [2], Kuei-Chih Feng [2], Chi-Shun Tu [3]

[1] *Department of Mechanical Engineering, Hwa Hsia University of Technology, New Taipei, Taiwan*
[2] *Department of Mechanical Engineering, Ming Chi University of Technology, New Taipei, Taiwan*
[3] *Department of Physics, Fu Jen Catholic University, New Taipei, Taiwan*

Relaxor ferroelectric sodium bismuth titanate–barium titanate [92.5%($Bi_{0.5}Na_{0.5}$)TiO_3 - 7.5%$BaTiO_3$ (BNB7.5T)] solid solution co-doped with 2 mol% strontium (Sr) and 0.1 mol% manganese (Mn) have

shown enhanced stability of the material properties and piezoelectric responses, which show a large electric-field induced linear strain behavior. Sr and Mn co-doped BNB7.5T (BNB7.5T-Sr-Mn) crystals were grown by self-flux method. The as-grown BNB7.5T-Sr-Mn crystals show uniform color with dimensions around centimeter. Synchrotron X-ray diffraction (XRD) was used to measure temperature-dependent phase structure. High-resolution transmission electron microscope (TEM) was used to analyze microstructures and symmetries of unit cell. Dielectric permittivity, polarization hysteresis loop, strain vs *E* field, and piezoelectric coefficient d_{33} were measured to analyze dielectric, ferroelectric, and strain properties. The results showed that BNB7.5T-Sr-Mn crystals have a coexistence phase of *R*3*c* and *P*4*bm* symmetries. Temperature-dependent dielectric permittivity and polarization loops of BNB7.5T-Sr-Mn crystals exhibited an ergodic relaxor behavior. The curves of strain vs. *E* field display a strain up to 0.49% at room temperature, which result mainly from the relaxor–ferroelectric phase transition and electrostrictive response. Temperature-dependent *P-E* and *D-T* curves of BNB7.5T-Sr-Mn crystals show that the depolarization temperature T_d shifts toward lower temperature. Temperature-dependent *S-E* curves for BNB7.5T-Sr-Mn displayed a giant strain of 0.59% at 150 ^{o}C, indicating that BNB7.5T-Zr-Mn crystals possess excellent thermal stability and can be used as environmental friendly piezoelectric actuators.

Keywords: relaxor ferroelectric, sodium bismuth titanate, crystal growth, structure, electric-field induced strain

---

Tu-S-P-53

Universal energetic coupling in complex antiferroelectric and incommensurate perovskites

Kinnary Patel [1], Sergey Prosandeev [2], Yurong Yang [1], Bin Xu [1], Jorge Iñiguez [3], Laurent Bellaiche [1]

[1] *Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas 72701, United States*

[2] *Institute of Physics and Physics Department of Southern, Federal University, Rostov-na-Donu 344090, Rostov-na-Donu, Russia*

[3] *Materials Research and Technology Department, Luxembourg Institute of Science and Technology, 5 avenue des Hauts-Fourneaux, L-4362 Esch/Alzette, Esch/Alzette, Luxembourg*

An atomic interaction interatomic energy is identified in the ABO_3 perovskite structure[1]. The term is harmonic in nature and collaboratively couples the antiferroelectric displacement patterns of the A-site cations with O_6 octahedral rotations going beyond the traditional Glazer notations. Straightforward analytical derivations using such energy are able to explain the instability of the phonon modes associated with the unusual ground state of the prototype of antiferroelectric materials, that is $PbZrO_3$, as well as their striking atomistic characteristics. Similar derivations further account for the instability of other complex phonon modes in other antiferroelectrics, as well as provide a successful explanation for the occurrence of incommensurability in some perovskite oxides.

References

[1] Kinnary Patel, Sergey Prosandeev, Yurong Yang, Bin Xu, Jorge Íñiguez, and L. Bellaiche. Phys. Rev. B 94, 054107 (2016)

Keywords: perovskite, atomic interaction, antiferroelectric, antipolar, incommensurate phases

---

Tu-S-P-54

Ferroelectric domain structure and piezoelectric properties of highly textured $Pb(Fe_{0.5}Nb_{0.5})O_3$ thin films deposited by sputtering

José Juan Gervacio Arciniega [1], Mario Alberto Curiel Álvarez [1], C. I. Enrique Flores [2], Carlos E Ostos Ortiz [3], Reynaldo Font [4], F. J. Espinoza-Beltrán [2], Jesus M. Siqueiros Beltrones [1], Oscar Raymond Herrera [1]

[1] *Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, AP 14, Ensenada 22860, Baja California, Mexico*
[2] *CINVESTAV Unidad Querétaro, Lib. Norponiente 2000, Real de Juriquilla, Querétaro 76230, Querétaro, Mexico*
[3] *Instituto de Química, Universidad de Antioquia, UdeA, Calle 70 No. 52-21, Medellín, Colombia*
[4] *Facultad de Física, Universidad de La Habana, San Lázaro y L, La Habana 10400, La Habana, Cuba*

The single-phase multiferroic compound $Pb(Fe_{0.5}Nb_{0.5})O_3$ (PFN) is a good candidate for new nanoscale technologies; however, studies have focused mostly on PFN ceramics and little has been published about thin films. In this work, we are reporting the local ferroelectric and piezoelectric properties of highly textured [110]-oriented PFN thin films grown by rf-magnetron sputtering on $SrRuO_3/SiO_x/Si$ substrates, and the strong correlation existing with the crystalline structure. The crystallographic study was realized using X-ray diffraction with monochromatic CuKα radiation and by high-resolution transmission electron microscopy. Piezoresponse force microscopy (PFM) was used to determine *out-of-plane* and *in-plane* surface topography, ferroelectric domain structure, domain switching and ferroelectric hysteresis of as deposited PFN films. Using structural simulation and the surface representation of the piezoelectric tensor, the observed domain patterns are explained in terms of a complex configuration of 70º, 109º, and 180º domain walls, where the domains with *out-of-plane* <110> and/or <1-10> preferential orientations are connected through crystalline faces or edges. After poling with an optimal applied dc bias, sharp images of up-down domain switching, using PFM in resonance mode, are presented. A piezoelectric constant d_{33} of 10 pm/V and a coercive electric field of ~388 kV/cm (4.65 V) were calculated from local hysteresis loops.

This work was supported by PAPIIT-DGAPA-UNAM (Grants IN110315 and IN105317) and CONACYT (Grants Fronteras-2026, 282778 and 280309). Technical assistance from E. Aparicio, F. Ruiz, I. Gradilla, P. Casillas, and E. Murillo is duly acknowledged.

Keywords: Multiferroic PFN, thin films, ferroelectric domains, structure-properties relationship, piezoresponse force microscopy

---

Tu-S-P-55

Study of magnetoeletric coupling in $BiFe_{1-y}Co_yO_3$ compositons using ferroic characterizations

Anuar Mincache [1], Odair Oliveira [1], Eduardo Volnistem [1], Gustavo Dias [1], Ivair Santos [1], Luiz Cótica [1], Amar Bhalla [2], Ruyan Guo [2]

[1] *State University of Maringá, Maringá, Brazil*
[2] *University of Texas at San Antonio, San Antonio, United States*

With the expansion of the technology and science of nanostructured materials the search for the miniaturization of electronic components has increased. Particularly, multiferroic materials with magnetoelectric properties, due to their correlation between the electrical and magnetic properties have attracted the attention of many researchers to be used in micro and nano devices. Perovskite structured materials based on $BiFeO_3$ is a class of materials largerly considered in these studies. In this work, $BiFe_{1-y}Co_yO_3$ (y = 0.01, 0.015 and 0.02) ceramic compositions were synthesized aiming a better understanding of the structural, dielectric, magnetic and magnetoelectric properties of these materials. The samples were processed in a high-energy milling, fast sintering and fast cooling protocol. Measurements were made by X-ray diffraction, and Rietivield refinement evidencing the rhombohedral symmetry of the ceramics with space group R3c. The magnetization measurements showed a possible antiferromagnetic behavior. The results of dielectric constants and loss tangents decrease with increasing frequency and increase with increasing temperature. We have a linear increase in the value of the magnetoelectric coefficient for the system evidencing in itself a possible multiferroic interaction at room temperature.

Keywords: Bismuth ferrite, Multiferroics, Magnetoelectric Effect

---

Tu-S-P-56

Indications of an enhanced magnetoelectric coupling in nanostructured $BiFeO_3$-$PbTiO_3$ compounds

Valdirlei Freitas [1, 2], Ivair Santos [2], Luiz Cótica [2], Gustavo Sanguino Dias [2], Diana Navroski [1]

[1] *State University of Midwest, Guarapuava, Brazil*
[2] *State University of Maringá, Maringá, Brazil*

Magnetoelectric materials have been studied for several possible technological applications based in the exploitation of the magnetoelectric effect. In order to enhance the magnetoelectric response, nanoparticles production has been proposed as an alternative for enhancing the magnetic response, and consequently, the magnetoelectric coupling. In fact, the magnetic properties change with decreasing of the particle size and exotic magnetic orders or behavior, as the superparamagnetism, can emerge. In this way, strong magnetic responses may result in a strong coupling between magnetic and electric order parameters in magnetoelectric materials. In this work, nanostructured ceramic bodies (mean grain sizes lower than 50 nm) of $BiFeO_3$-$PbTiO_3$ compounds were synthesized by using a modified Pechini method followed by fast-firing. Structural analysis showed single phase materials. A remarkable change in the magnetic order was achieved by a drastic reduction of the nanoparticle size (for paticles of ~10 nm in

diameter, observed by Transmission Electronic Microscopy), whereas the magnetic hysteresis loops, obtained by vibrating sample magnetometry, revealed a typical superparamagnetic-like behavior. A phenomenological analysis of the magnetic hysteresis loops strongly suggest that the superparamagnetism is formed by the overlapping of weak-ferromagnetic and paramagnetic contributions of the magnetic ensemble. Finally, the thermal dependence of the electrical properties under external magnetic fields, such as conductivity, resistivity and resistance, was investigated and indicated an ehanced magnetoelectric coupling in these materials.

Keywords: Magnetoelectric, nanoparticles, superparamagnetism

Tu-S-P-57

Switchable thin film bulk acoustic wave devices based on ferroelectric films

Anatoliy Mikhailov

Saint-Petersburg State Electrotechnical University (LETI), Saint-Petersburg, Russia
Daghestan State Technical University, Makhachkala, Russia

Thin film bulk acoustic resonators (TFBAR) offer significant potential in the area of modern microwave electronics. They are widely used in miniaturized filters for communication and navigation systems. Modern TFBARs are multilayer thin-film structures containing one piezoelectric layer. The operating frequency of these resonators is determined by the thickness of the structure and by the elastic properties of layers, and as a rule have no electrical tuning. Therefore, the development of TFBARs with the capability of electrically controlling their resonance frequency is a challenging problem whose solution could lead to a significant improvement of the modern filter devices and microwave systems. A possible solution of this problem is to replace the piezoelectric materials traditionally used for TFBAR fabrication, with ferroelectric materials in the paraelectric phase. A good candidate is strontium titanate (STO). STO is a relatively low loss dielectric material with a centro-symmetric crystal structure, in which an external electrical field induces the piezoelectric effect. The magnitude of the applied field determines the value of the piezoelectric coefficient. This work presents a TFBAR architecture that allows significant improvement of the device's operational range by introducing multi-resonance frequency switching ability. In such a way it is possible to vary the magnitude and the sign of the induced piezoelectric coefficients together, hence to control the excitation efficiency of each normal acoustic mode in the structure.

Keywords: Thin film ferroelectric bulk acoustic resonator, strontium titanate

---

Tu-S-P-58

Magnetic and dielectric response of $Sr_{0.95}Nd_{0.05}Fe_{12-x}Al_xO_{19}$ (x = 0.36, 0.60, 0.84 and 1.08) obtained by hydrothermal synthesis

Andrzej Hilczer [1], Katarzyna Pasińska [2], Ewa Markiewicz [1], Adam Pietraszko [2], Bartłomiej Andrzejewski [1]

[1] *Institute of Molecular Physics Polish Academy of Sciences, Poznan, Poland*
[2] *Institute of Low Temperatures and Structure Research Polish Academy of Sciences, Wroclaw, Poland*

Hexagonal ferrites attracted recently great attention as candidates for microwave absorbers due to low electric conductivity and low eddy current losses. Moreover, doping and codoping can be used to study the exchange coupling and to adjust intrinsic and extrinsic magnetic properties of the ferrites to application requirements. We studied the magnetic and dielectric response of $Sr_{0.95}Nd_{0.05}Fe_{12-x}Al_xO_{19}$ (x = 0.36, 0.60, 0.84 and 1.08) obtained by hydrothermal synthesis. Single phase solid solution with $P6_3/mmc$ space group and Z = 2 has been confirmed for all samples by X-ray diffraction and the lattice parameters were unaffected by Al^{3+} doping. SEM images revealed that the samples consist of 10-20 nm thick agglomerated platelets. Magnetic studies showed that the codoping influences mainly the intrinsic magnetic properties. Analysis of the Al^{3+} induced changes in the magnetic properties points to the substitution of Fe^{3+} ions in octahedral $4f_2$ Wyckoff positions. Temperature variation of the magnetization M_{ZFC} in zero-field-cooled and M_{FC} in field-cooled experiments revealed a bifurcation and a maximum in $M_{ZFC}(T)$ dependences. The temperature of the maximum was found to be shifted towards higher temperatures with increasing x and we propose to relate the feature to cluster-glass-like behavior. The dielectric permittivity and electric conductivity measurements in the frequency range 1Hz – 1GHz show that the dielectric response of the solid solution can be described within the Koops model.

Keywords: hexaferrite, dielectric and magnetic response, effect of doping

---

Tu-S-P-59

Magnetic and ferroelectric properties of sol-gel synthesized Al and Mn doped $GaFeO_3$ ceramics

NANDNI SHARMA [1], Ashish Mall [2], Rajeev Gupta [2, 3], Ashish Garg [4], Sanjeev Kumar [1]

[1] *Applied Sciences Department, PEC University of Technology, CHANDIGARH, India*
[2] *Materials Science Programme, Indian Institute of Technology, Kanpur, India*
[3] *Department of Physics, Indian Institute of Technology, Kanpur, India*
[4] *Department of Materials Science & Engineering, Indian Institute of Technology, Kanpur, India*

Polycrystalline $Ga_{0.5}Al_{0.5}Fe_{1-x}Mn_xO_3$ (x=0.0, 0.025, 0.05) samples were synthesized using metal nitrates by sol-gel technique. Rietveld refinement of X-Ray diffraction data shows the presence of orthorhombic structured phase with space group $Pc2_1n$ without any secondary phase in all the samples. Reduction in the lattice constant and unit cell volume is observed upon the doping of Al and Mn in $GaFeO_3$ (GFO) samples. Room temperature ferroelectric measurements showed the improvement in ferroelectric hysteresis loops with the incorporation of Al and Mn doping in $GaFeO_3$ and this is attributed to the increase of orthorhombic distortion with increase in doping content and due to changes in the defect chemistry. Consequently, the leakage current is also reduced by three orders of magnitude as compared to pure GFO. However, there is a decrease in magnetization values and Curie temperature (T_c) as compared with pure $GaFeO_3$.

Keywords: Multiferroics, X-ray diffraction, Leakage current, Magnetization

---

Tu-S-P-60

Synthesis, structural, microstructural and ferroic properties of $CoFe_2O_4$:$BaTiO_3$ nanocomposites

Denise Alanis [1, 2], Raquel Bini [1], Eduardo Volnistem [1], Daniel Silva [1], Gustavo Dias [1], Ivair Santos [1], Ruyan Guo [2], Amar Bhalla [2], Luiz Cótica [1]

[1] *State University of Maringa, Maringa, Brazil*

[2] *University of Texas at San Antonio, San Antonio, United States*

Multiferroic materials have attracted interest due to the presence of more than one ferroic order, for example magnetic and electric orders, in the same phase. This particular coupling phenomenon is known as magnetoelectric (ME) effect. The composites combining piezoelectric and ferrite compositions exhibit unique properties observed neither in the ferrite nor in the piezoelectric phase. Thus, in order to enhance the ME effect, piezoelectric/magnetostrictive composites have been exploited. Among some different configurations to prepare composite materials, the core-shell nanoparticles are also investigated as a beneficial starting material for magnetoelectric nanocomposite (MENC) materials. Particularly, cobalt ferrite-barium titanate in a core-shell configuration has been investigated due to appropriate individual (magnetostrictive and piezoelectric) properties of the components at room temperature. In addition, their chemical and mechanical stability and nontoxic properties are also important in applications regarding the environment and biological applications. In this work we prepared MENC's in a core-shell configuration with a narrow size distribution. A combination of polymeric and citrate methods was used for the MENC's syntheses. The structural characterizations of the obtained MENC's were performed by X-ray diffraction and Fourier transform infrared spectroscopy (FTIR). A core-shell morphology of MENC's was observed by transmission electron microscopy. The topography of the surface was observed by atomic force microscopy. Finally, the ferrimagnetic character of the MENC's was observed in the magnetic characterizations obtained in a vibrating sample magnetometer and magnetic force microscopy.

Keywords: nanocomposites, magnetoelectric, core-shell

Tu-S-P-61

Size and shape effects in ferroelectric nanoparticles

Franco Di Rino, Marcelo Sepliarsky, Marcelo Stachiotti

Insttituto de Física Rosario CONICET-Universidad Nacional de Rosario, Rosario, Argentina

We applied a first-principles atomistic shell model to investigate the influence of size and shape in the formation of different polar structures in $PbTiO_3$ nanoparticles. The studies were carried performing molecular dynamics simulation in freestanding nanodots of cylindrical, spherical and ellipsoidal shape. We found that the topological transformations are mainly driven by the aspect ratio diameter/thickness of the nanostructures. The observed polar configurations include one- and multiple-vortex states, and different multi-domain structures as the aspect ratio of the particles increases.

Keywords: Nanoparticles, size effects, simulations

Tu-S-P-62

Background dielectric permittivity: material constant or a fitting parameter?

Arkady Levanyuk [1], Boris Strukov [2], Andres Cano [3]

[1] *Department of Physics, University of Washington, Seattle, USA, Seattle, United States*
[2] *Moscow State University, Moscow 119991 Russia, Moscow, Russia*
[3] *CNRS, University of Bordeaux, ICMCB, UFR 9048, F-33600 Pessac, France, Pessac, France*

The concept of background dielectric constant proposed by Tagantsev, together with the distinction between critical and non-critical electric polarizations as a natural extension for the order parameter of ferroelectric phase transitions, is critically discussed. It is argued and exemplified that, even if these quantities can be very useful for obtaining qualitative and semi-quantitative results from phenomenological modeling, they cannot be introduced in a self-consistent manner. In other words, the background dielectric permittivity has no quantitative meaning and is rather a fitting parameter than a material constant.

Keywords: order parameter, ferroelectric phase transition, dielectric constant

---

Tu-S-P-63

Investigation of non-linear susceptibility of some relaxor ferroelectrics

Dziugas Jablonskas, Maksim Ivanov, Robertas Grigalaitis, Juras Banys

Vilnius University, Vilnius, Lithuania

Relaxor ferroelectrics (RFs) are a specific type of polar dielectrics. The definition of RFs is rather vague. However, it is usual to associate it with exceptional properties of this group of materials. That is, a broad and usually enormously large peak and a strong frequency dispersion of dielectric permittivity as a function of temperature. In contrast to ordinary ferroelectrics, the dielectric anomaly is not connected with any macroscopic structural change. Yet, there are inorganic systems, which have a RF type behavior down to certain specific temperature, at which an actual structural phase transition occurs. A good example of such behavior is $PbSc_{0.5}Nb_{0.5}O_3$ and $PbSc_{0.5}Ta_{0.5}O_3$. It would be interesting to investigate, if RFs of different composition actually possess the complete set of features attributed to RF type materials. Furthermore, it is interesting to find out, if it is correct to have a term of "RF phase". Non-linear susceptibility is a powerful tool to characterize phase transitions. According to the theory of Landau-Ginzburg-Devonshire, ferroelectric systems, which display continuous (2^{nd} order) phase transition, have negative third order susceptibility (χ_3) in paraelectric state and, with decrease of temperature, χ_3 changes sign to positive at the temperature of the phase transition. In case of a

discontinuous phase transition (1st order) the sign of χ_3 is positive and remains unchanged throughout the vicinity of temperature of the phase transition. In this contribution we will present some examples of typical results of investigations of non-linear dielectric susceptibility of some RFs.

Keywords: Relaxor ferroelectrics, phase transition, non-linear susceptibility, dielectric spectroscopy, polar dielectric

---

Tu-S-P-64

Influence of the dynamic magnetization response in the magnetoelectric effect in multiferroic composites

Alexandre Gualdi [1], Fabio Zabotto [1], Ducinei Garcia [1], Amar Bhalla [2], Ruyan Guo [2], Paulo Cesar de Camargo [1], Adilson Jesus Aparecido de Oliveira [1]

[1] *Universidade Federal de São Carlos, São Carlos, Brazil*
[2] *University of Texas at San Antonio, San Antonio, United States*

The magnetoelectric effect (ME) is a combination of ferromagnetic and ferroelectric orders coupling magnetic and electric fields, which allows controlling the magnetic behavior with an electric signal and vice versa. For multiferroic composites, the ME effect can be explained by an indirect coupling between the ferroelectric and the ferromagnetic phases. The main characteristic of the ME is a peak in the DC magnetic field dependency, associated with the magnetostriction behavior of the ferromagnetic phase. In previous works, we reported that the ME voltage coefficient for composites based on $CoFe_2O_4$ shows a dependence with the frequency of the AC magnetic field. This effect was related to the trigonal field of the ferrite structure, which changes the magnetoelastic contribution at low temperatures, inducing a step-like behavior in the ME coefficient. In this work, the ME of the composites PMN-PT/CFO and PMN-PT/NFO with different frequencies of the AC magnetic field were studied. The results show that the ME coefficient, at low temperatures (5 K), for PMN-PT/CFO composite presents a hysteresis behavior for frequencies higher than 100 Hz. Contrasting these results, the ME coefficient for the PMN-PT/NFO composite shows the well-known peak-peak related to the magnetostriction coefficient. It was possible to explain the ME hysteresis behavior for the $CoFe_2O_4$ composite based on energy levels stabilization for each ferromagnetic phase. This effect was attributed to the degeneracy of the energy levels, which comes from the Spin-Orbit coupling, from which the dynamic properties of the magnetoelastic interactions are altered.

Keywords: Magnetostriction, Dynamic Magnetization, Magnetoelectric Effect

---

Tu-S-P-65

Study of birefringence and electro-optic effect in SBN60 thin film

Surbhi Gupta [1], Ayushi Paliwal [1], Vinay Gupta [1], Monika Tomar [2]

[1] *Department of Physics and Astrophysics, University of Delhi, Delhi, INDIA, Delhi, India*
[2] *Physics Department, Miranda House, University of Delhi, Delhi, India, Delhi, India*

Recent advances towards Electro-optic (EO) modulators make use of the Pockels effect in non-centrosymmetric crystals which allows the preferential selection of polarization. The large value of electro-optic (EO) coefficient of Strontium barium niobate has gained advances in field of electro optic devices by various researchers. Various deposition techniques have been utilized for depositing SBN thin films which includes Pulsed laser deposition (PLD) technique, Sol-gel and Metal organic chemical vapor deposition (MOCVD). In order to investigate the birefringence property, SBN60 thin films were deposited using PLD technique under optimized parameters. The field-induced birefringence was measured in the transverse geometry for 800 nm thin SBN film deposited on the fused silica substrate. The dc electric field was applied on Aluminum parallel electrodes deposited on the surface of SBN thin film. A small birefringence was induced in the as-deposited film by the alignment of the incident laser along *c*-axis in the film plane. The birefringence in the SBN60 thin film was enhanced by application of a dc electric field (up to 10 kV). The small phase shift, , of the (between s and p polarized) reflected light was then determined from the difference of the light levels at the two balanced detectors monitored using lock in amplifier. The values of were obtained from , where is the wavelength of incident laser light (633 nm), d is the total optical path length across the film. The value of was found to be in accordance to the reported values.

Keywords: Electro-optic, SBN, birefringence

Tu-S-P-66

Bipolar resistive switching in Pt/BFO/BTO/Pt sandwiched structures

Savita Sharma [1], Surbhi Gupta [1], VInay Gupta [1], Monika Tomar [2]

[1] *Department of Physics and Astrophysics, University of Delhi, Delhi, INDIA,, Delhi, India*
[2] *Physics Department, Miranda House, University of Delhi, Delhi, INDIA, Delhi, India*

Resistive switching (RS) memory effect holds great promise for the next generation logical and non-volatile memory devices. Ferroelectric materials can be used for non volatile memory applications, eg., ferroelectric random access memories (FeRAM) because of their switchable spontaneous polarization, but their destructive readout scheme limits their application. Ferroelectric materials such as $SrTiO_3$, $BiFeO_3$, PZT, $BaTiO_3$ and $Pr_{(1-x)}Ca_xMnO_3$ have been exploited for resistive switching applications because their spontaneous electrical polarization improves the tuning charge properties at ferroelectric/metal interface. However, until now the RS effect of the metal/BFO/BTO/metal sandwiched structure has not been investigated, though the sandwiched structure is very important for real technical applications. In this paper, the RS characteristics in Pt/BFO/BTO/Pt sandwiched structures deposited by pulsed laser deposition have been studied and bipolar RS behavior is observed which may be attributed to the formation/rupture of nanoscale metal filaments into the multiferroic material due to the diffusion of the top electrodes under a bias voltage. The Pt/BFO/BTO/Pt sandwiched devices show both the well-established P–E hysteresis loops, along with reliable and reproducible resistance switching behaviors. The resistance ratio between the high resistance state (HRS) and low

resistance state (LRS) for the Pt/BFO/BTO/Pt sandwiched structure was about 100. The device exhibited good retention characteristics and low switching voltages.

Keywords: Resistive switching, Ferroelectric, high resistance state (HRS), low resistance state

---

Tu-S-P-67

XPS resolved surface state analysis of ZnO and Ni doped ZnO films for quantum well applications

Sheetal Dewan [1], Monika Tomar [2], A.K. Kapoor [3], R.P. Tandon [1], Vinay Gupta [1]

[1] *Department of Physics and Astrophysics, University of Delhi, Delhi-110007, INDIA, Delhi, India*
[2] *Physics Department, Miranda House, University of Delhi, Delhi-110007, INDIA, Delhi, India*
[3] *Solid State Physics Laboratory, DRDO, Ministry of Defence, Lucknow Road, Timarpur, Delhi-110054, India, Delhi, India*

3d transition metal doping in ZnO is known to alter the physiochemical properties of ZnO to a great extent. Distinctive chemical stability of nickel on zinc sites, owing to their nearly close ionic radii, recognizes it as one of the most resourceful dopant to tailor material properties of ZnO. A comprehensive analysis of the surface chemistry can provide a deeper insight of the interfacial properties of NiZnO/ZnO system. In the present study, Zn LMM Auger peaks were examined in Pulsed Laser deposited ZnO and NiZnO films on sapphire. LMM Auger transitions give a clear know-how of surface chemical states because a single Auger transition involves three electrons and many body effects. The measurements were made in ultra-high vacuum conditions at a probing angle of . The relative concentration of interstitial zinc (Zn_i) and Zn-O bonds was estimated using area under the corresponding deconvoluted peaks. An enhancement in Auger LMM peak area of Zn_i was observed in case of NiZnO. Since Zn_i is donor impurity, it favours enhanced n-type conduction in the material. Hall-Effect measurements were carried out on ZnO and NiZnO, which revealed n-type conduction in both the systems. NiZnO exhibited relatively higher electron mobility and carrier concentration compared to ZnO, thus validating the XPS results. The optical bandgap of films evaluated using UV-Visible Spectroscopy, showed a decrease in bandgap from 3.28 (ZnO) to 3.16 eV (NiZnO). The obtained results favour the utilization of NiZnO as active well layer and ZnO as barrier layer in NiZnO/ZnO based Quantum Well applications.

Keywords: XPS, LMM Auger transitions, Ni doped ZnO,

Tu-S-P-68

Dielectric spectroscopy of barium titanate doped with Ce^{4+} at the Ti site

Dzmitry Adamchuk [1], Sarunas Svirskas [1], Juras Banys [1], Vincenzo Buscaglia [2]

[1] *Faculty of Physics, Vilnius University, Vilnius, Lithuania*
[2] *Institute for Energetics and Interphases, CNR, Genoa, Italy*

Ferroelectricity in barium titanate (BT) has already been studied for more than 70 years. Still this material attracts a lot of attention because some of its properties are not quite well understood. It is also important from the application point of view. Most of the recent studies are concentrated on the doping of barium titanate with various ions. A lot of studies are concentrated on the rare-earth metal ion doping. Such kind of lattice substation can affect the properties of BT quite drastically. The addition of different ions can lead to very complex behaviour. One of the best examples is the mixtures between barium titanate and barium zirconate. This system shows very complicated crossover in the phase diagram between ferroelectric, relaxor and incipient ferroelectric phases. This study is devoted to the investigation of broadband dielectric spectroscopy of barium titanate doped with different concentration of cerium ions. The investigation was carried in a broad temperature (50 - 500 K) and frequency range (5 mHz – 1 GHz). The study shows that the increase of Cerium dopants in the B-site of perovskite lattice diminishes ferroelectric order and the relaxor behaviour is enhanced. It resembles barium zirconate titanate (BZT) system but the random fields supposed to be much stronger in the case of BT doped with Ce^{4+} at the Ti site. The evolution of temperature and frequency dependences of dielectric permittivity will be discussed in this contribution.

Keywords: Barium titanate, dielectric spectroscopy, relaxors, dipolar glasses

---

Tu-S-P-69

Ferroelectric photovoltaic properties of multilayered PZT/BFO thin film system

Reema Gupta [1], Monika Tomar [2], Ashok Kumar [3], Vinay Gupta [1]

[1] *Department of Physics and Astrophysics, University of Delhi, New Delhi, India*
[2] *Physics Department, University of Delhi, Delhi, Delhi, India*
[3] *CSIR-National Physical Laboratory, Dr. K.S. Krishnan Marg, Delhi, India*

Ferroelectric photovoltaic is the emerging field in the area of energy harvesting for converting light energy into useful voltage. Among various ferroelectric materials, Bismuth ferrite (BFO) is the most suitable for photovoltaic applications in terms of narrow band gap. BFO is multiferroic material having ferroelectric and antiferromagnetic ordering at room temperature. Multiferroic materials, which exhibit simultaneously ferroelectric, ferromagnetic, and ferroelastic behaviors, provide opportunities for the potential applications in wide field including storage devices, spintronics, and sensors. But the existence of large leakage current weakens its ferroelectric properties and limits its usage in various applications. To overcome this problem, Lead Zirconium Titanate (PZT), good ferroelectric material has been coupled with BFO in the present work. The multilayered PZT/BFO thin film systems with different periodicity have been deposited using pulsed laser deposition (PLD) technique. The structural and ferroelectric properties have been studied and the effect of periodicity on the ferroelectric properties has been analyzed. The top electrode has been patterned on multilayered PZT/BFO thin film system to study its ferroelectric photovoltaic properties. The photovoltaic characteristics were studied using solar simulator and the results are found to be proficient as compared to bare PZT thin film.

Keywords: ferroelectric, photovoltaic, bismuth ferrite, lead zirconium titanate

---

Tu-S-P-70

Studies on the effect of integration of metal nanoclusters on the electrical and ferroelectric properties of barium titanate thin film

Savita Sharma [1], Monika Tomar [2], Ashok Kumar [3], Vinay Gupta [1]

[1] *Department of Physics and Astrophysics, University of Delhi, Delhi, INDIA,, Delhi, India*
[2] *Physics Department, Miranda House, University of Delhi, Delhi, INDIA,, Delhi, India*
[3] *CSIR-National Physical Laboratory, Dr. K.S .Krishnan Marg, Delhi, INDIA, Delhi, India*

Ferroelectrics are a special class of materials which undergo spontaneous electric polarization and possess reversible polarization under an applied electric field due to their inherent ferroelectric, dielectric and optical properties. Barium titanate, $BaTiO_3$ (BTO) is a technologically important material because of its variety of applications in microwave devices, multilayer capacitors, non-volatile ferroelectric memories, dynamic random access memories (DRAM), micro-electromechanical- system (MEMS), and so on. Recently, research has been started on studying the effect of top electrodes on the various properties of ferroelectric thin films such as photovoltaic properties however, detailed study on the effect of different metal nanoclusters on the electrical properties of the ferroelectric material is significantly required. In the current work, polycrystalline BTO thin films have been synthesized on $Pt/Ti/SiO_2/Si$ substrates using a versatile low temperature technique called Sol-gel hydrothermal method and different metal nanoclusters (Au, Ag, Cu, Al, In and W) have been fabricated over the surface of BTO thin film using thermal evaporation technique. The effect of metal nanoclusters on the electrical and ferroelectric properties of BTO thin films have been studied. The current conduction mechanism is found to be dependent on the work function of different metal nanoclusters deposited over BTO thin film. The induced ferroelectric polarization also exhibited significant change due to difference in surface charge collection with different metal nanoclusters.

Keywords: Ferroelectric, Nano-clusters, Barium titanate

Tu-S-P-71

Relaxor behavior analysis of rare-earth modified PZT ferroelectric ceramics

Suzana Pereira Hessel [1], Atair Carvalho da Silva [1, 2], Arthur Vinicius Oliveira Costa [1], Ruyan Guo [3], Amar S. Bhalla [3], José de los Santos Guerra [1]

[1] *Grupo de Ferroelétricos e Materiais Multifuncionais, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Brazil*
[2] *Departamento de Física e Química, Universidade Estadual Paulista, Campus de Ilha Solteira, Ilha Solteira, Brazil*
[3] *Multifunctional Electronic Materials and Devices Research Lab., Department of Electrical and Computer Engineering, The University of Texas at San Antonio, San Antonio, United States*

Ferroelectric systems based on $Pb(Zr_{1-y}Ti_y)O_3$, are probably one of the most investigated materials due to their excellent physical properties, which can even be easily improved when modified with some chemical additives. Such substitutions provide some relevant characteristics in the piezoelectric,

ferroelectric and pyroelectric responses. For specific compositions, a strong frequency dependence of the dielectric properties, well known as the relaxor behavior, can be observed, which has attracted the attention of the researchers because of the exciting physical characteristics revealed by these systems. The present work aims a careful investigation in the dielectric properties of rare-earth (RE) modified PZT ferroelectric ceramics. In particular, the relaxor behavior and the characteristics of the phase transition have been studied in details as a function of the RE content. The obtained results were analyzed within the framework of the models proposed in the current literature.

The authors wish to thank FAPEMIG and CNPq Brazilian agencies and NSF (Grant No. ECCS1002380) for the financial support.

Keywords: Ferroelectric ceramics, Dielectric properties, Relaxor behavior, Vogel-Fulcher

---

Tu-S-P-72

Synthesis and characterization of $0.5Ba(Ti_{0.8}Zr_{0.2})O_3–0.5(Ba_{0.7}Ca_{0.3})TiO_3$ thin films grown by chemical solution deposition

Nadia Mamana, Maria Luz Santiago, Nora Pellegri, Marcelo Stachiotti

Instituto de Física Rosario, FCEIyA , Universidad Nacional de Rosario., Rosario, Argentina

We developed a route to fabricate environmental friendly lead-free ferroelectric $Ba_{0.85}Ca_{0.15}(Ti_{0.9}Zr_{0.1})O_3$ (BCZT) thin films by chemical solution deposition. The precursor solution was prepared by mixing starting solutions of calcium and barium acetate, and alcoholic solutions of titanium (IV) butoxide and zirconium (IV) propoxide using acetoin (3-hydroxy-2-butanone) as chelating agent. The films were obtained by the spin coating method on platinum substrates ($Pt/TiO_2/SiO_2/Si$). Different strategies for the optimization of the route were tested by investigating the evolution of the crystal structure of films treated at different temperatures between 650 and 900 ºC. Atomic Force Microscopy was used to examine the morphology. Finally the films were electrically tested by dielectric and ferroelectric measurements.

Keywords: Thin films, Lead-free piezoelectric, BCZT.

Tu-S-P-73

Electrical properties of ceramic $Ba[(M_{0.05}Ta_{0.05})Ti_{0.9}]O_3$ with M = Sc, Cr, Mn, or Fe and $Ba[(M_{0.0333}Ta_{0.0666})Ti_{0.9}]O_3$ with M = Mn, Ni, or Cu

YuHsun Liao, V. K. Veerapandiyan, Steven M. Pilgrim, Walter A. Schulze, Steven C. Tidrow

Kazuo Inamori School of Engineering, Alfred University, Alfred, United States

Two general goals in multilayer ceramic capacitors (MLCC) have been the replacement of noble metal electrodes and avoidance of regulated and/or toxic materials. The former relates primarily to material cost while the latter relates to engineering, health, and environmental costs. Ideally, one would reach these goals with improved performance, i.e., accompanied by an increase in relative permittivity, material breakdown strength and resistivity, with a simultaneous decrease in dielectric loss and the temperature coefficient of permittivity. Attainment of the goals and desired performance clearly requires something other than an evolutionary approach. This work explores the efficacy of dipole-like substitutional pairs in achieving improved performance in a non-lead dielectric material. Specifically, dipole-like substituted ceramic $BaTiO_3$, $Ba[(M_{0.05}Ta_{0.05})Ti_{0.9}]O_3$ with M = Sc, Cr, Mn, or Fe, and more complex electric-field interaction ceramics, e.g., $Ba[(M_{0.0333}Ta_{0.0666})Ti_{0.9}]O_3$ with M = Mn, Ni, or Cu, are being investigated as potential candidate materials for MLCC technology. Here, we report the temperature dependent (from room temperature to 900°C) electrical properties, relative permittivity, dissipation factor, and resistivity of $Ba[(M_{0.05}Ta_{0.05})Ti_{0.9}]O_3$ with M = Sc, Cr, Mn, or Fe and $Ba[(M_{0.0333}Ta_{0.0666})Ti_{0.9}]O_3$ with M = Mn, Ni, or Cu.

Keywords: Electrical properties,Dipole-like substitute

Tu-S-P-74

Dielectric relaxation anomalies in ferroelectric nanocomposites

Hoai Thuong Nguyen [2], Alexander Sidorkin [1], Svetlana Milovidova [1]

[1] *Voronezh State University, Voronezh, Russia*
[2] *Industrial University of Ho Chi Minh City, Ho Chi Minh City, Vietnam*

In recent years, a number studies of nanoporous matrix composites with ferroelectric inclusions have been carried out. These composites satisfy high demands of modern technique and technologies due to large variations of properties by changing the material characteristics and geometry of the coupling of their components. The search for new nanoporous matrices for ferroelectric composites is going on together with attempts to improve the properties of existing nanostructured systems. Nanocrystalline cellulose is a promising material for creating matrix nanocomposite due to the presence of a large number of nanofibers and OH-groups on their surface, which determine the high sorption capacity of cellulose in relation to water-soluble compounds. Dielectric relaxation of nanocomposites prepared by using ferroelectric particles of triglycine sulfate and sodium nitrite embedded into the matrix of nanocrystalline cellulose in a large frequency range of 10^{-3} to 10^{6} Hz in a weak measuring field ~1 V/cm at different temperatures were investigated. The study of dielectric relaxation in the nanocomposite with triglycine sulfate showed the presence of two relaxation sections. The Debye-like relaxation is observed at higher frequencies, and the linear dispersion – at lower frequencies due to respectively the reversible and irreversible domain-wall motion of the TGS crystallites embedded into the matrix. The displacement of relaxation frequency of TGS nanoparticles to the range of lower frequencies in comparison with those of TGS single crystals was also detected. In the case of sodium nitrite, a significant dielectric dispersion caused by the interfacial polarization according to Maxwell-Wagner-Sillars mechanism was found.

Keywords: Dielectric relaxation, matrix composites, triglycine sulfate, nanocrystalline cellulose

---

Tu-S-P-75

Dielectric properties of ferroelectric barium titanate - barium zirconate superlattices obtained using pulsed laser deposition

Alexander Sidorkin [1], Yaovi Gagou [2], Pierre Saint-Gregoire [3, 4], Evgenii Vorotnikov [1], Lolita Nesterenko [1]

[1] *Voronezh State University, Voronezh, Russia*
[2] *Universite de Picardie Jules Verne, Amiens, France*
[3] *University of Nimes, Nimes, France*
[4] *Montpellier University, Montpellier, France*

The most physical characteristics of artificial layered structures – ferroelectric superlattices (Curie temperature, the spontaneous polarization, and the dielectric constant of its nonlinear field dependence) change significantly compared to single-layer materials. To determine the influence of size effects on the properties of ferroelectric superlattices in the present work we have investigated the dielectric properties of the superlattices with 32 layers of barium zirconate - titanate $BaZrO_3$ / $BaTiO_3$ on LaSrCo/MgO substrate with a thickness of the individual layers of 6.65 nm/7.506 nm, obtained with using of pulsed laser deposition. Carried out research of the temperature dependence of dielectric constant showed the presence of anomalies with a maximum dielectric constant ~200, corresponding to a phase transition with temperature ~400 $^{\circ}$C lying between the Curie points of the lattice components, thus indicating the emergence of a qualitatively new structure as compared with the initial components. Using a modified scheme Soyer - Tower with conductivity compensation, the dependencies on the coercive field and spontaneous polarization on temperature were obtained. The temperature dependence of polarization in the vicinity of the transition temperature changes rather smooth, which may be due to the ingomogeneity of the synthesized structure. Synthesized superstructures have little internal bias field in comparison with its coercive one. Experimental studies of the dynamics of switching processes in synthesized superlattices with using Merz techniques revealed the transition from the "creep" regime with an activation of switching processes to slip regime at field ~300 kV/cm.

Keywords: ferroelectric superlattices, artificial layered structures. barium zirconate - titanate

---

Tu-S-P-76

Effect of sintering temperature on relaxor ferroelectric behavior of BCZT ceramic prepared by sol-gel auto combustion

Piyaporn Jaimeewong [1, 2], Xiaotong Wang [3], Zenghui Liu [3], ZuO-Guang Ye [3], Anucha Watcharapasorn [1, 4]

[1] *Department of Physics and Materials Science, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand 50200, Chiang Mai, Thailand*
[2] *The Graduate school, Chiang Mai University, 239 Huaykeaw Road, Suthep, Chiang Mai, Thailand 50200, Chiang Mai, Thailand*
[3] *Department of Chemistry and 4D LABS, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6, British Columbia, Canada*

[4] *Materials Science Research Center, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand 50200, Chiang Mai, Thailand*

This work reports the effect of sintering temperature on dielectric and ferroelectric behavior of $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ or BCZT ceramic prepared by sol-gel auto combustion method. The BCZT ceramic exhibited large dielectric permittivity in the range of 5000-5900 at room temperature. The maximum dielectric permittivity of all samples decreased with increasing frequency coupled with accompanying shift in the temperature at maximum dielectric permittivity which confirmed its relaxor behavior. Ferroelectric hysteresis loop (P-E loop) as a function of temperature was also investigated. At room temperature, the slim P-E loop was observed and remnant polarization (P_r) was closed to zero but at low enough temperature, a large P-E loop with the P_r value of 20 mm/cm^2 was observed. The bulk density, grain size and ferroelectric properties increased with the increasing in sintering temperature. In addition, the characterization of the effect of sintering temperature on the relaxor ferroelectric behavior was discussed in terms of the Curie-Weiss law and Volger-Fulcher law.

Keywords: BCZT, Sintering temperature, Relaxor ferroelectric, Curie-Weiss law and Volger-Fulcher law

---

Tu-S-P-77

On the structural and dielectric properties of nickel ferrite based multiferroic composites

Roney Junio de Portugal [1, 2, 3], Atair Carvalho da Silva [3], Soutik Betal [4], Moumita Dutta [4], Ruyan Guo [4], Amar S. Bhalla [4], José de los Santos Guerra [1]

[1] *Grupo de Ferroelétricos e Materiais Multifuncionais, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia – MG, Brazil*
[2] *Instituto Federal de Educação, Ciência e Tecnologia do Triângulo Mineiro, Campus Patrocínio, Patrocínio – MG, Brazil*
[3] *Departamento de Física e Química, UNESP, Campus de Ilha Solteira, Ilha Solteira – MG, Brazil*
[4] *Multifunctional Electronic Materials and Devices Research Lab. Department of Electrical and Computer Engineering, The University of Texas at San Antonio, San Antonio – TX, United States*

The increasing interest in the research on materials with magneto-electric properties has been one of the most challenging tasks for the scientific community in the last years. Specially, the investigation of such materials has been conducted to the development of electronic devices, such as sensors, transducers and memory storage. The magnetoelectric effect presented in certain materials can be explained by taking into account the electrical polarization response due to the application of a magnetic field or magnetization response due to the applied electric field. Multiferroic materials can successfully exhibit these effects, favoring the advent of a class of materials called magnetoelectric multiferroics, which combine ferro/ferri-magnetism and ferroelectricity phenomena. The objective of the present work is to investigatie the structural and dielectric properties of multiferroic ceramic composites based on spinel structure-type $NiFe_2O_4$ system. The samples were obtained from the solid-state reaction method, by considering a stoichiometric ratio between the nickel ferrite ferromagnetic and a ferroelectric phase

matrix. The obtained results have been discussed considering the influence of the nickel ferrite content on the physical properties of the studied composite.

The authors wish to thank FAPEMIG and CNPq Brazilian agencies and NSF (Grant No. ECCS1002380) for the financial support. R. J. Portugal also thanks the Materials Science Post-Graduation Program (PPGCM), UNESP, Ilha Solteira, Brazil.

Keywords: Multiferroics, Spinel, Ferroelectrics

Tu-S-P-78

Dielectric and piezoelectric properties of (1-*x*)$Ba(Zr_{0.2}Ti_{0.8})O_3$-(*x*)$(Ba_{0.7}Ca_{0.3})TiO_3$ ceramics

Panupong Jaiban [1], Pimpilai Wannasut [2], Suwapitcha Buntham [2], Anucha Watcharapasorn [2, 3]

[1] *Faculty of Science, Energy and Environment, King Mongkut's University of Technology North Bangkok, Rayong campus, Rayong, Thailand*
[2] *Department of Physics and Materials Science, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand, Chiang Mai, Thailand*
[3] *Materials Science Research Center, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand, Chiang Mai, Thailand*

(1-*x*)$Ba(Zr_{0.2}Ti_{0.8})O_3$-(*x*)$(Ba_{0.7}Ca_{0.3})TiO_3$ ceramics where x = 0.3, 0.4, 0.5 and 0.6 were prepared employing a solid state sintering technique. X-ray diffraction patterns suggested a morphotropic phase boundary of rhombohedral and tetragonal structure. Upon increase of $(Ba_{0.7}Ca_{0.3})TiO_3$, the average grain size became smaller. The decrease of the phase transition temperature was observed in correlation with the $(Ba_{0.7}Ca_{0.3})TiO_3$ content. The coexistence of rhombohedral and tetragonal played an important role in enhancement of dielectric and piezoelectric properties. The result here suggested that electrical properties of these ceramics may be largely tunable and could be an attractive material for high-dielectric response and piezoelectric devices.

Keywords: Ferroelectric properties, Perovskites, Electrical properties

---

Tu-S-P-79

Temperature and composition-driven percolation in $BaTiO_3$-based relaxor ferroelectric solid solutions

Alexei Bokov [1], Jian Zhuang [1, 2], Wei Ren [2], Zuo-Guang Ye [1]

[1] *Department of Chemistry & 4D LABS Simon Fraser University, Burnaby, Canada*
[2] *Electronic Mater. Res. Lab. & Intl. Center for Dielectric Research, Xi'an Jiaotong University, Xi'an, China*

The percolation theory is often used to interpret the sequence of phases which is observed in relaxors with the change of temperature. In relaxors the polar nanoregions growing upon cooling from paraelectric to relaxor phases are considered as finite percolation clusters which transform to infinite cluster at the percolation threshold temperature associated with the glassy freezing temperature or the ferroelectric Curie temperature. In the present work we show that in relaxor ferroelectric solid solutions the percolation behavior can be observed not only for the size of polar clusters as a function of temperature, but also for the size of compositional clusters as a function of concentration of ferroactive ions. Using the experimental techniques of x-ray diffraction, dielectric spectroscopy and the measurements of polarization-field hysteresis loops, we studied the solid solutions of classical perovskite ferroelectric $(1-x)BaTiO_3$ -$xABO_3$ wwhere ABO_3 =$BaZrO_3$, $BaSnO_3$, $BaHfO_3$, and $DyFeO_3$. The analysis of experimental data based on the percolation theory revealed the existence of a critical concentration, x_c, which is larger than the relaxor-to-normal ferroelectric crossover concentration and above which the infinite percolation cluster and the related relaxor phase cannot be developed. The temperature of the transition into the relaxor ferroelectric cluster state was found to follow the critical behavior $T^* \sim (x_c - x)^{\zeta}$ with the critical exponent $\zeta = 0.5$. The characteristics of polar clusters are estimated from the electric field and frequency dependences of polarization.

Keywords: Rlaxor ferroelectrics, lead-free, perovskits, percolation

---

Tu-S-P-80

Microscopic Description of the Ferroism properties in $AlFe_{1-x}A_xO_3$ (A= Mn or Co) and $Al_{1-x}Ga_xFeO_3$ Magnetoelectric Compositions

Guilherme Maia Santos [1], Luiz Fernando Cótica [1], José Eduardo Padilha [2], Ivair Aparecido dos Santos [1], Amar Bhalla [3], Ruyan Guo [3]

[1] *State University of Maringá, Maringá, Brazil*
[2] *Campus Avançado de Jandaia do Sul, Federal University of Paraná, Jandaia do Sul, Brazil*
[3] *University of Texas at San Antonio, San Antonio, United States*

The microscopic changes of the ferroic and multiferroic properties of the $AlFeO_3$, $AlFe_{1-x}A_xO_3$ (with A = Mn or Co) and $Al_{1-x}Ga_xFeO_3$ compositions has been carefully investigated by add different dopant in your structure. *Ab initio* density functional theory calculations have been used to obtain electron density distributions and the electric polarization. The studies of chemical bonds shows how the atoms dopant interferes in the bonds between Fe(3d) and O(2p) ions, changing the shorter/longer and stronger/weaker bonds, which leads to changes in the electric polarization. Density of states calculations showed a magnetic polarization as a result of a weak ferromagnetic ordering. The results showed that $AlFeO_3$ and its derivatives compositions is a multiferroic material and can have an magnetoelectric coupling.

Keywords: AlFeO3, multiferroic, density functional theory, electric polarization

---

Tu-S-P-81

Temperature dependent local structure of $LiCoO_2$ determined by *in-situ* Co K-edge X-ray absorption fine structure

Chinawat Ekwongsa

Suranaree University of Technology, Nakhon Ratchasima, Thailand

Lithium cobalt oxide ($LiCoO_2$) currently has a great attention as active cathode material lithium ion batteries. In this work, lithium cobalt oxide was prepared by solid state reaction and co-precipitation method. The synthesis parameters and phase formation behavior were investigated in details via several techniques, including thermal analysis, X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS). A change in local structure was investigated using in-situ extended X-Ray absorption fine structure (EXAFS). The temperature ranged between 400 °C and 700 °C with air condition was applied for this study. The results will be presented and discussed in details.

Keywords: Lithium cobalt oxide; extended X-ray absorption fine structure.

Tu-S-P-82

In-situ observation of an electric-field-induced lattice distortion of $BiFeO_3$ thin films

Seiji Nakashima [1], Osami Sakata [2], Hiroshi Funakubo [3], Takao Shimizu [3], Daichi Ichinose [3], Yasuhiko Imai [4], Hironori Fujisawa [1], Masaru Shimizu [1]

[1] *University of Hyogo, Himeji, Japan*
[2] *National Institute for Materials Science, Sayo, Japan*
[3] *Tokyo Institute of Technology, Yokohama, Japan*
[4] *Japan Synchrotron Radiation Research Institute, Sayo, Japan*

Recently, lead-free ferroelectric materials have attracted much attention from a view point of environmental protection. A $BiFeO_3$ (BFO) is one of the lead-free ferroelectrics, which shows an excellent ferroelectricity, and has been expected as a material for lead-free piezoelectric sensors, actuators, and vibration energy harvester. However, piezoelectric properties of BFO still remains unclear because growth of high-quality bulk ceramics is difficult. We have already demonstrated growth of single-crystal BFO thin films by sputtering. In this study, electric-field induced lattice distortion of BFO thin film was investigated by time-resolved X-ray diffraction under electric fields using a synchrotron radiation at BL13XU in SPring-8, Japan. The 1-μm-thick single-crystal BFO thin film was grown on $SrRuO_3$-buffered vicinal $SrTiO_3$ (STO) (001) substrate by rf sputtering. Pt top electrodes with a diameter of 200 μm were prepared by sputtering and lift-off process. The time–resolved X-ray diffraction measurement of the Pt/BFO/SRO/STO capacitor structure was performed under application of voltage pulses with an amplitude and width of 150 kV/cm and 300 ns, respectively. The synchrotron X-ray with an energy of 12.4 keV was focused within Pt top electrode in which electric field pulses are applied. Reciprocal space maps of BFO 003, 114, and 1-14 diffraction spots were observed by the time-resolved X-ray diffraction. Modulations of the BFO 003 and 114 diffraction spots were observed under the electric-field application. The lattice constants of the BFO with/without electric field indicates that

the BFO lattice was expanded along vertical direction, and compressed along in-plane direction owing to the electric-field induced strain.

Keywords: Piezoelectricity, BiFeO3. Thin films, Time-resolved X-ray diffraction

---

Tu-S-P-83

The evidence of giant Surface Flexoelectric Field in (111)-oriented $BiFeO_3$ thin film

tieying yang

Shanghai Institute of Applied Physics Chinese Academy of Sciences, shanghai, China

In this work, the surface structure of a single-domain epitaxial $BiFeO_3$ film with (111) orientation is investigated by in-situ grazing incidence x-ray diffraction and X-ray reflectivity. We found that a large strain gradient exists in the surface region (2-3 nm) of the $BiFeO_3$ film. The strain gradient is approximately 10^7 m^{-1}, which is 2 or 3 orders of magnitude larger than the value inside the film. Moreover, we found that a surface layer with a lower electron density compared with the underlying $BiFeO_3$ layer exists on the surface of $BiFeO_3$ film, and this layer exhibits an irreversible surface structure transition occurs at 500 K, which should be associated with the surface flexoelectric field. We considered that this large strain gradient is originated from the surface depolarization field of ferroelectrics. Our results suggest a coupling between the surface structure and the flexoelectricity and implied that the surface layer and properties would be controlled by the strain gradient in ferroelectric films.

Keywords: Surface layer, Ferroelectric thin films, X-ray diffraction, Flexoelectrics, Microstructure

---

Tu-S-P-84

Pinched hysteresis behaviour in lead free ferroelectric ceramic BCT-BZT

Atal Bihari Swain

Department of Physics, Indian Institute of Technology Madras1, Chennai-600036, India, chennai, India

Lead free ferroelectric ceramic (1-x) $Ba(Zr_{0.2}Ti_{0.8})O_3$-x$(Ba_{0.7}Ca_{0.3})TiO_3$ (BZT-BCT) of great interest in research community due to their triple point type morphotropic phase boundary(MPB) and high d_{33} value comparable with PZT. In this work we have investigated the influence of calcination temperature on ferroelectric property of BCT-BZT. We prepared the sample by conventional solid state reaction and calcined at different temperature ranging from 1200 ^oC to 1500 ^oC. Ferroelectric measurement reveals, solid solutions calcined at lower temperature gives rise to double hysteresis behavior whereas solid solution calcined at higher temperature displays typical ferroelectric hysteresis loop. The temperature dependent dielectric measurement shows that the system with low calcination temperature samples has lower Curie temperature compared to that of FE samples. The dielectric constant shows continuity in

Curie temperature and relatively not high value compare to FE sample. The structure, microstructure and dielectric analysis of these compounds are presented in this work.

Keywords: BCT–BZT ceramics, ferroelectrics, polymorphic phase transition, morphotropic phase boundary, dielectric.

Tu-S-P-85

Study on the interface behaviours between bismuth-based ceramics and electrodes

Xiukai Cai [1], Yuanxing Cai [2], Peng Deng [1], Zhiwei Xue [1], Sirui Cai [3]

[1] *College of Civil Engineering, Shandong Jianzhu University, Jinan, China*
[2] *School of Materials Science and Engineering, Shandong Jianzhu University, Jinan, China*
[3] *8615 SW 68th Ct., Apt 21, Miami, United States*

Although bismuth-based ceramics are promising candidates for the utilization for the electronic industry, it is absolutely essential to make it clear that many fundamental physical and chemical problems lied in the practical materials system. Aiming to understand bismuth-based low-firing dielectrics for the co-firing multilayer ceramic capacitor's application, the interface behaviors between bismuth-based dielectrics and deposited silver electrodes have been studied. It was found that bismuth-based dielectrics show a deteriorated tendency of dielectric properties towards higher silver firing temperatures. Perhaps poisoned in the vicinity of the interface layer, the metallic electrode silver, has been detected by scanning electron microscopy equipped with energy dispersive X-ray spectroscopy for the samples prepared in the higher silver-firing temperatures, which explains why the dielectric data turn to be bad.

Keywords: Bismuth-Based Ceramics, Dielectric Properties, Dielectric-Electrode Interfaces, Electrodes' Diffusion

---

Tu-S-P-86

NSMM Review – Part II: Development of structural relations using geometric considerations

YuHusn Liao [1], Vignaswaran K. Veerapandiyan [1], V. Mitic [2], Walter A. Schulze [1], Scott T. Misture [1], Steven M. Pilgrim [1], Steven Tidrow [1]

[1] *Alfred University, Alfred, United States*
[2] *University of Nis, Nis, Serbia*

We review the physical geometric constraints of the new simple material model (NSMM) and compare them with Goldschmidt's tolerance factor formalism, a correlation relation. NSMM geometric constraints serve as an important template for determination of coordination and temperature dependent elemental, genome-like, ion properties, and ionic radii, as shown in "NSMM Review – Part III". While

temperature dependent geometric considerations, including ionic radii, are not sufficient for ultimate determination of crystal structure, importantly, the coordination and temperature ionic radii, which significantly improve the accuracy and precision of lattice volume as a function of temperature, are essential inputs to the Clausius – Mossotti relationship for determination of coordination and temperature dependent ionic polarizability, as shown in "NSMM Review – Part IV". Importantly, the combined genome-like ion properties, radii and polarizability provide the temperature dependent relative permittivity of materials and the temperature of polarization-induced structural phase transitions. Further, another type of phase transition, a geometrically constrained volume-induced structural phase transition, has been recently identified, see "NSMM Review – Part V. In totality, geometric considerations when coupled with temperature dependent ionic properties, radii and polarizability allow us to physically understand why the majority of "simple" and "simply mixed" Perovskites are not cubic at room temperature and why so many of them undergo structural phase transition from a high temperature cubic-prototype.

Keywords: ionic radii space, planar and volume constraints, ionic radii and polarizability, Goldschmidt's tolerance factor,

Wednesday, September 6th, 2017 - Plenary Room - 08:10 - 09:00

Plenary -

Wednesday, September 6th, 2017 - Plenary Room - 09:00 - 09:50

Plenary - PLENARY 02

We-S-O-01

(INVITED) Large coupling ferroelectricity through polarization rotation

R.E. Cohen

Extreme Materials Initiative, Geophysical Laboratory, Carnegie Institution for Science, Washington, D.C., United States
LMU Munich, Munich, Germany

High coupling oxide ferroelectrics are generally optimized through polarization rotation. Rather than the simple collinear piezoelectric coupling involving stretching of the polarization by applying an electric field or strain, larger coupling is obtained by applying an oblique field or shear strain that causes the polarization to change direction. The response is much softer for rotations of the polarization, so that much larger response can be achieved for the same field. This principal applies both to conventional piezoelectrics like PZT near the MPB and to relaxor ferroelectrics. What improvements can we look for from here, and what kind of studies are needed? Defect dipoles in oxides can greatly enhance electromechanical coupling when aligned. This is also due to the polarization rotation mechanism. Changes in bulk properties that can be unexpectedly large even for small concentrations of defects. We

have simulated ferroelectric perovskites such as BaTiO3 as functions of defect dipole concentration and orientations. We have also performed experiments on Mn-doped samples as functions of aging. In an aging process, the defects align spontaneously, whereas in applied fields this process can be better controlled and accelerated. Now we have a detailed microscopic understanding of the effects of defect concentration, distribution and defect dipole alignment on polarization and strain response. This work is supported by the US Office of Naval Research and the European Research Council Advanced Grant ToMCaT.

Keywords: polarization rotation, first-principles, defects, ageing

Wednesday, September 6th, 2017 - Room1 - 10:20 - 10:50

keynote speaker - THEORY II

We-S-O-01

(INVITED) Polarization twist in perovskite ferrielectrics: A study on (Bi,Na)TiO_3-$BaTiO_3$ single crystals

Yuji Noguchi, Yuuki Kitanaka, Masaru Miyayama

The University of Tokyo, Tokyo, Japan

Because the functions of polar materials are governed primarily by their polarization response to external stimuli, the majority of studies have focused on controlling polar lattice distortions. In some perovskite oxides, polar distortions coexist with nonpolar tilts and rotations of oxygen octahedra. The interplay between nonpolar and polar instabilities appears to play a crucial role, raising the question of how to design materials by exploiting their coupling. Here, we introduce the concept of 'polarization twist', which offers enhanced control over piezoelectric responses in polar materials. Our experimental and theoretical studies provide direct evidence that a ferrielectric perovskite exhibits a large piezoelectric response because of extended polar distortion, accompanied by nonpolar octahedral rotations, as if twisted polarization relaxes under electric fields. The concept underlying the polarization twist opens new possibilities for developing alternative materials in bulk and thin-film forms.

Keywords: ferrielectric, polar, nonpolar, phase transition, ferroelectric, polarization, single crystal

Wednesday, September 6th, 2017 - Room2 - 10:20 - 10:50

keynote speaker - DIELECTRICS II

We-S-O-01

(INVITED) The bulk photovoltaic effect in the crystals without symmetry center and solar harvesting

Vladimir Fridkin

Shubnikov Institute of Crystallography of Federal Scientific Research Center "Crystallography and Photonics" of Russian Academy of Sciences, Moscow, Russia
Drexel University, Philadelphia, United States

The Bulk Photovoltaic Effect (BPE) is a new quantum mechanical phenomenon, which could be observed in the 20 symmetry points group crystals without symmetry center (ferro - and piezo electrics). Up to now the BPE was observed only in the bulk crystals and shows very low conversation efficiency of light energy (e.g. solar) to electricity. The last works have shown that in ferroelectric films with nanoscale thickness the conversion efficiency could be much higher. It opens very perspective application of BPE. There two microscopy mechanisms of BPE. The first one called ballistic mechanism is connected with asymmetric distribution of non-thermalized carrier momentum and violation of Boltzmann principle of detailed balance. The second one is the shift mechanism is a new quantum mechanical phenomenon obtained by accounting for the non-diagonal elements of density matrix. The BPE in ferro- and piezoelectric crystals and films is considered. The mechanism of BPE in topological insulators and in plasmonics is discussed. The special attention is paid to the PBE in the nanoscaled perovskites and hybrid perovskites and influence of screening field of the conversion energy efficiency.

References

[1] B. Sturmann and V. Fridkin, The Photovoltaic and Photorefractive Effects in Noncentrosymmetric Materials (Gordon and Breach, Philadelphia, 1992).

[2] S. Young and A. Rappe, Phys.Rev.Lett. 109, 116601 (2012).

[3] S. Young, F.Zeng, A. Rappe, Phys.Rev.Lett. 109, 236601 (2012).

[4] A. Zenkevich et al, Phys.Rev.B 90, 161409 (2014).

[5] Z. Gu et al, Phys.Rev.Lett. 118, 096601 (2017).

6] J. Spanier et al, Nature Photonics, 10, 610-616 (2016).

Keywords: photovoltaics, ferroelectrics, piezoelectrics, topological insulators, plasmonics, energy conversion efficiency

Wednesday, September 6th, 2017 - Room3 - 10:20 - 10:50

keynote speaker - RELAXORS II

We-S-O-01

(INVITED) On the relationship between materials properties and short-range order in highly piezoelectric lead-based relaxors

Peter Gehring [2], Matthew Krogstad [1], Daniel Phelan [1], Stephan Rosenkranz [1], Raymond Osborn [1], Feng Ye [3], Yaohua Liu [3], Jacob Ruff [4], Haosu Luo [5], Zuo-Guang Ye [6], Justin Wozniak [1]

[1] *Argonne National Laboratory, Lemont, United States*
[2] *National Institute of Standards and Technology, Gaithersburg, United States*
[3] *Oak Ridge National Laboratory, Oak Ridge, United States*
[4] *Cornell University, Ithaca, United States*
[5] *Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China*
[6] *Simon Fraser University, Burnaby, Canada*

Four different forms of local order that give rise to diffuse neutron and x-ray scattering in the relaxor ferroelectric series PMN-xPT are identified via broad, three-dimensional surveys of reciprocal space. Compositionally-dependent measurements reveal how the local ordering correlates with dielectric and electro-mechanical properties as well as with long-range polar order.

Keywords: Relaxors, PMN-xPT, short-range order, diffuse scattering

Wednesday, September 6th, 2017 - Room4 - 10:20 - 10:50

keynote speaker - FERROICS/MULTIFERROICS II

We-S-O-01

(INVITED) $EuTiO_3$: a possible multiferroic with unusual magneto-optical properties and applications

Annette Bussmann-Holder [1], Krystian Roleder [2], Jürgen Köhler [1]

[1] *Max-Planck-Institute for Solid State Research, Stuttgart, Germany*
[2] *Institute of Physics, University of Silesia, Katowice, Poland*

Thin films of $EuTiO_3$ deposited on a $SrTiO_3$ substrate have been fabricated which are insulating and transparent with a band gap of 4.53eV. Both materials are non-magnetic at room temperature. The films have been shown to be single crystalline with the cubic c-axis in the growth direction. At $T_S = 282$ K, $EuTiO_3$ changes from cubic to tetragonal symmetry thereby allowing the observation of birefringence Δn caused due to symmetry lowering. Below T*=190K an upturn in the birefringence signals another up to now unknown structural phase transition. Upon applying a magnetic field of only 0.02 T, Δn can be tuned directionally whereby the magnetic field directed along the [110] direction completely suppresses it in contrast to the perpendicular direction $[11\bar{0}]$ where it remains active up to 240 K. Along

[100] and [010] the onset of Δn is observed below T_S as expected from symmetry considerations. An increase in the magnetic field to 0.1 Tesla leads to an enormous increase in Δn by a factor of 3 and a shift of its onset temperature from 240 K to almost room temperature with the field being aligned along [11$\bar{0}$] direction. In the perpendicular direction an enhancement of both Δn and its onset temperature takes place, however, much less pronounced compared to the [11$\bar{0}$] direction. From these data it is apparent that $EuTiO_3$ thin films are magneto-optically active and suited for device applications. The magneto-optical properties can be tuned by a magnetic field and temperature together with rotations of the sample and the magnetic field.

Keywords: magneto-optic devices, novel multiferroics

Wednesday, September 6th, 2017 - Room1 - 10:50 - 11:15

Invited talk - THEORY II

We-S-O-01

(INVITED) Role of random electric fields in lead-free relaxor ferroelectrics

Zuo-Guang Ye [1], Jian Zhuang [2], Alexei Bokov [1], Wei Ren [2]

[1] *Simon Fraser University, Burnaby, Canada*
[2] *Xi'an Jiaotong University, Xi'an, China*

Lead-oxide relaxor ferroelectrics are widely used as materials for numerous applications due to extremely large dielectric constant and unparalleled piezoelectric coefficients. It has been shown that strong quenched random local fields caused by the disordered heterovalent cations establish the relaxor phase, identify the order parameter and lead to the dramatic enhancement of piezoelectric coefficients. On the other hand, the role of random fields in lead-free analogs is not clear. In this work we analyze the results on the concentration-induced crossover from ferroelectric to relaxor state in lead-free $BaTiO_3$-based homovalent and heterovalent solid solutions recently obtained in our laboratory and published in the literature to underline the characteristics and microscopic mechanisms specific to each group of materials. We demonstrate, that similar to classical lead-oxide relaxors, strong quenched random electric fields suppress the macroscopic ferroelectric ordering and promote relaxor behavior in lead-free oxides. We observe different types of the crossover behavior with increasing concentration x, including a gradual transformation from a sharp ferroelectric phase transition to a diffuse phase transition and to relaxor transition. Furthermore, the relaxor behavior vanishes if the strength of random fields becomes large enough. Alongside the widely known relaxor features such as the cubic macroscopic symmetry, the Vogel-Fulcher law for the frequency dependence of T_m and the Curie-Weiss law for e(T) at $T >> T_m$, we verify in lead-free relaxors some other specific relaxor phenomena, such as the scaling of slim-loop polarization curves and the Vogel-Fulcher scaling of the temperature/frequency dependences of permittivity.

Keywords: Lead-free relaxor ferroelectrics, random field, Ferroelectric to relaxor crossover

Wednesday, September 6th, 2017 - Room2 - 10:50 - 11:15

Invited talk - DIELECTRICS II

We-S-O-01

(INVITED) Thermodynamic stability of polar vortices in ferroelectric superlattices

Long-Qing Chen, Zijian Hong

The Pennsylvania State University, University Park, United States

This presentation will discuss the recent observations and predictions of new thermodynamically stable mesoscale polar states that might emerge from ferroelectric heterostructures at the nanoscale. In presentation, we focus on the determination of thermodynamic conditions and geometric length scales that are critical for the formation of ordered polar vortex lattice in ferroelectric superlattices of $PbTiO_3/SrTiO_3$ using phase-field simulations and analytical theory. We show that the stability of these vortex lattices involves an intimate competition between long-range electrostatic, long-range elastic, and short-range polarization gradient-related interactions leading to both an upper- and a lower- bound to the length scale at which these states can be observed. We found that the critical length is related to the intrinsic domain wall width, which could serve as a simple intuitive design rule for the discovery of novel ultrafine topological structures in ferroic systems.

Keywords: supserlattice, domains, vortices, phase-field simulation, modeling

Wednesday, September 6th, 2017 - Room3 - 10:50 - 11:15

Invited talk - RELAXORS II

We-S-O-01

(INVITED) Manipulation of electric field effect by orbital switching

Feng Pan, Bin Cui, Cheng Song

School of Materials Scienec and Engineering, Tsinghua University, Beijing, China

Conventional switches, which control the on–off states of circuits in macroscale, can be seen everywhere in our daily life. The concept of switch is broadened in microelectronics with sharply reduced dimensions and advanced functionalities: the p–n junctions with the size of several hundred nanometers constitute the cornerstone of the information treatment and logic circuit, while molecular switches could exhibit the basic functions of digital electronics−rectification, amplification, and storage in molecular devices. Nevertheless, the further miniaturization is urgently required and intensely pursued in semiconductor industry, which calls for atomic even subatomic modulation of electrical behavior, especially with the emergent conductivity at atomic level. Here, an orbital switch formed at the interface

between $BaTiO_3$ (BTO) and $La_{0.5}Sr_{0.5}MnO_3$ (LSMO) is used to manipulate the electric field effect in the LSMO/BTO heterostructure. The orbital switch is based on the connection or breakdown of interfacial Ti–O–Mn bond due to the ferroelectric displacement under external electric field. This fi nding would pave the way for the tuning of the material performance or device operation at atomic level and introducing the orbital degree of freedom into the terrain of microelectronics.

Keywords: Orbital Switching, Ferroelectric, Electric Field Effect, Heterostructure

Wednesday, September 6th, 2017 - Room4 - 10:50 - 11:15

Invited talk - FERROICS/MULTIFERROICS II

We-S-O-01

(INVITED) Strain-induced polar-to-nonpolar transitions in layered perovskites

James Rondinelli

Northwestern University, Evanston, United States

Epitaxial strain engineering is a powerful approach to generate and tailor collective phenomena and new functionalities in thin film oxides with layered habits, e.g. those of the homologous series $A_{n+1}B_nO_{3n+1}$ (n=1-∞). Although large epitaxial strains are believed to always induce ferroelectricity (FE), here we demonstrate that biaxial strain induces an unanticipated polar-to-nonpolar (P-NP) structural transition in (001) thin films of layered hybrid-improper ferroelectrics with the n=2 Ruddlesden-Popper structure at experimentally accessible biaxial compressive and tensile strains [1]. We show in detail for $Ca_3Ti_2O_7$ that the origin of the P-NP transition originates from the interplay of trilinear-related lattice mode interactions active in the layered oxides, and those interactions are directly strain tunable. We use this understanding to show that the P-NP transition also occurs in (001) $Ca_3Mn_2O_7$ and $Sr_3Zr_2O_7$ thin films. Last, we propose a design principle for selecting the required A and B cation chemistries that ensure strained $A_3B_2O_7$ (001) oriented films exhibit P-NP transitions [2], which we substantiate with density functional calculations. Our results call for a careful re-examination of the role of strain-polarization coupling in FE films with nontrivial anharmonicities and offer a route to search for new functionalities in oxides through multimode coupling.

References

[1] X.-Z. Lu and J.M. Rondinelli, Nature Materials **15**, 951-955 (2016).

[2] X.-Z. Lu and J.M. Rondinelli, Advanced Functional Materials (2017). DOI: 10.1002/adfm.201604312

Keywords: Ruddlesden-Popper, Density Functional Theory, Titanates, Improper Ferroelectricity

Wednesday, September 6th, 2017 - Room1 - 11:15 - 12:35

Oral presentation - THEORY II

We-S-O-01

Spin-phonon couplings and lattice instabilities in complex oxides

Jiawang Hong

Beijing Institute of Technology, Beijing, China

In a magnetic system that has a strong spin-phonon coupling, i.e., a strong dependence of the polar phonon frequencies on spin order, the magnetic order may be capable of tipping the balance between paraelectric and ferroelectric states. This strong spin-phonon coupling effect is promising to be used to search for new multiferroics. An theoretical approach was developed to calculate reliable spin-phonon coupling effect in several complex oxides and we will discuss the prospects for bulk and superlattice forms to be useful as multiferroics. By combining first-principles calculation and inelastic neutron scattering measurement, the spin-phonon coupling effect and lattice instabilities in complex oxides will be discussed.

Keywords: spin-phonon coupling, first-principles, multiferroics

---

We-S-O-02

Elastic and optical properties of Ruddlestone-Popper perovskites - *ab initio* calculation

Selami Palaz [2], Husnu Koc [3], Gokay Ugur [4], Ekmel Ozbay [1], Amirullah Mamedov [1]

[1] *Bilkent University, Nanotechnology Research Center, Ankara, Turkey*
[2] *Department of Physics, Harran University, URFA, Turkey*
[3] *Department of Physics, Siirt University, SIIRT, Turkey*
[4] *Department of Physics, Gazi University, ANKARA, Turkey*

In the present paper we haveinvestigated the electronic structure of some orthorhombic$A_3X_2S_7$(X = Ti, Zr, and Hf) compounds based on density functional theory. Then we extend the Ruddlesden-Popper(RP) $A_3X_2S_7$sulfides and examine how ferroelectricity is induced by coupled octahedral rotation modes. The mechanical and optical properties have also been computed. The second-order elastic constants have been calculated, and the other related quantities such as Young's modulus, shear modulus, Poisson's ratio, anisotropy factor, sound velocities, Debye temperature, and hardness have also been estimated in the present work.The band gap trend in $A_3X_2S_7$ can be understood from the nature of their elec-tronic structures. The obtained electronic band structure for $Ba_3Zr_2S_7$and $Ba_3Hf_2S_7$compounds are semiconductor in nature, and the $Ba_3Ti_2S_7$ compound also is semi-metal. Similar to ferroelectric oxides, there are pronounced hy-bridization of electronic states between X-site cations and anions in

$A_3X_2S_7$. Based on the obtained electronic struc-tures, we further calculate the frequency-dependent di-electric function and other optical functions in different phases.

Keywords: Ruddlesden-Popper perovskites, ab initio

We-S-O-03

Pecularities of antiferroelectric phase transitions in $PbZr_{0.71}Sn_{0.29}O_3$ crystal by Mössbauer effect

Irena Jankowska-Sumara [1], Maria Podgórna [1], Jan Żukrowski [2], Andrzej Majchrowski [3]

[1] *Institute of Physics, Pedagogical University of Cracow, Kraków, Poland*
[2] *AGH University of Science and Technology, Academic Center for Materials and Nanotechnology, Kraków, Poland*
[3] *Institute of Applied Physics, Military University of Technology, Warszawa, Poland*

The study of the phase transitions in the antiferroelectric crystals has been a challenging task for several years because of the presence of competing interactions between ferroelectricity and antiferroelectricity at phase transition point. In ferroelectric crystals phase transition at T_C is usually considered to be the result of softening of a single soft optic mode at the center of the Brillouin zone and/or relaxational processes which can exist in a given material. In the case of antiferroelectrics the situation is more complicated since the unstable mode is not in the center of the Brillouin zone. Typical example of an antiferroelectric crystal is $PbZrO_3$ (PZO). However, the nature of PZO's transition is far from being settled, as new experimental results and conflicting physical pictures have recently been reported. Numerous Raman and Brilloiun scattering measurement of pure and doped PZO (inter alia $PbZr_{1-x}Sn_xO_3$) crystals has not solved the problem of the existence of a classical soft mode although some promising experimental results was reported. Among the other experimental techniques that are able to measure "local" properties of the ferroelectrics and antiferroelectric phase transitions, Mössbauer spectroscopy seems to be forgotten technique. Since lattice dynamics is involved in the temperature dependence of some parameters of Mössbauer spectra, it seems to be possible to use them to get some information about the lattice dynamics of antiferroelectric single crystal of $PbZr_{1-x}Sn_xO_3$ passing through its critical points, mainly because of a Mössbauer nuclei (Sn) implemented to the crystal lattice.

Keywords: antiferroelectrics, soft modes, lattice dynamics, Mössbaer effect

---

We-S-O-04

Controlling Jahn-Teller Distortions and Optical Properties in Rare-Earth Manganite Perovskites by Electric Fields

Michael Marcus Schmitt [1], Yajun Zhang [1, 2], Philippe Ghosez [1]

[1] *Physique Theorique des Materiaux, Q-Mat, Cesam, Université de Liège, Allée du 6 Aout 17 (B5a), 4000 Sart Tilman, Belgium*

[2] *Department of Engineering Mechanics, School of Aeronautics and Astronautics, Zhejiang University, 38 Zheda Road, Hangzhou 310007, China*

The Jahn-Teller distortion (JTD) in ABO_3 perovskite compounds is linked to various functional properties as the electronic band gap size and the magnetic order. Among the perovskite oxides, the rare-earth manganite series $R^{3+}Mn^{3+}O_3$ exhibits one of the largest amplitudes of JTD. In these compounds, the JTD is responsible for opening a band gap, which's size gradually decreases with increasing temperature and eventually disappears together with the JTD (at ~ 750 K for $LaMnO_3$). Our aim is to design materials in which the non-polar JTD is tunable by an applied external electric fields in order to control optical properties.
We discuss two approaches vis-a-vis the contradictory problem: Hybrid Improper Ferroelectricity (HIF) and manganite thin films epitaxially grown on piezoelectric substrates. In compounds showing HIF, the appearing polar lattice distortion is slave to two non-polar geometrical distortions expressed in a trilinear term in the Landau expansion of the free energy. The involvement of the JTD in this trilinear term indicates the geometrical allowance of manipulating the JTD amplitude with an electric field. The second concept relies on the idea of tuning the JTD by manipulating the strain state of a manganite thin film through an applied electric field onto a piezoelectric substrate. We show why the second approach is conceptually the most promising and discuss how the electro-optic response can be maximized on the basis of our ab-initio results.

Keywords: Jahn-Teller Effect, Optical-Properties, Rare-Earth Manganites

---

We-S-O-05

(INVITED) Phonon dynamics and phase transformations in bismuth titanate

Sanjeev Nayak [1], Kevin Co [1], S. Pamir Alpay [1, 2]

[1] *Department of Materials Science & Engineering and Institute of Materials Science, University of Connecticut, Storrs, United States*
[2] *Department of Physics, University of Connecticut, Storrs, United States*

First-principles modeling of materials is key to fundamental understanding of materials properties. $Bi_4Ti_3O_{12}$ (BiT) is a complex layered oxide belonging to the Aurivillius class with alternating layers of perovskite-like and anti-fluorite-like ionic arrangements in the crystal structure. We have modeled the phonon dynamics of BiT using density functional theory (DFT) in order to understand the origin of lattice instabilities and structural phase transitions. The low temperature ferroelectric phase is monoclinic with space group P_c and the high temperature paraelectric phase is tetragonal. *Phonopy* and the density functional perturbation theory have been used to study the phonon modes whereby terahertz frequency-domain spectroscopy for highly textured BiT films and theoretical results are matched. Three low-frequency optical phonon modes were observed at room temperature form the THz spectroscopy: 0.61 THz, 0.83 THz and 0.95 THz. The DFT calculations predict the optical phonon modes at 1.13 THz,

1.14 THz, and 1.37 THz. Further analysis showed that the three low frequency phonons shifted by 7.1%, 2.6% and 1.3%, respectively, as temperature is increased from −273 °C to 527 °C. The corresponding displacement of phonon frequencies for hydrostatic expansion of the lattice by 1% is found to be 12.9%, 5.3% and 2.6%, providing the clue that the phonon softening is associated with the volume expansion of the lattice. In addition to that, phonons in presence of point defects such as the oxygen vacancies are explored which show site dependent trends. The effect of impurities on bismuth and titanium sites within the perovskite layers on the polarization is also explored.

Keywords: Ferroelctrics, First-principles modeling, Bismuth titanate, phonons, phase transitions

Wednesday, September 6th, 2017 - Room2 - 11:15 - 12:35

Oral presentation - DIELECTRICS II

We-S-O-01

Dynamics of acoustic phonons in niobium doped $PbZrO_3$ single crystals

Dariusz Kajewski [1], Jae-Hyeon Ko [2], Irena Jankowska-Sumara [3], Anette Bussmann-Holder [4], Byoungwan Lee [2], soohan Oh [2], Andrzej Majchrowski [5], Iwona Lazar [1], Andrzej Soszyński [1], Janusz Koperski [1], Krystian Roleder [1]

[1] *Institute of Physics, University of Silesia, ul. Uniwersytecka 4, Katowice, Poland*
[2] *2Department of Physics, Hallym University, 1 Hallymdaehakgil, Chuncheon, Gangwondo 24252, Korea, Republic of (South)*
[3] *Institute of Physics, Pedagogical University, ul. Podchor??ych 2, Kraków, Poland*
[4] *Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
[5] *Institute of Applied Physics, Military University of Technology, ul. Kaliskiego 2, 00-908 Warszawa, Poland*

Lead zirconate, $PbZrO_3$, has been of interest for dozens of years since its discovery [1-5]. Defects seem to play an important role regarding the microscopic origin of the formation of the so-called intermediate phase. Introduction of heterovalent cation Nb into crystal lattice of lead zirconate can create defects or may compensate charges produced by other defects. Additionally the low concentration of niobium leads to the existence of a new intermediate phase, properties of which depend on the dopant concentration [6]. Acoustic anomalies and precursor dynamics in high-quality niobium-doped lead zirconate single crystals investigated by Brillouin light scattering will be presented. Anomalous behaviour of the acoustic phonons was found to correlate with unexpected properties of the birefringence and piezoelectric effect in the temperature range in which permittivity does not obey the Curie-Weiss law. Moreover, temperature properties of acoustic phonons point to existence of the above-mentioned new intermediate phase. The Brillouin light scattering experiment was carried out on two $PbZrO_3$:Nb single crystals grown by two different flux methods.

References

[1] G. Shirane, E. Sawaguchi, A. Takeda, Phys. Rev. 80, 485 (1950).

[2] V. J. Tennery, J. Electrochem. Soc. 112, 1117 (1965).

[3] L. Benguigui, J. Solid State Chem. 3, 381 (1971).

[4] Z. Ujma and J. Hańderek, Phys. Stat. Solidi (a) 28, 489 (1975).

[5] J.-H. Ko, M. Górny, A. Majchrowski, K. Roleder, A. Bussmann-Holder, Phys. Rev. B, 87, 184110 (2013).

[6] D. Kajewski, Z. Ujma, P. Zajdel, K. Roleder, Phys. Rev. B 93, 054104 (2016).

Keywords: Lead zirconate, Brillouin light scattering, phase transitions, precursors,

---

We-S-O-02

Porous ferroelectric ceramic with novel aligned pore structures for energy harvesting

Yan Zhang, Mengying Xie, James Roscow, Chris Bowen

Department of Mechanical Engineering, University of Bath, BATH, United Kingdom

Energy harvesting from ambient energy sources and converting it into useful electrical power continues to receive increasing amounts of industrial and academic interests[1]. This research demonstrates the significant benefits of using highly aligned porosity in energy harvesting piezoelectric and pyroelectric materials. Porous lead zirconate (PZT) ceramics with highly aligned pore channels and varying porosity were manufactured via a unidirectional freezing method, termed 'freeze casting' [2]. It was observed that on increasing the porosity level from 20 to 60 vol.%, the compressive strengths of the porous PZT were 200%-580% higher than the conventional randomly distributed porous materials, respectively. Due to the introduction of porosity and air into the ceramic, the permittivity in the porous freeze-cast PZT decreased significantly, which is beneficial to achieving a high piezoelectric and pyroelectric performance figures of merit, compared with the dense PZT. A complete thermal energy harvesting system, composed of a parallel-aligned PZT harvester unit and an AC/DC converter unit was constructed to successfully demonstrate the real-time operation of charging a storage capacitor. These results indicated that the porous materials generated significantly more energy than the dense material when subjected to thermal oscillations, which are of benefit for the further design and selection of promising porous ferroelectric materials in devices for energy harvesting applications. The maximum voltage of 14.7 V can be obtained in the capacitor utilising the porosity of 60 vol.% PZT with the fastest charging speed.

References

[1] Chris Bowen, et al. Energy Environ Sci. 7, 25 (2014)

[2] Yan Zhang, et al, J. Am. Ceram. Soc. 98, 2980 (2015).

Keywords: aligned porous, PZT, piezoelectric, pyroelectric, energy harvesting

---

We-S-O-03

The influence of defect type and configuration on the electrical properties of PZT based ceramics

Jiangtao Zeng, Guorong Li, Liaoying Zheng

Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China

There are many types of defects and defect dipoles in PZT based ferroelectric ceramics and these defect dipoles can make the ceramics soft or hard, so they can be used for different applications. It is still debating that the interaction of defect dipole with domain is a boundary effect or a volume effect. In this study, we designed different doping strategies to obtain different defects. It was found that both boundary efffect and volume effect could appear in acceptor doped PZT ceramics. The electrical properties can be modifed by adjusting the concentration or configuration of defect dipoles.

Keywords: ferroelectric, defect, PZT

We-S-O-04

In situ dielectric spectroscopy and Brillouin scattering study of lithium niobate

Julita Piecha [1], Jae-Hyeon Ko [2], Krzysztof Szot [1]

[1] *Institute of Physics, University of Silesia, Katowice 40-007, Poland*
[2] *Department of Physics, Hallym University, Gangwondo 24252, Korea, Republic of (South)*

Physical and chemical properties of the $LiNbO_3$ can be modified during redox process and proton exchange reaction (PE). As a result of this treatment the significant lithium deficiency and concentration of defects in the surface of reduced lithium niobate crystal was observed. In our study we have analyzed an influence of reduction (*in situ*, under UHV, temperature: 20 - 800 °C) and oxidation (*in situ*, pure oxygen pressure (99.9999%): 6.4 x 10^{-7}-100 mbar, T = const.) processes on dielectric properties of the crystal. Dielectric spectroscopy investigation was obtained *in situ* at the frequency range from 1MHz to 1mHz for two set of samples: congruent and congruent with modified surface using proton exchange reaction (PE). The similar investigation of dielectric properties was obtained for sample modified with PE. Analysis of Cole-Cole plots showed that an equivalent circuit for reduction and oxidation reaction could be described as a typical Maxwell–Wagner capacitor. One of the Maxwell–Wagner inset was assigned to interior part of sample, second one to the crystal surface. Our study of temperature dependence vs Z' and Z'' with respect to the thermal and chemical treatment showed various characters

of activation energy for both contributions. Brillouin scattering study was used to enhance dielectric spectroscopy study. The $T_c \sim 1120$ °C value, determined in terms of the *ex situ* Brillouin scattering, was similar for all samples. However, unexpected anomaly in the Brillouin frequency shift was observed for proton exchange samples in vicinity of T_c for the longitudinal acoustic mode in contrast to referenced sample without anomaly.

Keywords: LiNbO3, dielectric & Brillouin spectroscopy, defects

---

We-S-O-05

(INVITED) Electromechanical behavior of Strontium-modified Lead Zirconate Titanate ceramics

Raj Singh

School of Materials Science and Engineering, Oklahoma State University, Tulsa, United States

PZT ceramics are extensively used as sensors and actuators in a variety of applications. Typically, these ceramics show strains between 0.1-0.2% depending on the specific materials and compositions. In contrast, selected Sr-modified PZT compositions (95:5) situated at the antiferroelectric (AFE)-ferroelectric (FE) phase boundary display AFE-FE phase change upon application of the electric field and large strain capabilities (~0.8%). In addition, some of these compositions also show excellent stability against cyclic fatigue damage to over 106 electric cycles. The processing approaches and origins of the large strains and fatigue mechanisms in these ceramics will be presented and discussed.

Keywords: Electromechanical response, Sr-modified PZT, Antiferroelectric-Ferroelectric Phase Change, Strain

Wednesday, September 6th, 2017 - Room3 - 11:15 - 12:35

Oral presentation - RELAXORS II

We-S-O-01

Sintering and characterization of dielectric and thermal mechanical properties of $(Bi_{1/2}Na_{1/2})TiO_3$-$BaTiO_3$ ceramics

Manuel Lente Lente, Giovanna da S. Batista

Federal University of Sao Paulo Science and Technology Institute, Sao Jose dos Campos, Brazil

(1-x)BNT-xBT ferroelectric ceramics, with x = 0; 8 and 12% mol, were prepared by the conventional ceramic processing method. The determination of the optimized sintering conditions for each composition allowed to the production of high density ceramic bodies free from secondary phase.

Dielectric and thermal mechanical properties of unpoled (1-x)BNT-xBT samples were determined from cryogenic temperatures to 850 K in order to contribute to a better understanding of the phase diagram of the BNT-BT system. The results revealed that the temperature in which an anomaly is observed from the thermal strain curve coincides with the so-called depolarization temperature characterized by dielectric measurements for each composition. While the Burns temperature for traditional relaxors can be determined by both dielectric and thermal mechanical measurements and agree with each other, for the (1-x)BNT-xBT ceramics these measurements did not revealed such accordance.

Keywords: Ferroelectrics; relaxors; sintering; BNT-BT

We-S-O-02

Super tetragonal ferroelectric phase of $BiFeO_3$-$PbTiO_3$: A cause for several novel phenomena

Bastola Narayan, Rajeev Ranjan

Department of Materials Engineering Indian Institute of Science, Bangalore, India

In the past few years we have discovered a series of unusual phenomena in the super tetragonal compositions of the ferroelectric alloy system (1-x)$BiFeO_3$-(x)$PbTiO_3$ (BF-PT) which at x = 0.30 exhibits an anomalously high percentage tetragonality (c/a – 1)x100 ~ 18 %, a value three times of the classical ferroelectric $PbTiO_3$. The super tetragonal phase of BF-PT exhibits unusual phenomena such as (i) isostructural structural transformation with temperature and (ii) a size driven coupled magneto-ferroelectric criticality at an anomalous size of ~ 300 nm. We have also exploited the practical aspects of the super tetragonal phase. We investigated the photocatalytic properties of BF-PT with regard to dye degradation and discovered that the when the super tetragonal phase was stabilized as metastable phase it enhanced the dye degradation rate five-fold. In another remarkable discovery, we found that by suitable chemical modification of the super tetragonal compositions it is possible to achieve a colossally high electrostrain of 1.3 % - a value comparable to that reported in single crystals of high performance piezoelectric such as PZN-PT.

Keywords: Size effect, piezoelectricity, photocatalysis, Bismuth ferrite, lead titanate

---

We-S-O-03

Observation of multiple phases and incommensurate transitions in bismuth and lead oxide based complex perovskites leading to high temperature relaxor behavior

Akansha Dwivedi

Department of Ceramic Engineering, IIT-BHU, Varanasi, India, Varanasi, India

Bismuth and lead oxide based ternary perovskites have been studied extensively in the past decade as potential electronic materials for high temperature application. Most of these materials however exhibit

diffuse phase transition and relaxor like behavior at very high temperature, where the Burns temperature (Td) goes well above 500 ^{o}C. In this report, a review of various such solid solutions have been presented while exploring one such system in detail in which multiple phase transitions have been observed. Possibility of segregation in this system has been explored by presenting X-ray diffraction analysis combining with the TEM and dielectric measurements. Quenched defect states leading to classical ferroelectric switching have also been observed for these complex oxides. The presence of defects possibly combined with segregated phases lead to phase instabilities and relaxor-like behavior in these systems.

Keywords: Perovskite, Relaxor, Ternary oxide

We-S-O-04

Lattice dynamics of $Na_{1/2}Bi_{1/2}TiO_3$ as studied by dielectric spectroscopy and Brillouin light scattering

Alexander Fedoseev [1], Vyacheslav Zalessky [1], Pavel Syrnikov [1], Sergey Lushnikov [1], Seiji Kojima [2]

[1] *Ioffe Institute, Sainkt-Petersburg, Russia*
[2] *University of Tsukuba, Tsukuba, Japan*

$(Na_{1/2}Bi_{1/2})TiO_3$ (NBT) belongs to relaxor ferroelectrics with disorder in the perovskite A-sublattice. Investigations of the NBT structure and physical properties have not succeeded in obtaining a complete picture of the crystal lattice dynamics. Only the structural phase transition of its cubic phase into a tetragonal ferroelastic one near 813 K and the ferroelectric state below 560 K have been established. The behaviors of the dielectric response in the "isotropization" region (620-580 K) and acoustic phonons in the vicinity of the ferroelectric state onset in NBT are intriguing. This report presents investigations of the dielectric response, conductivity, domain structure, and low-frequency region of the vibrational spectrum of NBT single crystals in the temperature range 290-750 K for the [100], [110], and [111] crystallographic directions. It is shown that the temperature evolution of the domains arising at $T < 800$ K has a temperature region 620-540 K in which domains disappear completely ([100] and [111] directions) or partially ([110] direction). This isotropization region manifests itself in the behavior of the imaginary part of the dielectric response and is due to the isotropic nature of conductivity. As Brillouin scattering experiments showed, the ferroelectric state onset was accompanied by softening of longitudinal and transverse acoustic phonons. Analysis of the NBT light scattering spectra revealed multicomponent quasielastic scattering. Temperature dependences of relaxation time and susceptibility the anomalous behaviors of which correlated with the anomalies in the behaviors of velocity and susceptibility of long-wavelength acoustic phonons were plotted.

Keywords: Relaxors, Dielectric spectroscopy, Brillouin scattering

---

We-S-O-05

(INVITED) Probing short-range order in PZN-xPT and PMN-xPT relaxor ferroelectrics with neutron scattering

Guangyong Xu [1], Zhijun Xu [1], Chris Stock [2], Peter Gehring [1], Fei Li [4], Shujun Zhang [3], Zuo-guang Ye [5]

[1] *National Institute of Standards and Technology, Gaithersburg, United States*
[2] *University of Edinburgh, Edinburgh, United Kingdom*
[3] *University of Wollongong, Wollongong, Australia*
[4] *Pennsylvania State University,, University Park, United States*
[5] *Simon Fraser University,, Burnaby,, Canada*

PZN-xPT and PMN-xPT relaxor ferroelectric materials have been studied extensively due to their extraordinary piezoelectric and electromechanical responses. One of the key issues in these materials is the role of polar nano-regions (PNR), or, in other words, how the short-range orders coexist with long-range polar order and influence the bulk property. We have performed neutron scattering measurements on single crystal PZN-xPT and PMN-xPT samples. With elastic diffuse scattering measurements carried out under external field along different directions, we were able to monitor how the dominant part of the diffuse scattering - the "butterfly diffuse" that extends along <110> directions - change with field. There is a complete redistribution (of the diffuse scattering intensities) under [111] field, a partial redistribution under [110] field, and no major change under [001] field. Our results suggest that the polar nano-regions are robust local orders that are locked in within the surrounding polar environment below Tc, and also strongly interact with acoustic phonon modes that induces instability in these systems.

Keywords: relaxor, polar nano-regions, piezoelectric, short-range, inhomogeneity

Wednesday, September 6th, 2017 - Room4 - 11:15 - 12:35

Oral presentation - FERROICS/MULTIFERROICS II

We-S-O-01

Structural characterization of ferroic materials by advanced spectroscopy techniques

Rattikorn Yimnirun [1], Jaru Jutimoosik [1], Saroj Rujirawat [1], Santi Maensiri [1], Pablo Esquinazi [3], Jochen Stahn [4], Amitesh Paul [2]

[1] *School of Physics, Institute of Science and NANOTEC-SUT Center of Excellence on Advanced Functional Nanomaterials Suranaree University of Technology, 30000, Nakhon Ratchasima, Thailand*
[2] *Technische Universität München, Physik Department, Lehrstuhl für Neutronenstreuung, James-Franck-Strasse 1, D-85748 Garching b., München, Germany*
[3] *Division of Superconductivity and Magnetism, University of Leipzig, D-04103, Leipzig, Germany*
[4] *4Laboratory for Neutron Scattering Paul Scherrer Institut, CH-5232, Villigen, Switzerland*

The Synchrotron-based X-Ray Absorption Near-edge Spectroscopy (XANES) and Polarized Neutron Reflectivity (PNR) techniques were employed to investigate the structural properties of $BiFe_{1-x}Mn_xO_3$

ceramic and Co/CoO/Au multilayer, especially to study the local structure of Mn in $BiFe_{1-x}Mn_xO_3$ ceramic and to verify the formation of secondary phase in Co/CoO/Au multilayer. Theoretical XANES spectra calculations corroborate with the interpretation of the XANES experimental data. In addition, the Co/CoO/Au multilayer was examined to explore the degree of recovery of the untrained state after the first two field cycles. Such a recovery was expected by field cycling a reorientation field along a direction of orientation angle away from the initial field cooling direction. Measurements as a function of and the strength of (along each direction) map the influence of on the reversal mechanism in the layers and thereby the degree of recovery.

Keywords: Ferroics, XANES, PNR

We-S-O-02

Magnetoelectric properties of cement and mortar

Bartłomiej Andrzejewski [1], Agnieszka Ślosarczyk [2], Ewa Markiewicz [1]

[1] *Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland*
[2] *Faculty of Civil and Environmental Engineering, Poznan University of Technology, Poznan, Poland*

Cementing materials have been widely used throughout the history of humanity. In ancient Egypt stone blocks were fixed together with sand and burnt gypsum. The Romans discovered that *opus caementicium* could be made by mixing volcanic ashes from Pozzuoli village near Vesuvius with burnt lime and were using on a large scale in ancient constructions. Beside of its long history and common applications, cement presents also an attractive material for science. In this report, we present the results of magnetometric and dielectric measurements of dry and hydrated cements and mortars. In dry cements, the main magnetic phase is C_4AF (in cement chemistry notation) brownmillerite with formula $Ca_2Al_{2-x}Fe_xO_5$ and intriguing physical properties depending on iron content. $Ca_2Fe_2O_5$ oxide (x=2) is known as a good ionic conductor in which O^{2-} ions can easily migrate along FeO_4 tetrahedral layers. It exhibits also pronounced magnetoresistance effect and belongs to *G*-type canted antiferromagnets with the Néel temperature $T_N \approx 770$ K. For $x < 1.5$ this ferrite undergoes a phase transition to noncentrosymmetric *Ibm*2 structure and begins exhibit ferroelectric properties with strong magnetoelectric coupling and spin flop transitions. During the hydration reaction, C_4AF phase transforms and the properties of cement or mortar are dominated by magnetic nanoparticles of ferrith *i.e.* the ferrimagnetic phase of ferrihydrite $5Fe_2O_3 \cdot 9H_2O$. The evolution of magnetic moment of metastable ferrith and ferrihydrite phases allows investigating a progress of hydration reaction in cement.

Keywords: magnetoelectric coupling, antiferromagnets, ferroelectrics, spin-flop transition

---

We-S-O-03

Tunable magnetic pole inversion in multiferroic $BiFeO_3$-$DyFeO_3$ solid solution

Jiangtao Wu [1], Znzhen Liao [1], Ting Sun [1], Lun-Wei Su [1], Zhaoxiong Xie [3], Zuo-Guang Ye [2], Jian Bi [1], Guangyin Fan [1], Daojiang Gao [1]

[1] *College of Chemistry and Materials Science, Sichuan Normal University, Chengdu, China*
[2] *Department of Chemistry & 4D LABS, Simon Fraser University., Burnaby, Canada*
[3] *State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, College of Chemistry and Chemical Engineering, Xiamen University., Xiamen, China*

In ferromagnets, the magnetic moment can generally be reversed by applying a sufficiently high external magnetic field of opposite polarity. Temperature, on the other hand, is usually known to affect the magnitude of a magnetic moment only, rather than its sign or polarity (most magnets exhibit a monotonic increase in magnetization upon cooling below their magnetic phase transition temperature). As a result, the temperature-induced magnetization reversal (i.e. magnetic pole inversion) remains a very rare phenomenon which lacks proper understanding and explanation because of the extreme difficulties encountered in controlling the thermodynamics of magnetization of classical metal or metal oxide magnets. Herein, we report an unusual magnetic pole inversion behaviour in mutiferroic (1-x)$BiFeO_3$-x$DyFeO_3$ solid solution (alloy), which can be tuned by varying the concentration of the magnetic ion Dy^{3+} in the solid solution. It is found that the temperature-induced magnetic pole inversion occurs in a wide composition range (x = 0.14 - 0.90). Moreover, for the first time in any ferrites, multiple magnetic pole inversions are observed in the solid solution compounds of high Dy^{3+}-concentrations. Our results may provide a better understanding of the temperature- and composition-induced magnetic pole inversion and related phenomena and point to new potential applications for magnetic and multiferroic materials.

Keywords: BiFeO3 solid solution, Multiferroic, Magnetic Pole Inversion, DyFeO3

We-S-O-04

Development of an optical magnetic field sensorbased on Ce and Mn doped $BiFeO_3$ thin films using SPR technique

Anjali Sharma [1], Ayushi Paliwal [2], Monika Tomar [3], Vinay Gupta [2]

[1] *Department of Physics, Atma Ram Sanatan Dharma College, University of Delhi, Delhi, India*
[2] *Department of Physics and Astrophysics, University of Delhi, Delhi, India*
[3] *Department of Physics, Miranda House, University of Delhi, Delhi, India*

Bismuth ferrite (BFO) is the only multiferroic compound which shows simultaneous ferroelectric and G-type antiferromagnetic orders over a broad range of temperature making it appropriate for a variety of novel applications such as spintronics, magnetic field sensors and ultrafast optoelectronic devices. Optical properties of polar multifunctional oxides are also of great importance for possible photonic and photovoltaic applications. Surface Plasmon Resonance (SPR) is the most relevant technique to examine the optical properties of any material and could be easily modified for optical measurements under different ambient conditions. In this report, single phase $BiFeO_3$, Mn doped $BiFeO_3$(BFMO) and Ce doped $BiFeO_3$(BCFO) thin filmshave been fabricated on the surface of Au coated prism using pulsed laser deposition (PLD) technique and their optical properties were studied using SPR.The refractive index dispersion with incident wavelength for all the films is also investigated. Change in optical

properties of BFO, BCFO and BFMO have been determined with changing magnetic field using SPR measurements. The BFMO/Au/prism structure is found to exhibit maximum change in optical properties with magnetic field (sensitivity = 147 °/Tesla), indicating the potential of BFMO thin films for the realization of efficient optical sensor.

Keywords: Surface Plasmon Resonance, BFO, ferroics, magnetic field sensor

---

We-S-O-05

Magnetoelectric and magnetostriction properties in multiferroic composites: A phenomenological approach

Adilson J. A. de Oliveira [1], Alexandre J. Gualdi [1], Fábio L. Zabotto [1], Paulo C. de Camargo [2], Ducinei Garcia [1]

[1] *Physics Department - Federal University of São Carlos, São Carlos, Brazil*
[2] *Institute of Advances and Strategic Studies - Federal University of São Carlos, São Carlos, Brazil*

The multiferroism is characterized by the existence of two or more ferroic orders in matter. Magnetoelectric (ME) materials are the combination of ferromagnetic and ferroelectric orders that present a coupling between the magnetic and electric fields. This property allows to control the magnetic response due to an applied electric field and vice versa. An alternative to obtain multiferroic materials is the production of composite that combine ferroelectric and magnetic materials. The use of magnetostrictive materials as ferromagnetic phase in composites is very important because the mechanical stress applied in ferroelectric phase induces the appearance of magnetoelectric effect. Our group has been study multiferroic composite materials with goal to understand magnetostriction and magnetoelectric effects via magnetization and AC susceptibility measurements using a phenomenological approach. We show that the magnetostrictive behavior of these materials is influenced by the piezomagnetic response and the stress of the piezoelectric matrix [1]. The magnetoelectric response of composites, at low temperatures, can be understood proposing that the ferromagnetic and ferroelectric phases are coupled by the interaction of the spins of the ferromagnetic phase with the composite phonons through spin/lattice relaxation. This assumption expands understanding of ME effect response on dynamic magnetization, based on the magnetic relaxation [2]. These models were applied with successful for (1-x)Pb($Mg_{1/3}Nb_{2/3}$)-x$PbTiO_3$/$CoFe_2O_4$ (PMN-PT/$CoFe_2O_4$) of the 0-3 type magnetoelectric particulate biphasic.

References

[1] A. J. Gualdi et al., J. Appl. Phys. 114, 053913 (2013).

[2] A.J. Gualdi et al., J. Appl. Phys. 119, 124110 (2016).

Keywords: Magnetostriction, Magnetoelectric effect, Composite materials, mutiferroic materials

Wednesday, September 6th, 2017 - Room1 - 13:50 - 14:20

keynote speaker - DOMAINS II

We-S-O-01

(INVITED) Insight into structure, properties, and mobility of ferroelectric domain walls

Nava Setter

EPFL - Swiss Federal Institute of Technology, Lausanne, Switzerland

As interfaces that can be displaced *in-situ,* ferroelectric domain walls are a source of continuous fascination. We have been studying during the past 5 years some of their properties and internal structure and learning how to control domain wall patterns and ultimately functionalize them. Among the obtained results are dense patterns of arrays of domains and domain walls having <10 nm width /periodicity, controlled displacement of domain walls, charged domain walls with metallic conductivity inside the insulating matrix and their controlled creation and density and demonstrated reconfigurability. It has been found also that tailored bent neutral domain walls can be electrically conductive, and this metallic conductivity is sustained to ultra-low temperature (testifying the metallic nature of the conductivity). In addition, we have evidenced ferroelectric boundaries in non-ferroelectric, antiferroelectric materials, evidenced polarization rotation across wide walls, demonstrated ferroelectric switch for propagation of ferromagnetic domain walls at room temperature, and showed the possibility of elastic interaction between non-ferroelastic domain walls, promising new possibilities for domain-wall control.

Keywords: domain wall, domain wall mobility, domain wall patterns, conductivity in domain walls

Wednesday, September 6th, 2017 - Room2 - 13:50 - 14:20

keynote speaker - DESIGN & SIMULATION II

We-S-O-01

(INVITED) Atomistic simulations of relaxor ferroelectrics

Laurent Bellaiche

Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, United States

Relaxor ferroelectrics are characterized by some striking anomalous properties. For instance, they adopt a (frequency-dependent) peak in their ac dielectric response-versus-temperature function while they remain macroscopically paraelectric and cubic down to the lowest temperatures. Furthermore, this dielectric response deviates from the ``traditional'' Curie-Weiss law for temperatures lower than the so-called Burns temperature. Other examples of anomalous properties include the plateau observed in their static, dc dielectric response at low temperature, and the unusual temperature behavior of the Edwards-Anderson parameter. Determining the origin of these intriguing effects has been a challenge to scientists

for more than half a century. The aim of this talk is to report and discuss results of atomistic simulations [1-10] that not only reproduce anomalous features of relaxors but also offer a microscopic insight into the $Ba(Zr,Ti)O_3$ and $Pb(Mg,Nb)O_3$ relaxor ferroelectrics.

References

[1] A. R. Akbarzadeh et al, Phys. Rev. Lett. 108, 257601 (2012).

[2] S. Prosandeev et al, Phys. Rev. Lett. 110, 207601 (2013).

[3] S. Prosandeev et al, Phys. Rev. Lett., 111, 247602 (2013).

[4] D. Wang et al, Nature Communications 5, 5100 (2014).

[5] A. Al-Barakaty et al, Phys. Rev. B 91, 214117 (2015).

[6] S. Prosandeev et al, J. Phys.: Condens. Matter 27, 223202 (2015).

[7] D. Wang, et al, Nature Communications 7, 11014 (2016).

[8] Y. Nahas et al, Phys. Rev. Lett. 116, 127601 (2016).

[9] G. Geneste et al, Phys. Rev. Lett. 116, 247601 (2016).

[10] S. Prosandeev et al, Phys. Rev. B 94, 180102(R) (2016).

Keywords: relaxors, simulations

Wednesday, September 6th, 2017 - Room3 - 13:50 - 14:20

keynote speaker - GROWTH & MATERIALS II

We-S-O-01

(INVITED) Loss of elastic stability and formation of inhomogeneous states at phase transitions in thin films on substrates

Arkady Levanyuk

Department of Physics, University of Washington, Seattle, United States

All the known ferroelectric phase transitions in perovskite crystals are of the first order. However, in thin perovskite films on substrates the same phase transitions look continuous and somewhat smeared. There is no consensus about the reason of this difference. Most of the researchers seem to agree with conclusion of Pertsev et al. (1998) that partial clamping by the substrate converts the first order transition

in $BaTiO_3$ and $PbTiO_3$ crystals into a second order one. Alternatively, Roytburd (2014) argues that constrains on first order transitions provoke two-phase states, not homogeneous second order transition. However, his arguments are relevant only for thick films on substrates while thin films are of the main current interest and the focus of our attention. We demonstrate existence of another mechanism of inhomogeneity: loss of elastic stability due to anomalies of elastic moduli at what would be second order transitions in films on substrates if the assumption about homogeneity were correct. The stability loss occurs independently of the film thickness. Also, we numerically check for inhomogeneity near phase transitions in thin films of various thicknesses accounting for elasticity boundary conditions. Inhomogeneous structures similar to smeared two-phase states are observed in a broad interval of film thicknesses.

Keywords: thin films, phase transitions, loss of elastic stability, two-phase states

Wednesday, September 6th, 2017 - Room4 - 13:50 - 14:20

keynote speaker - ELECTROCALORICS II

We-S-O-01

(INVITED) Inverse barocaloric effects in ferroelectrics

Xavier Moya

Department of Materials Science, University of Cambridge, CB3 0FS, UK, Cambridge, United Kingdom
Departament de Física i Enginyeria Nuclear, ETSEIB, Universitat Politècnica de Catalunya, Diagonal 647, 08028 Catalonia, Barcelona, Spain
Facultat de Física, Departament de la Matèria Condensada, Universitat de Barcelona, Martí i Franquès 1, 08028 Catalonia, Barcelona, Spain

Giant barocaloric effects driven by hydrostatic pressure have been suggested for cooling applications, but they have been traditionally seen only in a small range of magnetic materials that are relatively expensive. Here I will present pressure-dependent calorimetry data to demonstrate giant inverse barocaloric effects in ferroelectric materials that are made of cheap abundant elements.

Keywords: Barocaloric effect, Electrocaloric Effect

Wednesday, September 6th, 2017 - Room1 - 14:20 - 14:45

Invited talk - DOMAINS II

We-S-O-01

(INVITED) Ferroelastic domain wall kinetics: old insights and new observations

A.S. Everhardt [1], S. Zhou [1], N. Domingo [2], G. Catalan [2, 3], B. Noheda [1]

[1] *Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, Groningen, Netherlands*
[2] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC, Barcelona, Spain, Barcelona, Spain*
[3] *Institute of Science and Technology Campus, Universitat Autonoma de Barcelona, Bellaterra, 08193 Barcelona, Spain; 3 ICREA, 08193 Barcelona, Spain, Barcelona, Spain*

Ferroelastic thin films under epitaxial strain relax by forming ordered domain patterns. Domains crucially affect the functional responses of the thin film and, thus, understanding the domain formation mechanisms is of much interest. The thermodynamic laws that determine the size of these domains are well established. However, only recently we are able to grow thin films with enough control in order to test in which cases do ferroelastic thin films behave according to thermodynamics. Indeed, the observed domain widths are often not statistically spread around the expected equilibrium value, nor they are typically related to the presence of random defects. These deviations are generally explained by kinetic effects, but determining such kinetic mechanisms is a challenge. We will show the evolution of ferroelastic domain structures in epitaxial $BaTiO_3$ films grown on $NdScO_3$ substrates during the phase transition between two ferroelastic phases. We observe that the equilibrium domain structure is achieved by halving of the domain widths sequentially as the temperature is decreased, as previously predicted [1]. We will show that this type of domain kinetics can also be inferred from other published reports in different materials. This knowledge can impact in the design of domain wall (DW) functionality: since the DW conductivity reflects the thermodynamic equilibrium oxygen vacancy concentration in the films, walls formed at different stages will show different conductivity. Thus the relative magnitude of conductivity at different DWS can be used to "date" DWs.

[1] E.K.H. Salje, Phase Transitions in Ferroelastic and Co-elastic Crystal, Cambridge University Press (1993).

Keywords: domain walls, memristors, conductivity, thin films

Wednesday, September 6th, 2017 - Room2 - 14:20 - 14:45

Invited talk - DESIGN & SIMULATION II

We-S-O-01

(INVITED) Metallic ferroics: Coexistence of noncentrosymmetry, metallicity, electron correlation and magnetism

Venkatraman Gopalan [1], Shiming Lei [1], Greg Stone [1], Danilo Puggioni [2], Rondinelli James [2], Zhiqiang Mao [3], Xiaoyu Ji [1]

[1] *Pennsylvania State University, University Park, United States*
[2] *Northwestern university, Evanston, United States*
[3] *Tulane University, Tulane, United States*

Metals are defined in condensed matter as materials that possess a Fermi surface. There is a distinct lack of bandgap, and the high electrical conductivity therefore screens the driving force for any polar displacement modes. However, in correlated electronic oxides, one can simultaneously possess a condensed noncentrosymmetric mode as well as a metallic Fermi surface. I will discuss one such material that is a room temperature metal, exhibits polar domains, charged and uncharged domain walls, a metal insulator transition, and magnetism. Thus such materials can possess a remarkable coexistence of polar metallicity, correlation physics, and multiferroicity.

Keywords: Metallicity, noncentrosymmetry, magnetism, electron correlation

Wednesday, September 6th, 2017 - Room3 - 14:20 - 14:45

Invited talk - GROWTH & MATERIALS II

We-S-O-01

(INVITED) Composition and crystallization control in lead-free ceramic and polymer ferroelectrics derived from non-crystalline precursors

Kui Yao [1], Yumei Wang [1, 2, 3], Shuting Chen [1], Weng Heng Liew [1, 2, 3], Kun Guo [1, 2], Chee Kiang Ivan Tan [1], Meysam Sharifzadeh Mirshekarloo [1], Francis Eng Hock Tay [2]

[1] *Institute of Materials Research and Engineering, A*STAR (Agency for Science, Technology and Research), Singapore, Singapore, Singapore*
[2] *Department of Mechanical Engineering, National University of Singapore, Singapore, Singapore*
[3] *NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, Singapore, Singapore*

Our experimental results and analyses on the relationship among the compositions, crystalline structures and properties will be presented for two types of ferroelectric materials: potassium sodium niobate (KNN)-based lead-free ceramics and polyvinylidene fluoride (PVDF)-based polymers, both derived from non-crystalline precursors. The lead-free ceramic films were obtained by chemical solution method and thermal spray method, respectively, with controlled composition and crystallinity, and outstanding piezoelectric performance properties. In the chemical solution method for producing the KNN-based thin films, combinational chemical stabilizing agents were dedicatedly selected and introduced in the precursor solution for effectively suppressing volatile compositional loss; In the thermal spray process for the ceramic thick films, the extremely high melting and cooling rate significantly restricted the volatile loss and decomposition at high temperature. The mechanism of forming the high quality piezoelectric perovskite crystalline phase from the non-crystalline precursors will be analyzed in contrast to that of ceramic synthesis through solid state reaction of the oxide reactants. For the ferroelectric PVDF-based thin films and nanotubes, the crystallization of the polar phase and polarization orientation were controlled by addition of selective hydrated salts and an interesting nano-confinement effect, respectively. Superior piezoelectric performance properties will be highlighted in our nanostructured ferroelectric PVDF-based polymers with highly aligned polarization. The strategy for obtaining the excellent piezoelectric performance properties in the ferroelectric lead-

free ceramic and polymer materials from the non-crystalline precursors will be addressed. Finally, examples of piezoelectric devices realized with our obtained high performance ferroelectric materials will be introduced.

Keywords: Ferroelectric, piezoelectric, crystallization, ceramic, polymer

Wednesday, September 6th, 2017 - Room4 - 14:20 - 14:45

Invited talk - ELECTROCALORICS II

We-S-O-01

(INVITED) Strontium titanate based double perovskites: A new paradigm for high temperature thermoelectrics

Tanmoy Maiti

IIT Kanpur, India, Kanpur, India

Thermoelectric materials are considered as cleanest source of energy generation by converting waste heat into electricity. Recently we investigated wide range of $SrTiO_3$ based double perovskites to evaluate their potential for high temperature thermoelectric applications. In this report, overview of $A_xSr_{2-x}TiBO_6$ (A = Ba, La and B= Fe, Co, Mo) based double-perovskites were presented to understand the role of crystal structure, microstructure, multiple oxidation states of constituent atoms in order to achieve better figure of merit (ZT) for thermoelectric power generation. The thermo-power (S), electrical conductivity (σ) and thermal conductivity (k) were measured in the temperature range 25 K-1273 K. Exceptionally high thermopower (~ 800 μV/K) was obtained in some compositions. On the other hand metal-like electrical conductivity (~105 S/m) was achieved in some of these double-perovskites. It was observed that these oxides invariably demonstrated semiconductor ($d\sigma/dT > 0$) to metal ($d\sigma/dT < 0$) transitions. Manipulating the dopants in A-site and B-site of these $SrTiO_3$ based double-perovskites, both n-type and p-type behaviors were observed. Moreover some compositions exhibited temperature driven p-n type conduction switching along with colossal change in thermopower, which could be useful to develop next generation multifunctional electronic devices like switches, diodes, thermistors. Dielectric study confirmed that these double-perovskites exhibited relaxor ferroelectric like behavior. Moreover, it was shown that inducing dipolar glassy phase due to relaxor ferroelectricity could be an alternative way of designing thermoelectric materials similar to popular “phonon-glass electron-crystal” model.

Keywords: Double Perovskites, Relaxor ferroelectrics, Thermoelectrics, SrTiO3

Wednesday, September 6th, 2017 - Room1 - 14:45 - 16:25

Oral presentation - DOMAINS II

We-S-O-01

Electrostrain enhancement at an "invisible boundary" in a single ferroelectric phase

LUO ZHAO [1, 2], Xiaoqin Ke [1], Xiaobing Ren [1, 2]

[1] *Multidisciplinary Materials Center, Frontier Institute of Science and Technology, Xi'an Jiaotong University, Xi'an, China*

[2] *National Institute for Materials Science, Tsukuba, Japan*

A common method to enhance electrostrain effect of ferroelectric materials is to place the composition to a ferroelectric-ferroelectric phase boundary (often called morphotropic phase boundary). Naturally it would be a surprise if appreciable electrostrain enhancement effect can appear in a single phase, i.e., without a phase boundary. In this talk we report such an unexpected phenomenon. We found electrostrain enhancement appears in a single rhombohedral phase region of $(1-x\%)Ba(Ti_{0.8}Hf_{0.2})O_3$-$x\%(Ba_{0.7}Ca_{0.3})TiO_3$ system. The property enhancement occurs at an "invisible boundary" in the single rhombohedral phase region in the phase diagram, which starts from the quadruple point of the system. Unlike morphotropic phase boundary or polymorphic phase boundary, there is no composition-induced or temperature-induced phase transitions associated with the "invisible boundary". Other property anomalies are also detected at the "invisible boundary", including maximum coercive field. The electrostrain at the "invisible boundary" exhibits better temperature stability as compared with that at a real phase boundary in the same system. The electrostrain enhancement at "invisible boundary" is discussed from Landau model and tricriticality at quadruple point. The "invisible boundary" may provide a new way to enhance electrostrain effect with better temperature stability.

Keywords: electrostrain enhancement, invisible boundary, quadruple point

---

We-S-O-02

Large electrostrains in ferroelectric crystals/ceramics via reversible domain switching

Faxin Li, Qiangzhong Wang, Yingwei Li, Hongchen Miao

College of Engineering, Peking University, Beijing, China

Ferroelectric material based piezo-actuators had been widely used in modern industries due to their quick response, large actuation force, compact size, and the electric-driven style which is more convenient than magnetic driven or thermal driven ones. However, the widely used PZT-based actuators suffered from the rather small actuation strain, typically ~0.1%. Non-180^0 domain switching can cause large strains up to ~1% in $BaTiO_3$ crystals and over 0.5% in PZT ceramics. However, these strains are usually irreversible and cannot be used in actuators. In this work, we firstly realized large actuation strains in ferroelectric single crystals via reversible domain switching under uniaxial electromechanical loading. The reversible strain can be up to 0.93% in $BaTiO_3$ and 0.66% in PMN-PT crystals. However, the crystals turn fractured after several hundred or thousand circles of operation. Recently, we realized large actuation strains up to 0.45% in a domain-engineered PZT ceramics at low field (2 kV/mm). Self-stressing occurs in this hybrid-domain PZT ceramics upon electric loading and the generated stresses

caused back switching upon removing the electric field. The large reversible strain is stable after circles of operation, which is more promising for next generation large-strain actuators.

Keywords: domain switching, actuation, ferroelectric crystal, ferroelectric ceramics

---

We-S-O-03

Polar nature at the domain boundary

Hiroko Yokota [1], Shogo Niki [1], Raphael Haumont [2, 3], Yoshiaki Uesu [4]

[1] *Chiba University, Chiba, Japan*
[2] *Université Paris Sud, Orsay, France*
[3] *Ecole Centrale Paris, Chatenay-Malabry, France*
[4] *Waseda University, Tokyo, Japan*

The recent progress on the high-resolution observation technique guides us towards the new research direction on domain boundary. Now we are able to measure the physical properties of domain boundaries and it turns out that they exhibit different properties from the bulk. For example, the superconductivity, high defect mobility, photovoltaic effect, unusual vortices, and ferroelectricity have been reported in many oxides. Here, we present the second harmonic generation microscope (SHGM) observation results on ferroelastic CaTiO3 single crystal. SHG is very powerful method since it is very sensitive to detect the lack of spatial inversion and time reversal. Using the confocal system with piezo-stage, we are able to construct the three dimensional image of the specimen. Our SHGM observation of CTO single crystal tells that the domain boundary in CTO shows the polar nature. A compressive uniaxial mechanical stress is applied on CTO and the change in the domain structure is observed under the polarizing microscope and SHGM. New domain boundaries appear perpendicular to the original ones under the stress. The SHG microscope observations and analyses confirm that this type of stress-induced domain boundaries are polar similar to the original ones and crystallographically prominent with the monoclinic symmetry m. The quantitative estimation of this stress-induced effect reveals that CTO is hard ferroelastic in the sense that the domain boundary movement requires a large stress. Possible application of this phenomenon is discussed.

Keywords: domain boundary

We-S-O-04

Domain Evolution and Ferroelectric Properties of (1-*x*)$BiFeO_3$-*x*$PbTiO_3$ Single Crystals

Jian Zhuang [1], Alexei Bokov [2], Nan Zhang [1], Zuo-Guang Ye [2, 1], Wei Ren [1]

[1] *Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education & International Center for Dielectric Research, Xi'an Jiaotong University, Xi'an, China*
[2] *Department of Chemistry and 4D LABS, Simon Fraser University, Burnaby, Canada*

As a promising piezoelectric system with high ferroelectric Curie temperature (T_C) and stable perovskite structure, the (1-*x*)$BiFeO_3$-*x*$PbTiO_3$ (BF-*x*PT) binary solid solution has attracted increasing interest as high-temperature piezoelectrics. In this work, a series of BF-*x*PT single crystals with different compositions have been successfully grown using high temperature solution method. Structural characterization by powder *X*-ray diffraction (XRD) shows a crossover with increasing *x* from a dominant rhombohedral *R3c* phase to a pure *P4mm* phase. The T_C determined from the temperature dependence of dielectric constant decreases with increasing PT concentration, from 675 ºC to 525 ºC. By comparing the lattice parameters and T_C of single crystals with those of polycrystalline ceramics, the actual compositions of the as-grown single crystals have been determined. The static domain structures have been studied by various techniques, including etching method, Polarized Light Microscopy (PLM) and Piezoresponse Force Microscopy (PFM). The switching behaviors of domains under electric field and their evolution with temperature have been investigated and discussed using PFM and PLM, respectively. The difference between domain patterns inside and domain structures on the surface of the single crystal platelets supports the existence of a skin layer. In addition, our single crystals of good quality enable the application of high enough electric field to obtain the square-shaped ferroelectric hysteresis loops.

Keywords: (1-x)BiFeO3-xPbTiO3, single crystal, skin effect, domain structures

---

We-S-O-05

Molecular dynamics simulations of polarization ´switching at ferroelectric domain walls

Xiaowei Zeng

University of Texas at San Antonio, San Antonio, United States

Ferroelectrics have a spontaneous polarization that can be switched in direction by applying an external electric field, display coupling between mechanical strain and electric field, and have nonlinear constitutive response. The switchability of ferroelectrics is exploited in the design of non-volatile ferroelectric random-access memories. Since domain walls play an important role in this switching process, the motion of domain walls is critical to the application of high-density non-volatile random-access memory devises. In this research, based on a shell model potential obtained from first principles calculations, molecular dynamics simulations are performed to investigate the domain wall motion of a ferroelectric perovskite under finite temperature and electric field. The process of polarization rotation versus domain wall motion for switching is captured and the domain wall speed has been obtained from the simulation.

Keywords: Polarization switching; domain wall; Molecular Dynamics simulation

---

We-S-O-06

(INVITED) Natural domains of $BaTiO_3$ in ultrahigh vacuum, air and acid: Properties & invariant domain-size proving intrinsic screening and A review of polarization induced conduction

Yukio Watanabe [1], Hiroshi Nakahara [1], Shigeru Kaku [1], Daisuke Matsumoto [2], S.W. Cheong [3]

[1] *Kyushu Univ., Fukuoka, Japan*
[2] *Hitachi Central Lab, Kodaira, Japan*
[3] *Rutgers Univ., New Brunswick, United States*

Conduction at $SrTiO_3/LaAlO_3$[1] is intensively studied. Before this, conduction at clean surface of fully oxygenated $BaTiO_3$ in UHV (ultrahigh vacuum) was reported.[2] This verified conduction at charged domain-boundaries and ferroelectric interfaces.[2] These conductances are too small for electronics but are fundamental for domains, because they screens depolarization field.[3] Using nm-scale and macroscopic probes, we'll clarify ***static*** and ***dynamic properties*** of natural domains of *unpolished* atomically flat surface of fully oxygenated stoichiometric $BaTiO_3$ single crystal in UHV, air, and acid, which are explained by DFT/GL calculations: The electrostatic domain patterns agree excellently with piezoelectric force response images (PFM) with nearly complete screening of electric field from domains of atomically cleaned surface in UHV without extraneous screening. Both $+P_S$ and $-P_S$ surface show conduction: The location of each conduction is titanium of one unitcell deeper than top surface and the outermost oxygen, respectively. The domain patterns in UHV, air and acid are mutually very similar. In particular, we find a perfect agreement of domain patterns obtained by etching and PFM for the first time and invariance of domains of air in acid. The domain size/width in UHV, air, and acid was the same despite 100-times difference of permittivity (screening efficiency) between UHV and acid. These results verify intrinsic screening of depolarization field is inside ferroelectric, consistently with the evidence by conduction.[2] This screening explains the absence of natural vortex domains on free surface and nano-ferroelectrics such as compulsory nano-domain.

[1]Ohtomo-Hwang, Nature427(2004), [2]Watanabe et al, PRL86(2001), [3]Watanabe, PRB57(1998).

Keywords: 2D electron,etching, ferroelectric,depolarization, screening

Wednesday, September 6th, 2017 - Room2 - 14:45 - 16:25

Oral presentation - DESIGN & SIMULATION II

We-S-O-01

Atomic-level understanding of the structure-property connections in perovskite-based ferroelectric systems

Kaustuv Datta [1], Reinhard Neder [2], Jun Chen [3], Andreas Richter [4], Mathias Göbbels [4], Jörg Neuefeind [5], Boriana Mihailova [1]

[1] *Department of Earth Sciences, University of Hamburg, Hamburg, Germany*
[2] *Department of Crystallography and Structural Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg,*

Staudtstra?e 3, Erlangen, Germany
[3] School of Metallurgical and Ecological Engineering, University of Science and Technology Beijing, Beijing, China
[4] Department of Minerologie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Schlossgarten 5a, Erlangen, Germany
[5] Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, United States

Perovskite-based ferroelectric materials are an important class of functional materials and a key topic in materials science. One of the challenges remain however to build rigorous structure-property relationships based on the atomic-level information. In this context, we have applied total elastic scattering technique which manifests pair distribution functions, and inelastic Raman scattering to a series of popular ferroelectric solid solutions such as $BiScO_3$-$PbTiO_3$, $BiMg_{1/2}Ti_{1/2}O_3$-$PbTiO_3$, and $NaBiTiO_3$-$BaTiO_3$, in order to understand the much-debated topic of composition-driven structural phase transitions leading to enhancement of the physical properties at a critical composition, termed as 'Morphotropic Phase Boundary' (MPB). In particular, we have refined structural models implementing reverse Monte Carlo technique against the experimental PDFs to depict the composition-induced structural changes in term of magnitudes and directions of the local polarization vector derived from the analysis of the local environment of the individual cation. Combined with concomitant development of the phonon modes, the results not only provided atomistic features to relate the observed properties, but also a new approach to conceive the structure-property connections for complex ferroelectric systems.

Keywords: Perovskite, ferroelectrics, Pair distribution functions, Raman scattering, structure-property connections

---

We-S-O-02

Investigation of the response of nanoscale ferroelectric material through Molecular Dynamics simulation

Meng Li, Xiaowei Zeng, Ruyan Guo, Amar Bhalla
University of Texas at San Antonio, San Antonio, United States

Over the past decade, the significant development in manufacturing technology enables to obtain nanostructure material in various forms such as ultrathin films, nanowires, nanotubes, and nanoparticles. The extensive use of microelectromechiancal systems (MEMS) and nanoelectromechanical systems (NEMS) in pressure sensors, accelerometers, micromirrors, miniature robots enforces the importance of nanotechnology as one of the major trends in future and a wide range of potential industrial application of ferroelectric nanostructures. Intensive experimental and computational efforts have been made recently to understand the response of ferroelectric nanostructures. However, due to the quantum effects, nanoscale materials show significant differences in mechanical, thermal, electrical, magnetic, or optical properties etc, when compared to their corresponding bulk state. At nanoscale, even a slight atomic displacement strongly affects their properties, leading to critical malfunction of devices in some cases. Thus, a reliable design of nanoscale devices requires a better understanding of the behavior of nanoscale materials. To further elucidate the relation between property and performance of ferroelectric nanostructures, this study aims to investigate the coupling effect of ferroelectric nanostructures under

electric and mechanical fields through molecular dynamics simulation by applying shell model. In this study, the deformation process and the ferroelectric response of ferroelectric nanostructures lead titanate are investigated.

Keywords: Ferroelectric, Nanoscale, Molecular Dynamics, Shell model.

We-S-O-03

Impact of thermal vibrations on polarization reversal: a Monte-Carlo model

Andreas Leschhorn, Herbert Kliem

Saarland University, Germany, Saarbruecken, Germany

To simulate the polarization dynamics of ferroelectrics, the model of local fields is improved by considering thermal vibrations. The local electric field at a dipole is the superposition of the external field, the fields of all other charges and dipoles and the fields of the image charges at the electrodes. The model is based on a sequence of single dipole flips which are thermally activated. The time to flip a single dipole depends on its deterministic transition rate depending on the local field and on a probabilistic factor. In each step, the dipole with the shortest flip time is switched. Thermal vibrations change the distances between the dipoles. The variation of distances modifies the local fields at the dipoles. The extended model considers these variations by multiplying the local fields in each step with Gaussian distributed random numbers. The model is applied to compute the polarization of two and of three dimensional systems based on the barium titanate structure. Polarization switching, hysteresis loops and the decay of the polarization during heating are simulated.The simulations yield intrinsic dead layers close to the electrodes and around defects which cannot be switched even in very strong fields. These nonswitchable layers are nuclei for domains and thus nuclei for polarization switching. The switching time of the system vastly decreases with the amplitude of the thermal vibrations. Moreover, the thermal vibrations enable the polarization switching in low external fields, decrease the coercive fields and cause a sharp phase transition from ferroelectric to paraelectric.

Keywords: simulation, ferroelectric switching, polarization hysteresis, domain growth, defect and dead layer

---

We-S-O-04

Strain and switching behavior in doped BZCT system

Zhen Liu [1, 3], Ruihao Yuan [2], Dezhen Xue [2], Wenwu Cao [1, 4], Turab Lookman [3]

[1] *Condensed Matter Science and Technology Institute and Department of Physics, School of Science, Harbin Institute of Technology, Harbin 150080, China, Harbin, China*

[2] *State Key Laboratory for Mechanical Behavior of Materials,Xi'an Jiaotong University, Xi'an 710049, China, Xi'an, China*

[3] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, Los Alamos, United States*
[4] *Materials Research Institute and Department of Mathematics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, University Park, United States*

The lead-free $Ba(Zr_{0.2}Ti_{0.8})O_3$-x$(Ba_{0.7}Ca_{0.3})TiO_3$ (BZT-*x*BCT) solution has been reported to show excellent piezoelectric performance comparable to that of soft PZT at room temperature (e.g., d_{33} = 580~620 pC/N for BZT-50BCT at room temperature). For the BZT-*x*BCT system, the piezoelectric properties can be further optimized by ion doping. In this work, we consider variants of this system by including additional dopants and develop parameterized phase field simulations to study domain evolution. We investigate switching with increasing field to study factors leading to large piezoelectric enhancement. Our simulation results indicate that the domain rotation behavior can be greatly influence by dopants. Small changes of the elastic constants due to ion doping can lead to about 50% enhancement of the piezoelectric property.

Keywords: dopants, phase field simulation, domain rotation behavior, piezoelectric property

---

We-S-O-05

(INVITED) Room-temperature relaxor ferroelectricity and photovoltaic effects in SnTiO*x*/Si thin film heterostructures

Seungbum Hong [1, 3], Radhe Agarwal [2], Yogesh Sharma [2, 3, 4], Siliang Chang [5], Krishna Pitike [6], Changhee Sohn [4], Serge Nakhmanson [6], Christos Takoudis [5, 7], Ho Nyung Lee [4], James Scott [8], Ram Katiyar [2]

[1] *Department of Materials Science and Engineering, KAIST, Daejeon, Korea, Republic of (South)*
[2] *Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, San Juan, Puerto Rico*
[3] *Material Science Division, Argonne National Laboratory, Lemont, United States*
[4] *Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, United States*
[5] *Department of Chemical Engineering, University of Illinois at Chicago, Chicago, United States*
[6] *Department of Materials Science and Engineering, Institute of Materials Science, University of Connecticut, Storrs, United States*
[7] *Department of Bioengineering, University of Illinois at Chicago, Chicago, United States*
[8] *School of Physics and Astronomy, University of St. Andrews, St. Andrews, United Kingdom*

We studied ferroelectricity and photovoltaic effects in 40-nm-thick $SnTiO_x$ films grown directly onto a p-type (001) Si substrate by atomic layer deposition (ALD). These films showed well-saturated, square, repeatable hysteresis loops with 1.5 mC/cm^2 remnant polarization at room temperature, as detected by out-of-plane polarization versus electric field (P-E) and field-cycling measurements. A photo-induced enhancement in ferroelectricity was also observed as the spontaneous polarization increased under white light. The $SnTiO_x$ films exhibited relaxor characteristics with the dielectric constant peak shifting from ca. T = 600 K at f = 1 MHz to ca. 500 K at 100 Hz. Moreover, our films showed ferroelectric photovoltaic behaviour under the illumination of a wide spectrum of light, from visible to ultraviolet regions. A

combination of experimental and theoretical calculations determined the optical band gap of the $SnTiO_x$ films, which was found to lie in the visible range of the white light spectrum. Our study paves the way for the development of green ferroelectric $SnTiO_x$ thin films that are compatible with semiconducting processes and can be used for various ferroelectric and dielectric applications.

Keywords: Lead-free, SnTiOx, relaxor ferroelectricity, photoferroelectricity, photovoltaic, ferroelectric-semiconductor integration

Wednesday, September 6th, 2017 - Room3 - 14:45 - 16:25

Oral presentation - GROWTH & MATERIALS II

We-S-O-01

Lithium niobate thin films of stoichiometric composition doped with Ho^{3+} ions.

Edvard Kokanyan [1, 2], Anush Movsesyan [1, 2], Marco Bazzan [3]

[1] *Armenian State Pedagogical University After Kh. Abovyan, Yerevan, Armenia*
[2] *Institute for Physical Research, National Academy of Sciences of Armenia, Ashtarak, Armenia*
[3] *Physics and Astronomy Department, Universita di Padova, Padova, Italy*

Stoichiometric composition powders and alkoxide of lithium niobate doped with different concentrations of Ho^{3+} ions were prepared by solid and wet reactions respectively. Thin films of $LiNbO_3$:Ho^{3+} were grown by Sol-Gel method on a sapphire substrate of (001) orientation. The obtained powders and fired alkoxides were investigated by X-ray diffraction analyses and corresponding lattice parameters were obtained. X-ray reciprocal space mapping, which has been recently established as a powerful method for strain and structural characterization of epilayers and heterostructures, was realized on grown thin films of $LiNbO_3$ doped with different concentration of Ho^{3+} (0.1 mol% and 1.0 mol%) ions and having different thickness (130 nm and 300 nm). By comparing the maps obtained from different independent Bragg reflections, the deformation matrix was solved. The lattice parameters of thin films were obtained and compared with those of corresponding powders and bulk crystals.

Keywords: lithium niobate, thin film, X-ray

We-S-O-02

X-ray spectroscopic evidence for the coexistence of ferroelectric and antiferrodistortive orders in $SrTiO_3$ thin films

Cong Lu, Nobuo Nakajima

Graduate School of Science, Hiroshima University, Higashihiroshima, Japan

The ferroelectric order in $SrTiO_3$ (STO) thin films induced by structural transformation and external stimuli such as pressure or bending stress has attracted much attention, since it is expected to be used in lead-free ferroelectric applications. We prepared STO thin films sputtered on various substrates and investigated the local distortion of the films from the electronic point of view by using Ti *K*-edge X-ray absorption spectroscopy. In all the films, the enhancement of the Ti-3*d* e_g pre-edge peak was observed due to the off-center displacement of Ti ions, indicating the potential for ferroelectricity. We also observed two minor changes in the spectra depending on the films: an enhancement of the main absorption edge and a clear separation of the e_g and t_{2g} peaks. A simple model which simulates these features was coexistence of the antiferrodistortive order of TiO_6 octahedra and the local ferroelectric order caused by Ti off-centering.

Keywords: SrTiO3, X-ray absorption spectroscopy, ferroelectricity, antiferrodistortive rotation

---

We-S-O-03

Effects of the deposition temperature of Nd-doped $Bi_4Ti_3O_{12}$ thin films prepared by pulsed laser deposition

Eun Young Kim [1], Sungkyun Park [2], Sang Don Bu [1]

[1] *Chonbuk National University, Jeonju, Korea, Republic of (South)*
[2] *Pusan National University, Busan, Korea, Republic of (South)*

Recently, the deleterious environmental impact of the lead used in many ferroelectric and piezoelectric materials has stimulated research into lead-free alternatives with comparable properties. Bismuth titanate-based materials are considered to be candidates for use as lead-free piezoelectrics. We investigated the $Bi_{3.15}Nd_{0.85}Ti_3O_{12}$ (BNdT) thin film fabricated by Pulsed Laser Deposition (PLD), which is a relatively easy method for fabrication of thin films. The samples were grown on $Pt/Ti/SiO_2/Si$ substrates using a KrF laser (248 nm). To find an optimal condition of this sample, we varied the PLD deposition conditions, including the substrate temperature, oxygen gas pressure, repetition frequency, target-substrate distance and pulse energy density. The BNdT thin films were measured by X-ray diffraction (XRD), Field effect-scanning electron microscope (FE-SEM), T-F analyzer, and Sawyer-Tower Circuit for structural and electrical properties. As the films deposited at different temperature up to 750 □ in our system, the main peak (117) is highest at 700 □. Also, that peak is suddenly increased from 600 □. we found (004) and (006) peaks rose from 650 □. Especially, the second phase is disappeared from 600 □. So we thought the deposition temperature is the most important parameter of BNdT thin films. Unfortunately, we couldn't measure the electrical properties yet. We think because of the effect of Bismuth's volatile property so that we will overcome that problem using the Bi excess in extra experiments.

Keywords: BNdT thin films, PLD,

We-S-O-04

Formation of epitaxial ferroelectric thin films on graphene: mechanism and properties

Wei Liu [1], Bin Zou [1], Olena Shaforost [1], Nicholas Harrison [2], Norbert Klein [1], Neil Alford [1], Peter Petrov [1]

[1] *Department of Materials, Imperial College London, London, United Kingdom*
[2] *Department of of Chemistry, Imperial College London, London, United Kingdom*

The transfer process of graphene onto the surface of ferroelectric thin films is well known. However, for many devices, is required high quality oxide thin films to be grown on the surface of graphene. This step is not understood. It is not clear why the oxide should adopt the epitaxy of the underlying oxide layer when it is deposited on graphene where there is no lattice match. To date there has been no explanation or suggestion of mechanisms which clarify this step. Here we present a mechanism, supported by first principles simulation and structural characterisation results, for the growth of oxide ferroelectric thin films on graphene. We describe the growth of epitaxial $SrTiO_3$ (STO) thin films on a graphene and show that local defects in the graphene layer (e.g. grain boundaries) act as bridge-pillar spots that enable the epitaxial growth of STO thin films on the surface of the graphene layer. In this study, $SrTiO_3$ layers with thicknesses varying from 10nm to 100 nm were deposited using pulsed laser deposition. To measure its electrical properties, the STO film was covered with a 50 nm Au layer using dc magnetron sputtering; and MIM capacitor structures were formed with photo-lithography followed by ion-milling. The surface of the STO film was analyzed using AFM, while its crystal structure was examined by x-ray, SEM and TEM. Results of the electrical measurements carried out within a temperature range of 77K up to 100^{o}C will be presented.

Keywords: SrTiO3 thin films, epitaxial growth on graphene, growth mechanism

---

We-S-O-05

Growth and characterization of PLD grown large area $PbZr_xTi_{1-x}O_3$ thin films

Martando Rath

IIT Madras, Chennai, India

Lead Zirconate Titanate ($PbZr_xTi_{1-x}O_3$) (PZT) is an inorganic ceramic processed at high temperature, and it crystallizes in perovskite cubic structure in its paraelectric phase where Pb^{2+} ions occupy the cube corners, Zr^{4+}/Ti^{4+} ions are at the body center and O^{2-} ions are at the face center positions. Below the Curie temperature, depending on the compositional ratio of Zr/Ti and crystallographic structure, it deforms to rhombohedral (Zr rich) or tetragonal (Ti rich) structure. It has been found that the saturation polarization and piezoelectric coefficient of PZT ceramics are around 40 $\mu C/cm^2$ and 500 pC/N respectively near the morphtrophic phase boundary (MPB). In the present work, ferroelectric large area (20 mm x 30 mm) PZT thin films were grown on (111) oriented Pt coated Si (001) substrate using off-axis pulsed laser deposition (PLD) with a beam-rastering mechanism. In this mechanism, a focused laser beam sweeps across the rotating target which covers the entire 2 inch target surface area. The phase purity of the film was confirmed from X-ray diffraction study. Root means square (RMS) surface roughness of PLD grown PZT thin film were determined to be ~ 5.0 nm using atomic force microscopy. The electrical characterization i.e polarization vs electric field mapping of the PZT thin films was carried

out using ferroelectric loop tracer with gold (Au) as top electrode and piezo force microscopy (PFM). . Results will be presented and discussed in detail.

Keywords: Large area, PLD, Polarization mapping, raster mechanism,PFM

We-S-O-06

(INVITED) Structure and dielectric analysis of hybrid copolymers of PVDF/Metal-Organic frameworks composite film

Hathaikarn Manuspiya, Samanya Paramee

Petroleum and petrochemical college Chulalongkorn University, Thailand, Bangkok, Thailand

A piezoelectric composite is growing in various applications. Generally, metal-organic frameworks (MOFs) with perovskite-like structure, ABX_3, $[(C_3N_2H_5)(M(HCOO)_3)]$ with M= Mn^{2+} and Mg^{2+}, were provided as an appropriate filler to enhance the dielectric constants of composites. Synthesis of $[(C_3N_2H_5)(Mn(HCOO)_3)]$ (ImMn) and $[(C_3N_2H_5)(Mg(HCOO)_3)]$ (ImMg) were prepared using a solution diffusion method at room temperature. TGA technique was performed under N_2 atmosphere and temperatures ranging from 30 - 800 ^oC. Two weight loss steps were observed the removal of imidazolium and M(Mn^{2+} and Mg^{2+})$(HCOO)_2$. Morphology observed from SEM of each MOFs depend on type of metal ion. ImMn exhibits the polygon-like structure while ImMg clearly shows cubic-like structure. Frequency dependent dielectric properties was measured in the range of 10 kHz – 1 MHz. Dielectric constants of ImMg was higher than that of ImMn. However, brittleness and difficult to process limited its application. Poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP)/MOFs composites were fabricated by mixing in brabender and pressing in compression mold. The increment in β-phase crystalline presented with higher amount of MOFs. The dielectric constant showed that the values of composite film were enhanced from 37 of neat PVDF-HFP to 43 with 5 wt.% of ImMn. To further investigate the piezoelectric properties of the PVDF-HFP/MOFs composite, the type of MOFs and volume fraction of MOFs are also optimized.

Keywords: Metal organic framwork, Composite, Dielectric constant, Polyvinylidene fluoride

Wednesday, September 6th, 2017 - Room4 - 14:45 - 16:25

Oral presentation - ELECTROCALORICS II

We-S-O-01

Abnormal electrocaloric effect in the presence of defect dipoles

Yangbin Ma [1], Anna Grünebohm [2], Kai-Christian Meyer [1], Karsten Albe [1], Bai-Xiang Xu [1]

[1] *Technical University of Darmstadt, Darmstadt, Germany*
[2] *University of Duisburg-Essen, Duisburg-Essen, Germany*

In acceptor doped perovskite ferroelectrics, the A site or B site ions can be substituted by ions with a lower valence, e.g., Ti ions in $BaTiO_3$ are substituted by Mn. The associates of the acceptors and the compensating oxygen vacancies form non-switchable or hardly switchable defect dipoles, which shift or pinch the dielectric hysteresis, and might affect or even enhance the electrocaloric effect (ECE) significantly.An analytical model based on the entropy change calculation is utilized to investigate the influence of the defect dipoles on the ECE, while the lattice-based Monte-Carlo simulations are applied to reveal the mechanism on the domain structure level. Additionally, for comparison, the Molecular Dynamics with the effective Hamiltonian are performed. All three approaches confirm that there is a competition between the external field and the internal field induced by the defect dipoles, and when the induced internal field is stronger than the external field, the positive ECE transfers to the negative ECE. More complex phenomena, e.g., the coexistence of the positive ECE and the negative ECE, and the double peak behavior of the ECE, are also revealed. Simultaneously, a modified electrocaloric cycle, which makes use of the negative electrocaloric effect in the presence of defect dipoles, is proposed to enhance the cooling effect.

Keywords: Electrocaloric effect, defect engineering

We-S-O-02

(INVITED) Skyrmion dynamics in multiferroics in the presence of a temperature gradient

Shizeng Lin
Theoretical Division, T-4 and CNLS, Los Alamos National Laboratory, Los Alamos, United States

A magnetic skyrmion is a swirling spin texture discovered recently in magnets without inversion symmetry. Because of their compact size, high mobility and the ability to create or destroy them by electric currents, skyrmions are regarded as promising candidates for applications in memory devices. We study the skyrmion dynamics in multiferroics subjected to a thermal gradient. The thermal gradient generates a spin current that flows from the hot region to the cold region. The spin current interacts with the skyrmion through the spin transfer torque, which drives the skyrmion the hot region to the cold region. When the sample is embedded in a circuit, the motion of skyrmion induces an ac electric current in multiferroic insulators. Our results demonstrate that skyrmions in multiferroics are a promising route for spin caloritronics applications.

Keywords: skyrmion, spin caloritronics

We-S-O-03

Flexocaloric and multicaloric effects in ferroic materials

Avadh Saxena [1], Antoni Planes [2], Teresa Castan [2]

[1] *Los Alamos National Lab, Los Alamos, United States*
[2] *University of Barcelona, Barcelona, Spain*

Flexoferroic materials are materials with interplay between a ferroic property such as polarization or magnetization and the gradient of a mechanical strain. Multi-caloric materials are those that simultaneously exhibit more than one caloric effect, e.g. electrocaloric and magnetocaloric (or barocaloric). Flexoelectricity is one of the most studied effects due to the fact that this effect is allowed by symmetry in any material. We develop the thermodynamics of both the flexoferroic and multiferroic class of materials and apply the results to study flexocaloric and multicaloric effects in solids. Flexocaloric effect is the reversible component of the thermal response of a solid to deformation bending (in general inhomogeneous straining). The two limits of interest correspond to bending performed in isothermal and adiabatic conditions. In the first case, the flexocaloric effect is quantified by the change of entropy of the materials, which is related to the heat exchanged with the surroundings. In the second case it is quantified by the corresponding change of temperature. Very recently a number of studies have considered the possibility of a flexocaloric effect in ferroelectric materials. We address the nature of this phenomenon in ferroic and multiferroic materials.

Keywords: Flexocaloric effect, multicaloric effect, strain gradient, bending, thermodynamics

---

We-S-O-04

Electrocaloric effect in aging ferroelectric samples

Baixiang Xu [1], Yangbin Ma [1], Runqing Yang [1], Zhijian Zhou [2], Xiaobing Ren [2, 3]

[1] *Technical University of Darmstadt, Darmstadt, Germany*
[2] *Xi'an Jiaotong University, Xi'an, China*
[3] *National Institute for Materials Science, Ibaraki, Japan*

In an aged ferroelectric sample, a pinched hysteresis loop is present, the origin of which can be interpreted by the presence of the defect dipoles. The aging behavior influences multiple materials properties. To the best knowledge of the authors, the influence of aging on the electrocaloric effect (ECE) is not investigated. Using a direct calculation approach based on Monte Carlo simulation with a Landau-Ginzburg type Hamiltonian, the ECE of aged $BaTiO_3$ is evaluated. In the simulation setup, the defect dipoles with two opposite directions are placed perpendicular to the external field, which induces a perpendicular internal field. This leads to the phenomena that the characteristic pinched hysteresis loop appears below the Curie temperature T_C, and disappears above T_C. Below T_C, with the field applied the domain configuration is disordered close to the defect dipoles. After field removal, in the vicinity of the defect dipoles, the domain configuration becomes more ordered than with applied field, which leads to the decrease of the configurational entropy. Thus, the positive temperature change under field removal, i.e., the negative ECE, is observed. Above T_C, the initial configurational entropy with field applied is bigger when introducing defect dipoles. After field removal, the final configuration entropy in the case with defect dipoles is similar to the defect-free case. Therefore, the increase of the

configurational entropy is smaller in the case with defect dipoles, which leads to the degeneration of the positive ECE. Simulation results will be compared with experimental data.

Keywords: Aging, Electrocaloric effect

We-S-O-05

Direct measurements of electrocaloric $PbSc_{0.5}Ta_{0.5}O_3$ ceramics

Enric Stern-Taulats [1], Pol Lloveras2 [3], Maria del Barrio [3], Josep Tamarit [3], Lluís Direct electrocaloric measurements are challenging, and so the majority of electrocaloric studies are performed using indirect methods. We present direct measurements of isothermal heat Q and adiabatic temperature change ΔT using a bespoke calorimeter and [2], Antoni Planes [2], Alex Avramenko [1], Neil Mathur [1], Xavier Moya [1]

[1] *Department of Materials Science & Metallurgy, University of Cambridge 27 Charles Babbage Road, Cambridge CB3 0FS, UK, Cambridge, United Kingdom*
[2] *Departament de Física i Enginyeria Nuclear, ETSEIB, Universitat Politècnica de Catalunya, Diagonal 647, Barcelona, 08028 Catalonia, Spain., Barcelona, Spain*
[3] *Facultat de Física, Departament de la Matèria Condensada, Universitat de Barcelona, Martí i Franquès 1, E-08028 Barcelona, Catalonia, Spain, Barcelona, Spain*

Direct electrocaloric measurements are challenging, and so the majority of electrocaloric studies are performed using indirect methods. We present direct measurements of isothermal heat Q and adiabatic temperature change ΔT using a bespoke calorimeter and an ultrafast infra-red camera in the well-known electrocaloric material, $PbSc_{0.5}Ta_{0.5}O_3$ (PST). We find room-temperature values of $|Q| \sim 850$ J kg^{-1} and $|\Delta T| \sim 1.8$ K, for changes in electric field of 13.4 kVcm^{-1}. The values of Q and ΔT determined using these two independent techniques are in excellent agreement with each other, via values of specific heat measured at zero electric field.

Keywords: electrocaloric effect, direct temperature measurement, infra-red, refrigeration, phase transitions

---

We-S-O-06

(INVITED) Enhancement of bulk photovoltaic effect in $BiFeO_3$ thin films by Mn doping

Seiji Nakashima, Kota Takayama, Hironoori Fujisawa, Masaru Shimizu

University of Hyogo, Himeji, Japan

Recently, photovoltaic effect in ferroelerctrics have been attracted much attention because of its high voltage generation. We have investigated bulk photovoltaic effect in single-domain $BiFeO_3$ (BFO) thin films, and have reported that Pt/single-domain BFO/Pt coplanar capacitor with a interelectrodes distance of 260 μm shows open circuit voltage (V_{OC}) of 41 V under a blue-violet laser (λ= 405 nm) illumination. In this study, enhancement of bulk photovoltaic effect in single-domain BFO thin films by Mn doping

was investigated. 1-μm-thick Mn-doped BFO (BFMO) thin films with various Mn-doping amount of 0 – 10 at% were grown by RF magnetron sputtering. Vicinal $SrTiO_3$ (STO) (001) with vicinal direction and angle of <110> and 4°, respectively, was used as a substrate for growing single-domain BFMO thin films. Pt electrodes were deposited on BFMO thin films, and Pt/BFMO/Pt coplanar capacitors with interelectrodes distance of 260 μm were prepared. I-V characteristics of the Pt/BFMO/Pt coplanar capacitors were measured under blue-violet laser illumination. Maximum V_{OC} of 287 V was found in Pt/1-at%-doped BFO/Pt coplanar capacitor at RT. This value corresponds to electric field of 11 kV/cm.

Keywords: BiFeO3, bulk photovoltaic effect, thin films

Wednesday, September 6th, 2017 - Poster Room - 16:30 - 18:30

Poster session - Poster Session 2

We-S-P-01

Preparation, characteristics and temperature as well as frequency dependence dielectric and complex impedance spectroscopic studies on composite multiferroic of $PbTiO_3$ – $SrFe_{12}O_{19}$

Krishan Kumar Bamzai

Crystal Growth & Materials Research Laboratory, Department of Physics and Electronics, University of Jammu, Jammu, India

Multiferroic composite, such as ferromagnetic – ferroelectric heterostructures offer a novel route for integrating ferroelectric and ferromagnetism which can produce large magneto-electric (ME) effect due to coupling interaction between the constituent phases. Single phase multiferroic materials possess ferroelectric and magnetic ordering in the same phase, thus the choice of single phase multiferroic exhibiting coexistence of strong ferro - / ferrimagnetism and ferroelectricity is limited. With a view to understand the multiferroic composite phenomenon, lead titanate as a ferroelectric phase and strontium hexaferrite as ferromagnetic phase was taken in the present investigations. This multiferroic composite with general formula (x)PbTiO3 - (1-x)SrFe12O19 (where x = 0.10, 0.30 and 0.50) was prepared using solid state sintering method. Lead titanate and strontium hexaferrite phase formation was identified using X-ray diffraction technique, thus establishing diphase system without any secondary phase. Calculation of lattice parameter shows that the composite prefers hexagonal structure. The morphology of the formation of composite was seen through scanning electron microscopic technique. The morphological investigations show that the composites are dense, have fewer pores and ferroelectric grains are homogenously distributed in the ferrite matrix. The ferroelectric and ferromagnetic grains are identified on the basis of energy dispersive spectroscopy (EDS) studies. The magnetic behavior of the composites at room temperature display magnetic hysteresis loop, indicating that the composites are ferromagnetic. The value of saturation magnetization decreases with increase in ferroelectric content from x = 0.10 to 0.30, whereas for x = 0.50 it shows an increase. The magneto-capacitance shows a decrease in its value due to magnetostriction.

Keywords: Multiferroic, lead titanate, strontium hexaferrite, electric properties, magnetic properties.

We-S-P-02

Diisopropylammonium halides – new family of lead-free ferroelectric materials

Anna Piecha-Bisiorek, Ryszard Jakubas

Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland

The poster deals with a member of the halide derivatives of diisopropylammonium abbreviated as DIPA. This family presents a practical interest due to its spectacular dielectric properties. Namely, DIPA bromide discovered simultaneously by two groups: Xiong R. –G. (Science, 2013, 339, 425.) and Jakubas R. (Cryst. Eng. Comm., 2013, 15, 940), possesses the spontaneous polarization about 23 $\mu C \cdot cm^{-2}$ which is the highest among organic ferroelectrics and is comparable with classical inorganic ferroelectrics. The DIPA derivatives are, thus, attractive for further studies, and are potential candidates for superseding the lead-based toxic inorganic ferroelectrics which are widely used till now. The results obtained for iodide analog (DIPAI) are surprising and qualitatively different from those for the remaining compounds. Although the dielectric response is typical for a ferroelectric phase transition, when approaching the unique phase transition (T_c = 364 K) from below, the spontaneously polarized phase does not occur. Instead, the system transforms into another phase of a symmetry that is not group-subgroup related to the initial phase. A particular attention has been paid to the elucidation of the mechanism of the phase transition where in spite of a strong dielectric response a spontaneously polarized phase does not occur. The assembly of experimental data has allowed us to propose a general symmetry-based scheme of the related phenomena observed in the whole family of compounds. The proposed phenomenological Landau-type theory explains the mechanism of this behaviour in a unified way encompassing all the members of the diisopropylammonium family.

Keywords: diisopropylammonium, ferroelectric, phase transition

---

We-S-P-03

Order-disorder phenomenon in a ferroelectric Jahn-Teller phase transition

Jiri Hlinka

Institute of Physics, Czech Acad. Sci., Prague, Czech Republic

Possibility of ferroelectric Jahn-Teller phase transitions was largely neglected in the ferroelectric community so far. Only very recently a nice example has been demonstrated in the crystal of GaV_4S_8 and in closely related materials. Here we shall address the mechanism and the order-disorder nature of this ferroelectric Jahn-Teller phase transition in terms of a simple phenomenological model. Discussion will be supported by comparison with the results of recently available spectroscopic studies, partly reported in a recent publication[1].

This work was supported by the Czech Science Foundation (Project GACR 17-11494J).

References

[1] J. Hlinka, F. Borodavka, I. Rafalovskyi, Z. Docekalova, J. Pokorny, I. Gregora, V. Tsurkan, H. Nakamura, F. Mayr, C. A. Kuntscher, A. Loidl, S. Bordács, D. Szaller, H.-J. Lee, J. H. Lee, and I. Kézsmárki, Phys. Rev. B 94, 060104(R) (2016).

Keywords: Jahn-Teller effect, order-disorder phenomenon

We-S-P-04

Flexible crystals of perovskite-like coordination polymers with tunable and switchable organic guests

Magdalena Rok, Grazyna Bator

University of Wroclaw, Faculty of Chemistry, Joliot-Cure 14, 50-383, Wroclaw, Poland

A family of the cyano-bridged coordination polymers (CPs), which undergo a phase transition between high and low dielectric states upon thermal stimulus, are promising materials for potential application in electrical and electronics devices. The inorganic cage compounds, with the organic guest molecules as cations, may give materials, where solid-to-solid phase transitions with different nature like order-disorder or displacive-type can be observed. The carefully designed guest/host materials, where into well-matched host framework the switchable guest is placed, leads to crystals with interesting physicochemical properties, i.e. the large dielectric/magnetic susceptibility, spontaneous polarization and/or non-linear optical ones. We would like to present the dielectric, optical and thermal properties of the novel crystals, which are classified as an elpasolite family. These materials have a double perovskite-type structure, ones the cage framework is formed (with the general formula: $A'_4A''_4(CN)_{12}$, A'-monovalent metal, K^+, and A''-trivalent metal, Fe^{3+}/Co^{3+}) the cationic organic guest are embedded in the cage. We would like to prove that the mechanism of the phase transition is related both to a change in dynamics of cations and a deformation of the inorganic structure. It is worth to highlight that in our work not only the cationic/guest but also anionic/host-framework dynamics has been described and the appropriate models of the molecular disorder are proposed. The detailed analysis of the structural properties allows us to describe a correlation between the microscopic structure and the dielectric and optical properties of the crystals.

Keywords: dielectric properties, guest/host crystal, phase transition

---

We-S--05

Keywords:

We-S-P-06

On the influence of the synthesis temperature on the fluorescence dependence of doped PVDF/Er films

Evaristo Falcao [1, 2], Glauciane Leite [1], Eriton Botero [1], Ruyan Guo [2], Amar Bhalla [2]

[1] *Federal University of Grande Dourados, San Antonio, United States*
[2] *University of Texas at San Antonio, San Antonio, United States*

Ferroelectric polymers as PVDF has attracted great interest in photonic area because of the possibility to be usefull as hosts for rare-earth ions. However, their preparation parameters, as temperature and time of drying can influence the fluorescence of the samples. Although, few works can be found in the literature concerning the study of the fluorescence in ferroelectric materials. In this way, PVDF samples were doped with erbium oxide to verify the improvement in the optical fluorescence of the polymeric matrix. The FT-IR measurements confirmed the incorporation of dopant in the polymeric matrix host. The optical measurements in those samples shonw a dependence of fluorescence intensity as a function of the synthesis temperature. This behavior can be related to the losses of the ferroelectricity of PVDF as a function of the temperature. In summary, the experimental results revealed that the ferroelectric PVDF/Er is a potential candidate for optical and photonic applications.

We are grateful to the Brazilian Agencies, CAPES, CNPq (process 483683/2010-8 and 208232/2014-1), for the financial support of this work. E. A. Falcão also acknowledges UTSA and MeMDRL for hosting him under the NSF/INAMM and NSF ECCS 1002380 programs.

Keywords: PVDF, Optical Fluorescence, Erbium, Optical Properties

---

We-S-P-07

Improvements of the PVDF fluorescence spectrum caused by Nd and Ce addition

Evaristo Falcao [1, 2], Lais Aguiar [1], Eriton Botero [1], Claudio Carvalho [1], Ruyan Guo [2], Amar Bhalla [2]

[1] *Federal University of Grande Dourados, Dourados, Brazil*
[2] *University of Texas at San Antonio, San Antonio, United States*

Poly(vinylidene fluoride) (PVDF) possesses large application in technological areas due to ferroelectricity, that permits their use as electro-mechanical and electro-thermal transducers, speakers, sensors and to stimulate the growth of bone tissue in animals. However, in the last years the researchers are giving attention to the possibility of their use as a host for rare earth ions to be used in optical devices. Though, in certain cases it becomes necessary the utilization of ligands to promote the process of energy transfer from ligand to rare earth ions to get some improvements in the fluorescence spectra. In this sense, this work presents a study of the optical properties of PVDF doped with 2-amino terephthalate (AMT), Nd-AMT and Ce-AMT. The measurements of FT-IR confirmed the incorporation of dopant in the polymeric matrix. In the optical measurements in PVDF doped samples was observed a broadening in absorption as well as the fluorescence spectra with the increase of the Nd-AMT and Ce-AMT content.

In summary, the experimental results revealed that the PVDF/Nd-MCA is a potential candidate for optical and photonic applications.

We are grateful to the Brazilian Agencies, CAPES, CNPq (process 483683/2010-8 and 208232/2014-1), for the financial support of this work. E. A. Falcão also acknowledges UTSA and MeMDRL for hosting him under the NSF/INAMM and NSF ECCS 1002380 programs.

Keywords: PVDF, Optical Properties, Fluorescence

We-S-P-08

Study of the phase transition in PLZT samples by the Interferometric Method

Evaristo Falcao [1, 4], Ivair Santos [2], Jose Pereira [2], Alysson Steimacher [2], Antonio Medina [2], Mauro Baesso [2], Jose Eiras [3], Garcia Ducinei [3], Ruyan Guo [4], Amar Bhalla [4]

[1] *Federal University of Grande Dourados, Dourados, Brazil*
[2] *Universidade Estadual de Maringá - UEM, Maringa, Brazil*
[3] *Universidade Federal de Sao Carlos, São Carlos, Brazil*
[4] *University of Texas at San Antonio, San Antonio, United States*

Transparent ferroelectric ceramic lanthanum modified lead titanate zirconate ceramic or (PLZT) presents high optical transmittance, ranging from 0.37 up to 6.5 μm that have a wide range of application for different in optical area. It is possible to find some reports showing the use of PLZT as host for rare earth to be applied as photonic material. In this way, the thermo-optical properties such as the temperature coefficient of the optical path length change (ds/dT) plays an important rule to evaluate the figure of merit of optical materials. Therefore, in this work it was used the Optical Interferometric Method to determine the ds/dT parameter of the PLZT samples as a function of temperature. The experimental results shown a peak at 96 °C for PLZT 9/65/35 and a peak at 86 °C for PLZT 9/65/35 that were related to the maximum temperature of the dielectric constant (Tm) of these materials. The results shown that the IO can be used to determine the phase transition in transparent ceramic samples.

Acknowledgement: We are grateful to the Brazilian Agencies, CAPES, CNPq (process 483683/2010-8 and 208232/2014-1), for the financial support of this work. E. A. Falcão and I. A. Santos also acknowledges UTSA and MeMDRL for hosting him under the NSF/INAMM and NSF ECCS 1002380 programs.

Keywords: PLZT, Optical Interferometry, Thermo-Optical Properties

---

We-S-P-09

Temperature dependent magnetoelectric and magnetodielectric response of multiferroic cobalt ferrite and Pb(Zr,Ti)O3 multilayered structure

Brandon Young

University of Texas at San Antonio, San Antonio, United States

Multiferroic and magnetoelectric materials have become increasingly popular due to the functionality they could provide in the sensing and medical fields. Single-phase multiferroic/magnetoelectric materials are incapable of large responses due to limitations imposed by various physical constraints. Multiphasic multiferroic/magnetoelectric materials are able to produce outputs many orders of magnitude higher than their physical counterparts as they rely on the coupling between the magnetostrictive and piezoelectric phases. These multilayered structures possess their own unique problems such as difficulty of deposition, and serial electrodes reducing dielectric performance. The effect of temperature on the magnetoelectric response of these multilayered multiferroics has not been thoroughly studied. The temperature dependence of the magnetodielectric and magnetoelectric properties of a $CoFe_2O_4$/PZT/$CoFe_2O_4$ trilayer laminate structure has been investigated. The experiments where performed using an AC magnetic field of 5 Oe, with increasing DC magnetic field biases. The measurements were taken at three temperature conditions: room temperature, the temperature decreasing slowly to 100 K, and then increasing the temperature up to room temperature again.

Keywords: Multiferroics, Magnetoelectrics, Multilayered Magnetoelectric,

---

We-S-P-10

Upconversion in co-doped SBN for supercontinuum light generation

Moumita Dutta [1], Michael Williams [2], Rohit Prasankumar [2], Amar Bhalla [1], Ruyan Guo [1]

[1] *The University of Texas at San Antonio, San Antonio, United States*

[2] *Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Albuquereque, United States*

SBN:60 crystal grown by the Czochralski method with a doping concentration of 0.03%weight (0.015% Cr : 0.015% MO) when excited with 800 nm Ti:Sapphire femtosecond laser pulses, found to emit light with wavelengths varying across the entire visible range. The emitted light can be tuned both by the intensity and the polarization of the excitation beam. The upconverted emission is polarized and of appreciable intensity. While the unpoled crystal gives planar SHG, the upconversion gives conical emissions. The novel phenomena are attributed to the level splitting due to double doping at the B-site along with localized trapping centers formed by the donor and acceptor concentration gradient.

Keywords: Upconversion,SBN,Supercontinuum,ferroelectric

We-S-P-11

Structure and properties of $Pb(Mg_{1/4}Nb_{1/2}Ti_{1/4})O_3$ nanodots from first principles

Abdullah Albarakati [1], Sergey Prosandeev [2, 3], Dawei Wang [4], Laurent Bellaiche [2]

[1] *Physics Department, Umm Al-Qura University, Makkah, Saudi Arabia*
[2] *Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, United States*
[3] *Research Institute of Physics, Southern Federal University, Rostov on Don, Russia*
[4] *School of Electronic and Information Engineering and State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, China*

Relaxor ferroelectric systems (bulk/nanostructure) are very important because of their unusual properties and potential applications [1,2]. Atomistic simulations can reveal many interesting features of bulk or nanostructured materials that may lead to new applications [3,4]. In this study, Monte-Carlo (MC) and Molecular Dynamics (MD) methods, within the framework of Effective Hamiltonian (Heff), are used to simulate $Pb(Mg_{1/4}Nb_{1/2}Ti_{1/4})O_3$ nanodots (PMN-25PT NanoDot) for various cases, such as the size of nanodots and the distribution of B-site atoms. We summarize our work as the follows. First, we extend the Heff developed in reference [5] to include the influence of surfaces by adding terms that characterize the interaction of surfaces with local dipoles and strains. Second, we perform MC and MD simulations under ideal open circuit condition from high to low temperature for various nanodots. During each simulation, the size of dots, the distribution of B-site atoms, and the temperature are kept fixed. The outputs of our simulations are local mode u (which are directly proportional to polarizations) and strains. Third, we compute static/dynamic dielectric susceptibilities, toroidal and hyper-toroidal moments as well as their susceptibilities using the methods shown in reference [6]. Results of these MC/MD simulations reflect the importance of the size of nanodots and the distribution of B-site atoms. These results will be discussed in details.

This work is supported by King Abdulaziz City for Science and Technology under grant number 11-NAN1414-10 and ONR Grant N00014-12-1-1034.

Keywords: effective Hamiltonian, perovskite PMN-xPT, Nano structure, Monte-Carlo, Molecular Dynamics

---

We-S-P-12

Physical, electrical and magnetic properties of ferrite modified PZT-based composite ceramics

Jiradtakeat Dechawuttikul [1], Anurak Prasatkhetragarn [1], Pongsakorn Jantaratana [2], Rattikorn Yimnirun [3]

[1] *University of Phayao, Phayao, Thailand*
[2] *Kasetsart University, Bangkok, Thailand*
[3] *Suranaree University of Technology, Nakhon Ratchasima, Thailand*

Composite materials of $(1-x)PZT-(x)Fe_2O_3$, when x = 0.1, 0.3, 0.5, 0.7 and 0.9, were prepared by solid-state reaction technique. PZT powder was first synthesized with calcination temperature of 900 °C in air. Phase formation, densification, morphology and magnetic properties of $(1-x)PZT-(x)Fe_2O_3$ composites were investigated and discussed. The XRD technique was used to analyze the phase formation behavior. Fe_2O_3 reach phase was found with increasing Fe_2O_3 content. Interestingly, for high sintering temperature of 1100 °C, the major gramma - Fe_2O_3 phase was found for all Fe_2O_3 substitution

in PZT system. Densities of the sintered specimens tend to decrease with increasing Fe_2O_3 content. In addition, the superparamagnetic behaviors were observed using a Vibrating Sample Magnetometer (VSM), which reached maximum value at x = 0.7. More importantly, Fe_2O_3 addition has been found to affect the phase formation, microstructure and ferromagnetic properties of PZT ceramics.

Keywords: microstructure, magnetic properties, composite ceramics, PZT-Fe2O3

We-S-P-13

Study on dielectric and magnetic properties of the organic-inorganic hybrid layered structure halide material

Yonghwan Kim, namjung hur

Inha university, phsics, Incheon, Korea, Republic of (South)

Organic-inorganic hybrid materials with the layered perovskite structure were known to have the possibility of the multiferroicity. In the unique layered structure consisting of organic layers and inorganic layers, the symmetry of organic molecules determines the electrical properties, and the magnetic properties depend on the magnetic ordering in metal-halogen octahedral layers. Therefore, physical properties of these hybrid materials depend on the type of organic molecule and composition of metal halide octahedral site. Here, we studied dielectric and magnetic properties of various organic-inorganic hybrid materials including $(CH_3NH_3)_2MnCl_4$ and $(C_6H_5CH_2NH_3)_2CuCl_4$ to search for new type of multiferroic materials.

Keywords: layered perovskite structure, halide, metal-organic frameworks, magnetism, dielectric properties

---

We-S-P-14

Environmental friendly $SrTi_{1-x}Mo_xO_3$:15Nb perovskites for high temperature thermoelectric applications

Mandvi Saxena, Ritwik Banerjee, Tanmoy Maiti

Plasmonics and Perovskites Laboratory, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, Uttar Pradesh, India 208016, Kanpur, India

Thermoelectric (TE) power generator generally consists of p-type and n-type thermoelectric elements, which are connected thermally in parallel and electrically in series. There are not many options available among oxide-based materials at present to choose as n-type element in the thermoelectric module. Nb doped $SrTiO_3$ ($SrTiO_3$: Nb) has show lot of promises as an n-type thermoelectric material. Recently, authors have reported that molybdenum can be used to increase the electrical conductivity of $SrTiO_3$ perovskite. In the present work, we have doped Mo in place of Ti in $SrTiO_3$:15%Nb in anticipation of increasing its electrive conductivity which can pave way for attaining higher ZT values. Polycrystalline

samples of $SrTi_{1-x}Mo_xO_3$:15Nb (0 x 0.3) have been synthesized by solid-state reaction process. Sintering has been done at 1673-1773 K under reducing atmosphere. X-ray diffraction pattern has confirmed single phase solid solution. Scanning electron microscopy has confirmed dance microstructure. Seebeck coefficient and electrical conductivity have been measured from room temperature to 1173 K. Conductivity mechanism of these perovskites has been found to be governed by variable range hopping model.

Keywords: Perovskits, Oxides, Thermoelectric, SrTiO3

We-S-P-15

Relaxor ferroelectric $Ba_xSr_{2-x}TiCoO_6$ double perovskite material for high temperature thermoelectric application

Nirma Kumari, Mandvi Saxena, Pinku Roy, Tanmoy Maiti

Plasmonics and Perovskites Laboratory, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, Uttar Pradesh, India 208016, KANPUR, India

In this work, thermoelectric property of double perovskite $Ba_xSr_{2-x}TiCoO_6$(BSTC) materials has been studied. $Ba_xSr_{2-x}TiCoO_6$ for $0 \leq x \leq 0.2$ ceramic samples were synthesized by solid-state reaction route. Phase purity, crystal structure and elemental composition were confirmed by XRD and SEM/EDS respectively for those samples. Average grain size, grain orientation and distribution were investigated by EBSD. Dielectric measurements were carried out for all BSTC samples in the range of 10 K - 700 K. Frequency dispersion behavior in the dielectric constant and dielectric lost curve suggested the relaxor behavior in samples. Seebeck coefficient and electrical conductivity of BSTC were measured in the temperature range of 300 K to 1273 K. Maximum value of Seebeck coefficient achieved was 345 μV/K at 1222 K for BSTC with x = 0.15 and positive Seebeck coefficient which indicate p-type semiconductor behavior. Thermal conductivity of BSTC samples was measured in the temperature range of 300 K to 1250 K. Thermal conductivity of all BSTC samples varied from 0.01 W/mK to 0.55 W/mK. Maximum dimensionless TE figure-of-merit ZT obtained was 0.29 at 1223 K for BSTC composition with x = 0.2. Further p-type behavior of samples was confirmed by X-ray Photoelectron Spectroscopy (XPS). It happens due to variation in oxidation state of Ti and Co both. We have shown that dipolar glassy phase induced by relaxor ferroelectric in BSTC results in low thermal conductivity. Hence a very good figure of merit ZT values was obtained.

Keywords: Double Perovskites, Dielectric,Thermoelectric,oxides

---

We-S-P-16

Metal-like electrical conductivity in double perovskite $A_xSr_{2-x}TiMoO_6$ (A = La, Ba) oxides for high temperature thermoelectric power generation

Mandvi Saxena, Tanmoy Maiti

Plasmonics and Perovskites Laboratory, Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, Uttar Pradesh, India 208016, Kanpur, India

Recently oxides have been used as thermoelectric materials with a good combination of several parameters such as high Seebeck coefficient, good electrical conductivity and low thermal conductivity. Oxides materials, in general, demonstrate high Seebeck coefficient, however they suffers from low electrical conductivity. Hence, electrical conductivity of oxide materials need to be improved for developing efficient thermoelectric devices. In the present work, the thermoelectric properties of La and Ba doped Sr_2TiMoO_6 (STM) double perovskites have been studied. Polycrystalline samples of these double perovskites have been synthesized by solid-state reaction process. Sintering has been done at 1573 - 1673 K under reducing atmosphere. X-ray diffraction has confirmed single phase solid solution. Seebeck coefficient and electrical conductivity have been measured from room temperature to 1273 K. These compounds have high electrical conductivity in the range of 10^4 - 10^5 S/m at room temperature and have large carrier concentrations ($\sim 10^{22}/cm^3$) which are generally found in metals. These oxides exhibit p-type to n-type conduction switching at higher temperature. To evaluate the source of charge carries and oxidation state of cations in these double perovskites XPS measurement has been carried out. Temperature dependent Seebeck coefficient has been explained using an analytical model for coexistence of high mobility electrons and low mobility oxygen vacancies in these oxides. Conductivity mechanism of these double perovskites has been found to be governed by small polaron hopping model.

Keywords: Double perovskite, Oxides, Thermoelectric

We-S-P-17

Gamma-ray irradiation effects on the ferroelectric domain structure of epitaxial $Pb(Zr_{0.52}Ti_{0.48})O_3$ thin films

Sang Don Bu, Sam Yeon Cho, Eun Young Kim

Chonbuk National University, Jeonju, Korea, Republic of (South)

Ferroelectric thin films have attracted considerable attention because they are used for non-volatile ferroelectric random access memories (FERAM). In particular, as the development of the aerospace industries, investigation on ferroelectric domain behavior of memory devices in exposed to high-energy radiation such as in space is required. In previous study, the ferroelectric thin films has been reported degradation behavior of polarization and dielectric properties by gamma-ray irradiation. Therefore, we investigated a change in the ferroelectric domain structure of epitaxial $Pb(Zr_{0.52}Ti_{0.48})O_3$ (PZT) thin films by gamma-ray irradiation. Epitaxial PZT thin films were prepared on the $SrRuO_3/SrTiO_3$ (001) substrates by using a sol–gel method with a spin-coating process. The x-ray diffraction analysis show that fully c-axis oriented epitaxial PZT films were grown. The prepared epitaxial PZT thin films were subjected to gamma-ray radiation with various total doses. Piezoelectric force microscopy (PFM) is employed to study the ferroelectric domain structure in epitaxial PZT thin films. We have prepared 3 μm x 3 μm square patterns in PZT films, which areas were formed through the electrical poling with the cantilever by applying a + 5 V dc bias. By combining the perpendicular and in-plane piezoresponse data, we found that the ferroelectric domain structure is mainly described by one polarization directions. There patterns were investigated a change in the ferroelectric domain structure by repeated PFM

measurements with various irradiation total doses. Based on these results, gamma-ray irradiation effects on ferroelectric domain structure in epitaxial PZT thin films will be discussed.

Keywords: Gamma-ray irradiation effects, Ferroelectric thin films

---

We-S-P-18

Ferroelectric-based synapse devices with oxide heterostructure

Joonbong Lee [1], Hojin Lee [1], Yeogyun Yoon [1], Youjung Gill [1], Yunseok Kim [2], Taekjib Choi [1]

[1] Hybrid Materials Research Center, Department of Nanotechnology and Advanced Materials Engineering, Sejong University, Seoul 05006, South Korea, Seoul, Korea, Republic of (South)
[2] School of Advanced Materials Science and Engineering, Sungkyunkwan University, Suwon 16419, South Korea, Suwon, Korea, Republic of (South)

Ferroelectric polarization related charge transport have been utilized for novel electronic devices, such as ferroelectric tunnel junction, switchable diode, and ferroelectric memristor. Recently, ferroelectric-based oxide heterostructure has been proposed for synapse device that exhibits a high on/off ratio, low power consumption and short process time. In ferroelectric-based synapse devices, gradual electroresistive modulation is associated with change of ferroelectric domain configuration, providing the controllability of the electric conductance for the effective operation of synapse devices. In this work, we fabricated a ferroelectric-field-effect transistor based synapse devices with channel layer of metal to semiconducting transition (MST) oxide. Ferroelectric polarization reversal can control the amount of applied energy to MST oxide phase transition and channel conductance at the same time. Our ferroelectric heterostructure with analog-like electroresistive modulation is highly desirable for realizing a new synapse device.

Keywords: Synapse device, Ferroelectric, Metal-Semiconducting transition, ferroelectric-field-effect transistor, Oxide heterostructure

---

We-S-P-19

Enhanced thermoelectric figure of merit in environment friendly nanocomposite of $SrTi_{0.85}Nb_{0.15}O_3$ and graphene oxide for clean energy generation

Tanmoy Maiti [1], Pinku Roy [2], Farheen Anjum [3]

[1] IIT Kanpur, Kanpur, India
[2] IIT Kanpur, Kanpur, India
[3] IIT Kanpur, Kanpur, India

n-type thermoelectric material with good Figure of Merit ($ZT = S^2\sigma T/k$) is need of the hour to design a thermoelectric power generator which consists of p-type and n-type TE module connected electrically in series and thermally in parallel configuration. In this investigation we report high temperature

thermoelectric properties of $SrTi_{0.85}Nb_{0.15}O_3$ (STN) and Graphene Oxide (GO) nanocomposites prepared via Spark Plasma Sintering (SPS). The oxidation state of Ti and Nb in these ceramics were studied by XPS. Rietveld refinement of these oxides defined them as cubic crystal with *Pm*-3*m* space group. TEM study confirmed the existence of GO in the grains as well as in the grain boundaries of these nano composites. The temperature dependent electrical conductivity of pure STN exhibits semiconducting nature ($d\sigma/dT > 0$) from room temperature to 1223 K. Addition of little amount of GO in the matrix causes increase in the electrical conductivity however, with further increase in wt% GO, electrical conductivity changes in the order of 10^2 with metal like behaviour ($d\sigma/dT < 0$), without major change in Seebeck coefficient (ranges between -80 μV to -180 μV) and resulted maximum power factor of 1300 $\mu W/mK^2$ for 1.5 wt% GO. The Seebeck coefficient was negative throughout the temperature range of measurement, indicating n-type behaviour. The thermal conductivity was measured to calculate the ZT value of these nano composites and maximum ZT of more than 1 was observed. Further the conduction mechanism in the composites were discussed by Variable Range Hopping and Small Polaron hopping mechanisms.

Keywords: Thermoelectrics, Oxide electronics.

We-S-P-20

Synthesis of orthorhombic SnO_2 and effect of the cerium doping on the structural properties

Ernesto Pereira, Maria Helena Costa, Adilson de Oliveira

Federal University of Sao Carlos, Sao Carlos, Brazil

The SnO_2 is an intrinsic n-type semiconductor that at ambient pressure commonly crystallizes as cassiterite, which has the rutile structure with tetragonal symmetry (space group P42 / mnm). Another polymorph of SnO_2 is with the orthorhombic structure which is a metastable phase originally obtained in experiments with high pressures and temperature. In this work, we have investigated the formation of the orthorhombic phase of α-PbO_2-type SnO_2 in the nanoparticle system x = 0, 0.05, 0.1 and 0.3 synthesized at 750 °C in an air atmospheric by the Pechini's method. We studied the formation of the α-PbO_2-type phase as a function of the synthesis temperature and Cerium concentrations. The structural and morphological characterization was performed using experimental techniques such as X-ray diffraction (XRD), allied to the Rietveld refinement, field emission scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM). The reflections in the XRD pattern and clear lattice fringes observed by HRTEM confirm the formation of the orthorhombic SnO_2 phase. Through the Rietveld refinement analyzes it can be observed that the sample with 0.3 moles of cerium reaches a significant mass fraction of the orthorhombic phase, approximately 36%. The reducing atmosphere generated by the heat treatment process of the samples and the strain originated due to the difference of ionic rays between the tin and cerium ion can play a crucial role in the formation of α-PbO2-type SnO_2.

Keywords: SnO2, orthorhombic phase, sol-gel route

We-S-P-21

Spectral insights of newly synthesized environmentally benign bismuth based lead free organic inorganic hybrid perovskite solar cell

Tanmoy Maiti [1], Pritam Dey [2], Harish Singh [3], Shubham Gautam [4]

[1] *Indian Institute of Technology Kanpur, UP-208016, India, Kanpur, India*
[2] *Indian Institute of Technology Kanpur, UP-208016, India, Kanpur, India*
[3] *Centre for Nanotechnology, Central University of Jharkhand, Jharkhand 835205, India, Ranchi, India*
[4] *Indian Institute of Technology Kanpur, UP-208016, India, Kanpur, India*

Organometallic halide based perovskite solar cells (PSC) have shown exponential growth in energy conversion efficiency over the past couple of years making it one of the breakthrough materials of this decade. However there are some serious issues like toxicity of lead, poor durability in hot and humid conditions which are needed to be addressed before it can be used commercially. In the current investigation we synthesized environmentally benign lead-free novel bismuth based photo absorbers with double perovskite ($A_2B_2I_6$) as well as single perovskite (ABI_3) crystal structure having methylammonium and formamidinium in the A-site. The thin films perovskites were synthesized by solution chemistry and spin coating technique followed by annealing at optimized temperature. Transient photoluminescence (trPL) measurement exhibits high recombination time in these materials. Micrometer range large single crystals with hexagonal morphology were found in FESEM and fluorescence image analysis. Incorporation of Bi in the B-site of these perovskites provided superior moisture and temperature stability without compromising the high recombination time of lead based perovskites. The large single crystal formation was attributed to anti-solvent treatment in the thin-film processing. UV-Vis spectroscopy measurement demonstrated very high absorption coefficient in the visible spectrum and low optical band gap around 1.7 eV were obtained. Furthermore, ferroelectric properties of these materials were investigated by P-E loop measurement. The C-N, N-H bonds have been analyzed from FTIR spectra. TGA-DSC measurement of these samples confirmed good temperature stability.

Keywords: PSC, trPL, Ferroelectric, Hexagonal morphology

We-S-P-22

Colossal change in thermopower with temperature driven p–n type conduction switching in La and Ca doped Sr_2TiFeO_6 double perovskites

Tanmoy Maiti [1], Pinku Roy [2]

[1] *IIT Kanpur, Kanpur, India*
[2] *IIT Kanpur, Kanpur, India*

Double perovskite materials have interesting structural, electronic and magnetic properties which have driven the researchers to study the thermoelectric material properties of such materials for efficient and clean energy conversion. In this work Sr has been substituted by La and Ca separately to check its effect on the thermoelectric properties of Sr_2TiFeO_6 double perovskite. Crystal structure of these double

perovskites have been determined as Pm-3m space group by rietveld refinement of XRD data. Microstructure was investigated by SEM. The electrical conductivity of these oxides exhibit a semiconductor ($d\sigma/dT > 0$) to metal ($d\sigma/dT < 0$) transition behaviour for all the compositions. Further the conduction mechanism of these oxides were studied with respect to polaron hopping model and non-degenerate semiconductor model was used to calculate the activation energy associated with carrier generation. Both $La_xSr_{2-x}TiFeO_6$ (LSTF) $Ca_xSr_{2-x}TiFeO_6$ (CSTF) composition exhibit p-type to n-type conductivity switching at elevated temperature. Moreover, this accompanied by a large change in thermopower with 2516 $\mu W/mK^2$ for $La_{0.1}Sr_{1.9}TiFeO_6$ and 4239 $\mu W/mK^2$ for $Ca_{0.2}Sr_{1.8}TiFeO_6$. A colossal change in thermopower associated with p–n type conduction switching driven by temperature in the same oxide compound provides a great potential to develop next generation, high temperature multifunctional electronic devices like switches,diodes, thermistors, etc.

Keywords: Thermoelectrics, p-n switching, Oxide Electronics

We-S-P-23

Ambient processing of P(VDF-TrFE)-based thin-film capacitors

Hamed Sharifi Dehsari, Jasper Michels, Kamal Asadi

Max-Planck Institute for Polymer Research, Mainz, Germany

Solution casting of thin films of the ferroelectric copolymer poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)) under ambient conditions is highly attractive for cost-effective production of flexible ferroelectric memory devices. However, due to the typically rough and porous films obtained under ambient, the yield of functional devices is low. A major challenge is ambient water vapor condensing into the drying solution, causing vapor-induced phase separation (VIPS). In this contribution we have used a combined experiment-modeling approach and show that the hydrophilicity of solvent is a decisive factor in the morphology of the final film, as it determines the ingress rate of water into the drying polymer solution during the film formation process. We present our numerical study, to study the ternary phase diagram of the polymer/water/solvent blend. Our calculation show that how VIPS is influenced by the change in composition due to simultaneous solvent evaporation and water condensation. The numerical simulations render morphologies consistent with the experimentally observed structures. Furthermore, the model shows that how the domain size and the early-stage phase composition principally depend on the relative humidity of the environment. Based on the gained insight, we have processed transparent, closely packed smooth films under ambient and outside cleanroom conditions, and demonstrate functional device yield of 100% for devices operating at voltages compatible with flexible electronics.

Keywords: Ferroelectric polymer, solution processing, nonvolatile memory, ferroelectric capacitor

---

We-S-P-24

Ferroelectric response of phase pure PMN-PT thin films realized through pulsed laser deposition

Pius Augustine [1, 2], Martando Rath [2], M.S. Ramachandra Rao [2]

[1] *Sacred Heart College (Autonomous), Thevara, Kochi, Kerala, India. Indian institute of technology Madras, Chennai, India., Kochi, India*

[2] *Department of Physics, Nano Functional Material Technology Centre and Material Science Research Centre, Indian Institute of Technology Madras, Chennai-600036, India., Chennai, India*

0.65PMN-0.35PT thin films exhibits excellent ferroelectric and piezoelectric properties, which make it suitable for various device applications like sensors, actuators, energy harvesting *etc.* Although large number of research reports were available on PMN-PT, the unparallel electric properties and smartness of this material could not be explored and utilised completely, till date. Synthesizing good quality and single phase PMN-PT ceramic target and stoichiometric transfer of the material during thin film growth were reported as two prominent reasons. Lead evaporation and pyrochlore formation during thin film growth are two challenges, which repel the researchers from utilizing this excellent and smart material. Deposition window for PMN-PT thin film is very narrow and the phase formation and quality of the film depend on various factors like nature and quality of the substrate and target, buffer layer used, substrate temperature during deposition, energy fluence, laser frequency, throw distance, oxygen partial pressure during deposition, annealing time etc, which make the realization of PMN-PT thin film/optimization of the deposition parameters, a cumbersome process. We will present a systematic study of these various factors to realize high quality PMN-PT thin film using pulsed laser deposition. $La_{0.5}Sr_{0.5}CoO_3$ (LSCO) buffer layer was deposited on commercial platinised silicon substrate, prior to the deposition of PMN-PT thin films. XRD, Raman, SEM, AFM and XPS analysis were carried out on selected films to establish the phase formation and the quality of the films. Ferroelectric studies of the films attest the suitability of the deposited films for device fabrication and/or applications.

Keywords: pulsed laser deposition, thick film, ferroelectric response

---

We-S-P-25

Highly resistive fast-sintered $BiFeO_3$ multiferroic magnetoelectric ceramics

Gustavo S. Dias [1], Luiz F. Cótica [1], Ivair A. Santos [1], Valdirlei F. Freitas [2], Fabiano Yokaichiya [3]

[1] *Universidade Estadual de Maringá, Maringá, Brazil*

[2] *Universidade Estadual do Centro-Oeste, Guarapuava, Brazil*

[3] *Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany*

Over the past few years, the interest in intrinsic multiferroic materials has increased significantly due to the fact that these compounds present different ferroic orders in the same phase and a coupling between them. In particular, multiferroic materials with magnetoelectric multifunctional properties have experienced an exponential growth in research interest due to the fact that one single-phase presents (anti)ferromagnetic and (anti)ferroelectric orders and their coupling. Among them, $BiFeO_3$ is one of the

most studied. It has a rhombohedral distorted perovskite structure and presents ferroelectric and antiferromagnetic ordering below 1098 K and 643 K, respectively. Even after many years of synthesis research, the preparation of highly resistive $BiFeO_3$ ceramics remains a challenge. The main problems are related to the presence of impurities. Ceramics prepared through the conventional solid-state reaction tend to have undesired phases and exhibit high leakage currents that prevent technological application and hinder the study of its properties. Many alternative routes of synthesis were proposed and/or tried along the years, unfortunately, the formation of $Bi_{25}FeO_{39}$ from the solid state reaction of Bi_2O_3 and Fe_2O_3 precedes the formation of the $BiFeO_3$. In this sense, we propose the use of high-energy ball milling to obtain highly homogeneous $BiFeO_3$ powders, allied to the fast firing method followed by quenching to room temperature to prevent the segregation and peritectic decomposition of secondary phases. As a result, highly resistive monolithic $BiFeO_3$ samples were achieved, and strong evidences of magnetoelectric coupling could be observed.

Keywords: BiFeO3, Magnetoelectric, High-Energy Milling

We-S-P-26

Dielectric and ferroelectric properties of (1-(x/2))$BaTiO_3$-(1-(x/2))$BiFeO_3$-(x)$LaFeO_3$ ceramics synthesized via solid-state reaction method with NaCl salt as the surface active agent.

Narit Triamnak, Kunyarat Aryuyuen, Kiratiporn Boonkham, Chanatorn Patadoung

Department of Materials Science and Engineering, Faculty of Engineering and Industrial Technology, Silpakorn University, Nakornpathom , 73000, Thailand, Nakornpathom, Thailand

In this work, the dielectric and ferroelectric properties of (1-(x/2))$BaTiO_3$-(1-(x/2))$BiFeO_3$-(x)$LaFeO_3$ ceramics, where x = 0.6 - 1.0 were investigated. The ternary solid solutions were synthesized via solid-state reaction method with NaCl salt as the surface active agent. Crystal structure of this ceramic system which was examined by x-ray diffraction technique revealed the orthorhombic-rhombohedral transition at x = 0.1, approximately. In addition, the solid solutions were successfully synthesized by exhibiting single phase at these compositions and the calcination temperature was reduced because of the NaCl salt. Dielectric and ferroelectric properties were investigated as well as magnetic properties via vibrating sample magnetometer measurement.

Keywords: Barium Titanate, Ferrite, Bismuth, Dielectric

We-S-P-27

Physical characterizations of the high-bioactive PVDF-HAp ferroelectric composite

Valdirlei Freitas [1], Taiana Bonadio [1], Jaciele Rosso [2], Gustavo Dias [2], Luiz Cótica [2], Ivair Santos [2], Ludmilla Silva [1]

[1] *State University of Midwest, Guarapuava, Brazil*
[2] *State University of Maringá, Maringá, Brazil*

The search for innovative and advanced materials for biological applications has been intensified in the recent years. This is because the advances in modern medicine, especially in the orthopedic and traumatology, are directly linked to the specific properties of these materials and new techniques for their synthesis and characterization. However, for satisfying the expectations of future advanced medicine it is necessary to obtain completely revolutionary materials, which may indicate new directions and provide faster results than the current ones. In this sense, novel multifunctional materials emerge as strong candidates for fulfill these underserved biomedical applications. This is the case of (ferro)piezoelectric/bioactive compounds, as polyvinylidene fluoride-hydroxyapatite (PVDF-HAp), which can catalyze the bone growth by piezoelectric voltage and/or electro-mechanical distention/contraction stimuli. In adition, magnetic structures (Fe_4O_3-like) can be added to the composite to provide responses to external magnetic stimuli. In this work, an innovative bioactive polyvinylidene fluoride-hydroxyapatite ferroelectric composite was synthesized and characterized. Microstructural analyzes of samples immersed in simulated body fluid high-bioactivity by controlled times revel an elevated rate (210 nm per day) of synthetic osseous tissue (apatite) growing on the composites surface with and without external stimuli. At room temperature, the polar polyvinylidene fluoride (β2) phase besides elevated remnant polarizations (40 kV/cm2) and coercive fields (28 kV/cm) were observed in structural and ferroelectric investigations. These results indicate the high-potential for synthetic apatite growth on polyvinylidene fluoride-hydroxyapatite ferroelectric composites by using alternating electric fields in-vitro or in-vivo experiments.

Keywords: Bioactive Composite, Ferroelectric Polymer

We-S-P-28

Effect of Nb doping in $BaSrZrTiO_3$

Anju Dixit

Department of Physics, VSSD College, Kanpur, Kanpur, India
Department of Physics & Materials Science, UIET, CSJM University Campus, Kanpur, Kanpur, India

It has been widely investigated that the ferroelectric properties of BaSrTiO3 (BST) perovskites can be modified to exhibit relaxor behavior by Zr substitutions on Ti sites. Therefore, the relationship between the phase transition behaviors with Zr contents has been of great interest. Further the inclusion of Nb in BSZT lattice shows structural and corresponding phase changes. In this work, BSZT samples were prepared using sol gel technique and the effect of Nb doping in BSZT has been studied. Small amount of Nb changes structural, electrical and dielectric properties of BSZT. The inclusion of Nb in lattice has been verified by XRD and the influence of the dopant as well as associated effects on the physical and electrical characteristics are investigated and will be presented.

Keywords: Ferroelectric, Phase Transition

We-S-P-29

Rapid detection of transient currents in ferroelectric nanocapacitors via Bayesian Inference

Suhas Somnath [1], Kody Law [2], Anna Morozovska [3], Petro Maksymovych [1], Yunseok Kim [4], Xiaoli Lu [5], Marin Alexe [6], Richard Archibald [2], Sergei Kalinin [1], Stephen Jesse [1], Rama Vasudevan [1]

[1] *Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, OAK RIDGE, United States*
[2] *Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, United States*
[3] *Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine*
[4] *Sungkyunkwan University, Suwon, Korea, Republic of (South)*
[5] *Xidian University, Xi'an, China*
[6] *University of Warwick, Coventry, United Kingdom*

The investigation of displacement currents arising from polarization switching is a commonly employed method used to explore ferroelectric hysteresis. However, in the nanoscale measurement using an atomic force microscope (AFM) tip, traditional current-voltage (I-V) curve acquisition is generally too slow to measure this transient current, and thus nanoscale studies have focused on the use of complementary techniques such as piezoresponse force microscopy (PFM). Here we present a method to simultaneously increase the rate of acquisition of I-V curves by a factor of ~200x, through use of AC excitation to the tip, full information acquisition, and Bayesian inference. We successfully observe switching current in ferroelectric $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin-film nanocapacitors, with results indicating contamination towards the center of nanocapacitors, varying leakage levels, and also allow determination of the dielectric constant of the individual nanocapacitor structures. Analysis of the switching current profiles enables determination of degree of disorder, which can be spatially mapped and provides a complementary channel to supplement PFM. This study shows the utility of the full information acquisition and Bayesian inference approach, and can be extended to scanning tunneling microscopy for rapid electronic characterization. This research was sponsored by the Division of Materials Sciences and Engineering, BES, DOE (RKV, SVK, PM,SS). This research was conducted and partially supported (SJ) at the Center for Nanophase Materials Sciences, which is a US DOE Office of Science User Facility. The Bayesian inference was sponsored by the Applied Mathematics Division of ASCR, DOE; in particular under the ACUMEN project (KJHL, RA).

Keywords: Piezoresponse Force Microscopy, Switching current, Atomic Force microscopy, nanocapacitor

---

We-S-P-30

Long-wave optic phonons in $PbNi_{1/3}Nb_{2/3}O_3$ crystals.

Alexander Fedoseev [1], Tatyana Smirnova [1], Sergey Lushnikov [1], Ram Katiyar [2]

[1] *Ioffe Institute, St.-Petersburg, Russia*
[2] *University of Puerto Rico, San Juan PR, United States*

$PbNi_{1/3}Nb_{2/3}O_3$ (PNN) belongs to cubic relaxor ferroelectrics. Its lattice dynamics is poorly studied. It is known that a broad frequency-dependent anomaly of the dielectric and acoustic response is observed near 153 K [H. J. Fan, et.al. JAP, 91, 2262 (2002)]. The crystal symmetry changes near 153 K from the cubic to a rhombohedral ferroelectric phase. Investigations of PNN magnetic properties have shown that it is paramagnetic up to helium temperatures [T.Shirakami et.al. JJAP, 39, L678 (2000)]. This report presents Raman studies of vibrational spectrum of the PNN crystal in a wide temperature range, 600-90 K. The experiments used a T64000 spectrometer (Joben Ivon) in the backscattering geometry. It has been found that at high temperatures a well-polarized Raman spectrum is similar to the scattering spectra for PMN crystals. A temperature decrease affects the Raman spectrum. Additional lines appear, the low-frequency region considerably changes. This behavior of the Raman spectrum for the PNN crystal points to a crystal symmetry change. By using group-theoretical analysis of the experimental spectra, possible models of the PNN structure in the low-temperature phase are considered. Analysis of temperature dependences of frequencies of the first-order scattering lines revealed a significant "softening" of the low-frequency vibration in the VV polarization near 150 K and also the anomalous behavior of hard modes in this temperature range. Fitting of the low-frequency region of the spectra showed the existence of quasi-elastic light scattering the behavior of which exhibited a strong dependence on temperature.

Keywords: Raman spectroscopy, lattice dynamics, relaxor ferroelectrics

---

We-S-P-31

Investigation on a giant magnetoelectric effect in a hexaferrite via neutron scattering techniques

Yan Wu [1], Huibo Cao [1], Young Sun [2]

[1] *Oak Ridge National Laboratory, Oak Ridge, United States*
[2] *Institute of Physics, Chinese Academy of Science, Beijing, China*

Y-type hexaferrite $Ba_2Mg_2Fe_{12}O_{22}$ was reported recently to have a large magnetoelectric effect (ME). The magnetic structure of $Ba_2Mg_2Fe_{12}O_{22}$ consists of two groups of L- (large moment) and S- (small moment) blocks alternating stacked along the c-axis direction. The moments align ferrimagnetically in the same block. At zero field, it displays a proper screw magnetic structure with an incommensurate wavevector k along the c-axis below a ferrimagnetic-antiferromagnetic (FM-AFM) transition (195 K) and then transforms to a longitudinal conical phase below 50 K. Applying a small magnetic field, the material displays polarization in the conical phase. When doped with Sr, the material keeps its sensitivity to field while the ME coefficient is greatly enhanced with Sr doping. The transition temperatures are largely elevated and FM-AFM transition temperature goes above room temperature. Meanwhile, temperature dependent neutron diffraction investigation shows pinning effect emerging at heavy Sr doped sample that has an alternating longitudinal conical ground state. The study of size effect indicate that such simultaneously occurred effects can correspond to relatively independent mechanisms. Comparison study of the crystal and magnetic structure of the doped samples is performed to identify the moment interaction picture differences behind doping effects.

Keywords: hexaferrite, neutron scattering, magnetoelectric effect, conical phase

---

We-S-P-32

Synthesis and characterization of the perovskite compound $YFe_xCr_{1-x}O_3$ (0 < x < 1)

Roberto Salazar [1], Friedrich E. Wagner [2], Antonio Lazo [3], Rubén Puga [1], Juan Z. Dávalos [4], Américo Orccohuancca [1], Héctor Loro [1]

[1] *Facultad de Ciencias, Universidad Nacional de Ingeniería, Lima, Peru*
[2] *Technische Universität München, Physik Department E15, Garching, München, Germany*
[3] *Facultad de Ingeniería Geológica, Minera y Metalúrgica, Universidad Nacional de Ingeniería, Lima, Peru*
[4] *Instituto de Química Física Rocasolano CSIC, Madrid, Spain*

It was possible to synthesize the perovskite compound $YFe_xCr_{1-x}O_3$ by the combustion method using urea and glycine. The spongy and laminated appearance of the ocher colored material was characterized by X-ray diffraction indicating crystallization of the samples in a perovskite structure with orthorhombic deformation. Additionally the samples were studied by Mössbauer spectroscopy at 300 K and 4.2 K. All of them presented magnetic ordering at 4.2K with very narrow line widths. The value of the hyperfine field continuously decreased from the pure sample of $YFeO_3$ to $YFe_{0.25}Cr_{0.75}O_3$. At 300 K the samples of $YFeO_3$ and $YFe_{0.75}Cr_{0.25}O_3$ present a magnetic hyperfine splitting, but the samples with $YFe_{0.50}Cr_{0.50}O_3$ and $YFe_{0.25}Cr_{0.75}O_3$ show only an electric quadrupole splitting indicating superparamagnetism or the absence of magnetic order. We also report the result of first principle calculations of the electronic structure of $YFeO_3$ and $YCrO_3$.

Keywords: Multiferroics, Mössbauer Spectroscopy, Perovskite, Combustion

---

We-S-P-33

Inorganic ferroelectric/dielectric nanocomposite thin films

Yomery Espinal [1, 2], Brendan Hanrahan [1], Pamir Alpay [2]

[1] *Army Research Laboratory, Adelphi, MD, United States*
[2] *University of Connecticut, Storrs, CT, United States*

We have developed a simple, chemical deposition-based process for creating ferro-/dielectric nanocomposites to address leakage current issues associated with ferroelectric films. Ferroelectric thin films are attractive for energy conversion and memory devices but experience high leakage current and relatively low breakdown voltages, limiting their use. A ferroelectric nanocomposite consisting of an active ferroelectric phase within a low-loss dielectric matrix could provide a means to reduce loss, leakage, and breakdown while maintaining significant dielectric and pyroelectric properties inherent to ferroelectrics. In this work, 100 nm barium titanate (BTO) nanoparticles were co-deposited within a dielectric spin-on-glass titania matrix at <450 Celsius, resulting in a virtually crack-free ~ 200 nm composite film. The polarization and leakage current of the composite films were analyzed at room temperature between 0 - 250 kV/cm. Initial results showed low leakage current ($<10^{-7}$ A/cm^2) for the composite film while increasing the relative permittivity by 52% at only 9 area% loading of BTO

particles. This work demonstrates that it may be possible to combine the properties of an active ferroelectric and a low loss inorganic dielectric in a single nanocomposite film.

Keywords: Nanocomposites

We-S-P-34

Domain wall conductivity with a twist

Rama Vasudevan [1], Ye Cao [1], Nouamane Laanait [1], Anton Ievlev [1], Linglong Li [2], Jan-Chi Yang [3], Ying-Hao Chu [4], Long-Qing Chen [5], Sergei Kalinin [1], Petro Maksymovych [1]

[1] *Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, United States*
[2] *Frontier Institute of Science and Technology, Xi'an Jiaotong University, Xi'an, China*
[3] *Department of Physics, National Cheng Kung University, Tainan, Taiwan*
[4] *Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan*
[5] *Department of Materials Science and Engineering, Pennsylvania State University, University Park, United States*

Conduction isolated at ferroelectric domain walls has garnered substantial attention, due to both fundamental physics considerations, and the possibility of reconfigurable circuitry that such nanoscale functional elements could provide. However, the mechanism of conduction remains under active debate. Here, we present a new mechanism based on the formation of a polarization nucleus and a twisted structure at the domain wall, that does not rely on intrinsically different conduction mechanisms at the wall. Through investigations of I-V curves on a thin (~10 nm) epitaxial film of $BiFeO_3$ (BFO) on (001) $SrTiO_3$, in combination with phase-field modeling, we show that the formation of a twisted nucleus with nonzero curl leads to a field enhancement, which is sufficient to explain the variation in the I-V curves acquired within domains compared with those obtained at the nominally uncharged wall. This new mechanism is universal, suggests that different electronic properties at the domain wall are unnecessary to explain the literature results, and presents an unexpected merging of the dynamics of topological defects with domain wall conduction.

This research was in part sponsored by the Division of Materials Sciences and Engineering, BES, DOE (RKV, SVK). Research was conducted at the Center for Nanophase Materials Sciences, which also provided support (AI) and which is a DOE Office of Science User Facility. NL acknowledges support from the Eugene P. Wigner Fellowship program at Oak Ridge National Lab. X-ray data was collected at the Advanced Photon Source which is a DOE Office of Science User Facility.

Keywords: domain wall conduction, phase field modeling

We-S-P-35

Is ferroelastic $BiVO_4$ also antiferroelectric?

Nidal Banja, Hongjian Zhao, Jorge Iniguez, Mael Guennou

Luxembourg Institute of Technology, Belvaux, Luxembourg

$BiVO_4$ is known as one of the very few examples of a material exhibiting a "proper" ferroelastic transition, where strain is the primary order parameter. This tetragonal-to-monoclinic phase transition has been scrutinized in details in the past, mostly to reveal and confirm this original property [1]. More recently, $BiVO_4$ has regained interest for its optical properties and potential applications to photocatalysis, due to its absorption in the visible range. In this work we re-examine the ferroelastic transition in $BiVO_4$ in the light of its possible antiferroelectric character predicted in [2], and hinted at by its small but distinct dielectric anomaly [3]. We give a detailed description of the phonon spectrum across the transition, as measured by Raman spectroscopy, and discuss mode couplings in a hard-mode spectroscopy approach. From first-principle phonon calculations for the low- and high-symmetry phases, we give a full mode assignment of the phonon modes and vibration patterns, and discuss the behaviour of the low-lying polar and antipolar modes in relation with antiferroelectricity.

References

[1] Cummins and Levanyuk, Light scattering near phase transitions, Elsevier Science (1983).

[2] Tolédano and Guennou, Phys. Rev. B 94, 014107 (2016).

[3] Dudnik et al., Fiz. tverd. tela 16, 2733 (1974).

Keywords: antiferroelectricity

We-S-P-36

Preparation, characterization and dielectric properties of Mg-doped $CaCu_3Ti_4O_{12}$ ceramics

Eduardo Antonelli, Leonardo Arruda

UNIFESP - Universidade Federal de São Paulo, São Jose dos Campos, Brazil

Ferroelectric materials are fundamental to capacitors industry due to their dielectric properties. However, their excellent dielectric properties are closely related to structural phase transitions and their spontaneous polarization. Accordingly, ferroelectric capacitors present a large variation in capacitance with temperature, high dielectric loss near the Curie temperature, fatigue and aging when submitted at an alternating electric field. Recently, the cubic perovskite $CaCu_3Ti_4O_{12}$ (CCTO) has drawn a lot of attention due to their giant dielectric constant (GDC). There are some hypotheses to explain the origin of the GDC in CCTO that, in general, are based on intrinsic or extrinsic factors. In the present work, the CCTO pure and doped with Mg^{2+} was prepared by the conventional ceramic method. The results here presented and discussed refer to the trend of Mg^{2+} occupation on the CCTO structure and their influence on the dielectric and interfacial properties. The pure and doped ceramic were sintered at 1050^{o}C for 3,

6 and 12 hours in a furnace. The phase and microstructure developments were followed by X-ray diffraction (XRD) using a Rigaku Ultima IV diffractometer (CuK_α, $\lambda = 1.5406$ Å) and scanning electron microscopy (FEI), respectively. Electrical measurements were carried out with a Solartron SI 1260 impedance/gain-phase analyzer over a wide temperature range from 25 to 200 ^oC. In particular, Mg^{2+} was seen to inhibit the materials' grain growth process, besides promoting a decreasing of the GDC of CCTO. This decreasing on permittivity was related to the resistivity for grains and grains boundaries in doped-CCTO.

Keywords: CCTO, dielectric, capacitors

We-S-P-37

Refractive indices and birefringence of lithium niobate as a function of temperature and wavelenght

Abdallah Albarakaty, Nasser Moustafa

Physics Department, Umm-Al-Qura University, Makkah, SA, Makkah, Saudi Arabia

In this work, an experimental approach was used for measuring refractive indices and birefringence of $LiNbO_3$ singel crystal over a wide range of wavelength and temperature. We proposed a speckle photography method for the measurements. The main advantages of our method is the simplicity of optical set-up that uses a single refrence beam, thus reducing mechanical stability requirements of the set-up. Experimental results have been presented to validate the theoritical predictions. The values of refractive indices and birefringens were obtained with an acceptable degree of accuracy. Speckle photography , photo-refractive materials, refractive indices, birefringence.

Keywords: Speckle photography , photo-refractive materials, refractive indices, birefringence.

We-S-P-38

Molten salt synthesized $La_{1-x}Sr_xCoO_3$ as an efficient electrocatalyst for water splitting

Yuanbing Mao, Swati Mohan

University of Texas Rio Grande Valley, Edinburg, United States

Perovskite oxides are important and effective class of mixed oxide plays significant role in field of energy storage and conversion systems. Here we present a series of $LaCoO_3$ cobaltite perovskite samples which were synthesized by a combined sol-gel and molten salt method and doped with 5%, 10%, 20% and 30% of strontium. The combined sol-gel and molten salt procedure provided regular morphology of these particles, which act as a significant catalyst for oxygen evolution and reduction reactions (OER and ORR). The structural and morphological characterization of these Sr-doped $LaCoO_3$ samples was carried out by powder X-ray diffraction, Raman spectroscopy, Infrared spectroscopy, X-ray photoelectron spectroscopy, and scanning electron microscopy. Moreover, as good as our knowledge

till the date we are presenting first time some useful comparison in terms of specific capacitance, total charge, most accessible charge, electrochemically active surface area, and roughness factor by using rotating disk and rotating ring-disk electrode techniques of these $LaCoO_3$ particles for OER. $LaCoO_3$ doped with 30% Sr show enhanced electrocatalytic OER activity in 0.5 M H_2SO_4 media compared to the $LaCoO_3$ doped with 0, 5, 10, 20% Sr. Among all five $LaCoO_3$ catalyst samples, the doped $LaCoO_3$ demonstrated better OER and ORR activity than undoped $LaCoO_3$.

Keywords: LaCoO3, Molten salts, Electrocatalysis, OER

We-S-P-39

Structural analysis and thermoelectric properties of La-doped Sr_2CoMoO_6 double perovskites

Tanmoy Maiti [1], Khagesh Tanwar [1]

[1] *Department of materials science and Engineering, kanpur, India*
[2] *Department of materials science and Engineering, kanpur, India*

Nano-crystalline powders of La-doped and pure Sr_2CoMoO_6 (SCMO) have been synthesized by using conventional solid state route. The powders were calcined at 1150 ºC and pressed into pellets which were sintered at 1350 ºC in air. XRD and SEM analysis of prepared samples show single phase solid solution with negligible percentage of extra phases and dense microstructure of varying grain size. Rietveld refinement reveals the double perovskites crystal structure with *I*4/*m* Space group. Thermoelectric properties were measured in the temperature range of 0 - 900 ºC. It is interesting to notice that when pure SCMO samples were annealed in reducing atmosphere it induces n-type behaviour and triggers the conductivity into two order higher than the conductivity of normally sintered samples thus resulting into enhanced power factor. Furthermore, we have doped lanthanum at the place of strontium to provide more charge carriers into lattice.

Keywords: Double Perovskites, Rietveld refinement, Thermoelectrics

---

We-S-P-40

Sensing magnetic fields with an innovative smart probe composed by piezoelectric elements

José R D Pereira [1], Fernando J Gaiotto [1], Rogerio G Nespolo [1], Diogo Z Montanher [2], Ivair A Santos [1]

[1] *State University of Maringá, Maringá, Brazil*
[2] *Federal University of Technology, Guarapuava, Brazil*

In this paper, a probe that is sensitive to an external magnetic field was characterized and developed. This probe sensor was made with rectangular polarized piezoelectric ceramic elements and a copper wire coil located around it, which induces an alternating electrical response. The system consists in a

probe coupled to a microprocessor and a signal conditioning system with Wi-Fi technology, integrated with a smartphone application for magnetic field sensing in real-time. The operation principle of this sensor involves the Lorentz force and the direct piezoelectric effect. The basic principle of this probe is when a continuous magnetic field (HDC) is applied to the sensor, a Lorentz force is established due the interaction between magnetic field and electric current. This force transfers energy to the piezoelectric element, which promotes a mechanical deformation that is converted into electric voltage via direct piezoelectric effect. The Electric response voltage induces the linear output response of HDC between 0 and 1 kOe, with an excitation current in the coil of 100 mA. These sensors showed ability to measure magnetic fields of the order of 10 - 4 T, leading to the development of smart sensors for several applications. It can be used with magnetic transducers that are widely used in modern industry and electronic applications to sense the magnetic field, measuring current, position, and other physical parameters. To conclude, those innovations in magnetic field sensor probes are important for the development of new smart technologies with applications in current control and measuring in switching power supplies for industrial automation

Keywords: piezoelectric effect, magnetic transducers

We-S-P-41

Phase transitions studies in (1-x)($Ba_{0.77}Ca_{0.23}$)TiO_3-xBa($Ti_{0.75}Zr_{0.15}$)O_3 ceramics

Eduardo Antonelli, Renato Boschilia, Rangel Aredes, Andre Boaventura

UNIFESP - Universidade Federal de São Paulo, São Jose dos Campos, Brazil

The Lead has recently been expelled from many commercial applications and owing to concerns regarding its toxicity. Currently, piezoelectric ceramic materials in commercial use are based on lead titanate zirconate (PZT), which are widely used in sensors, actuators and other electronic devices. The basic approach to achieving high piezoelectricity is to place the composition of the material to the proximity of a composition-induced phase transition between two ferroelectric phases. Such a transition has been known as the morphotropic phase boundary (MPB) in the phase diagram. Therefore, in the present work, the compounds (1-x)($Ba_{0.77}Ca_{0.23}$)TiO_3-xBa($Ti_{0.85}Zr_{0.15}$)O_3 (1-xBCT-xBZT x = 0.25, 0.50 and 0.75) have been prepared through solid state reaction of BCT and BZT compounds. The compositions were sintered at 1320 ºC for 2 h in a furnace. The final density of each sintered specimen was determined by the Archimedes method and the grain sizes were investigated using a scanning electron microscopy (FEI). The phase transitions studies were performed in several temperatures using a Rigaku Ultima IV diffractometer (HT 1500 high temperature attachment). Electrical measurements were carried out with a Solartron SI 1260 impedance/gain-phase analyzer over a wide temperature range from 25 to 200 ºC. The phase transitions were also studied using the dilatometry technique (Netzsch-DIL 420C) and the differential scanning calorimetry (DSC) techniques (Netzsch-STA 409C). The combination of all these techniques allows us to have an overall view of the BCT-BZT phase transitions behavior.

Keywords: BCT-BZT, phase transitions, dielectric

We-S-P-42

Magnetoelectric properties of epitaxial $Sr_{0.5}Ba_{0.5}MnO_3$ films

Temuujin Bayaraa [1], Yurong Yang [1], Jorge Íñiguez [2], Laurent Bellaiche [1]

[1] *University of Arkansas, Fayetteville, United States*
[2] *Luxembourg Institute of Science and Technology, Luxembourg, Luxembourg*

(Sr,Ba)MnO_3 perovskites are expected to exhibit a strong coupling between electrical polarization and spin order. Tuning the lattice by strain engineering has the possibility to strongly modify such magnetoelectric coupling. Here, we use *ab-initio* calculations to predict structural, magnetic and magnetoelectric properties of epitaxial films made of multiferroic $Sr_{0.5}Ba_{0.5}MnO_3$ for different chemically-ordered arrangements, and under both compressive and tensile strain. In particular, some specific regions of misfit strain are identified to yield large magnetoelectric couplings. Effects of the value of the Hubbard U parameter on these predictions will also be discussed.

Keywords: ab-initio, epitaxial strain, magnetoelectric property

---

We-S-P-43

Induced Magnetic-anisotropy by the remanent electric polarization of PMN-PT/$CoFe_2O_4$ multiferroics particulates composites

Korllvary R.C. Parra-Jimenez, Fábio L. Zabotto, Ducinei Garcia, Adilson J. A. de Oliveira

Physics Department - Federal University of São Carlos, São Carlos, Brazil

Multiferroics magnetoelectric materials that present induced electric polarization due to an applied magnetic field or vice versa. These materials are classified in monophasic and biphasic multiferroics, respectively with intrinsic and extrinsic magnetoelectric response. The mechanisms to explain how to influence the electric field control of magnetic properties, magnetic-anisotropy, magnetic order and magnetic domain wall motion on biphasic composites. The possible mechanisms the electric field control on magnetic properties are magneto-elastic effect, and charge modulation effect depends on type composition and structure material. In this work we present a studied of the electric polarization influence on the magnetic properties in PMN-PT/$CoFe_2O_4$ of the 0-3 type magnetoelectric particulate biphasic. The samples were prepared by solid-state reaction method in concentration 80/20 in two condition sintering time of 1 hour and 10 hours at temperature of 1050 °C. The samples were characterized using magnetometry and magnetoelectric response on the two conditions of the remanent electric polarization {0,+20} kV/cm under electric field applied at room temperature (RTP) and 80 °C (TP). Our results showed that the saturation magnetization decreases with the electric polarization in ~ 2% (RTP) and ~ 5% (TP) to the field magnetic parallel to poled axis and increases ~ 4% (RTP) and ~ 6% at 80 °C to the field magnetic perpendicular to poled axis. However, the coercive field did not change. This is an indication that electric polarization not only stressed the system, but also induced magnetic-anisotropy caused by the electric polarization over strain interfacial mediated coupling between constituted phases.

Keywords: multiferroic materials, magnetic measurements, composites

---

We-S-P-44

Gradient-lead-excess crystallization process: A way to produce highly textured (111) PZT films

Alexander Sigov [1], Lyubov Delimova [2], Elena Guschina [2], Nina Zaitseva [2], Dmitry Seregin [1], Konstantin Vorotilov [1]

[1] *Moscow Technological University (MIREA), Moscow, Russia*
[2] *Ioffe Institute, Saint-Petersburg, Russia*

Nucleation at the Pt surface plays an important role in formation of CSD PZT films. The nucleation of (111) perovskite (Pe) grains occurs directly on the Pt (111) surface. The presence of TiO_2 or PbO on the Pt surface stimulates growth of Pe grains with (100) orientation. As a result, CSD PZT films on Pt demonstrate a mixed (111) and (100) Pe orientation. Pb-reach or Ti-reach seed layers are commonly used to enhance (100) orientation that is important, for example, for MEMS applications due to higher piezoelectric coefficient value. On the other hand (111) orientation may be preferable for FeRAM applications due to less elastic stress during domains switching. New crystallization technique for produce of PZT films with high (111) orientation is proposed in this work. It is based on deposition of layers with different Pb-excess in precursor solution. The first crystallization step (deposition of a seed layer) is performed at a low Pb excess (0 - 5 wt %) to form highly oriented Pe (111) grains. The next crystallization step is performed with a 30 wt % excess of Pb to prevent formation of pyrochlore particles and accelerate the growth of Pe grains. An effect of the low-Pb-excess seed layer on the film texture, hysteresis loops, grain size, polarization dependences of the transient currents, and local current distribution are discussed. It is shown, that in the case when first crystallization step proceeds at a low Pb content condition, Pe (111) texture is sufficiently enhances with complete suppression of others orientations.

Keywords: thin films, growth conditions, PZT, perovskite phase, pyrochlore phase.

We-S-P-45

Dielectric polarization in $BaSrTiO_3$ films modulated by THz electric field

Mikhail Agranat [2], Elena Mishina [1], Alexander Sigov [1]

[1] *Moscow Technological University (MIREA), Moscow, Russia*
[2] *Joint Institute for High Temperatures of Russian Academy of Sciences (JIHT), Moscow, Russia*

The switching rate of the order parameter in ferroelectrics has been the subject of intensive research for decades. In this paper, we present the results of experimental and theoretical study of the dynamic switching of polarization in ferroelectrics, as well as the creation of residual polarization upon action on a ferroelectric by short pulses of a high-intensity terahertz field. Sub-cycle terahertz field up to 1 MV/cm

is created by optical rectification of a short optical pulse in an organic crystal. As a measure of the dielectric polarization, the intensity of second harmonic generation is recorded as a function of the delay time between THz pump and femtosecond optical probe. Epitaxial (001) and (111) oriented 500 nm $(Ba_{0.8}Sr_{0.2})TiO_3$ films were grown on MgO substrate by RF sputtering. Experiments reveal that under the action of a short powerful THz pulse on a ferroelectric, two effects are observed: modulation of the SHG intensity with exactly the shape of THz pulse and a step-like change of the SHG intensity overlapped by oscillating signal after the THz pulse ended. The former reveals transient modulation of polarization within the THz pulse duration, the latter may indicate switching of the polarization and creation of remnant polarization. Both effects take place due to the displacements of ions under the action of short THz pulses which were earlier observed in experiments on synchronous X-ray structural analysis. The observed switching behavior can be described by the nonlinear Duffing equation.

Keywords: terahertz pulses, ferroelectric films, polarization switching, SHG.

We-S-P-46

Estimation of dead layer at the PZT - Pt interface

Alexander Sigov, Yury Podgorny, Pavel Lavrov, Konstantin Vorotilov

Moscow Technological University (MIREA), Moscow, Russia

Conception of a passive dead layer at the metal-ferroelectric interface plays an important role in electrical properties characterization of metal-ferroelectric-metal structures. It is commonly supposed that the dead layer is a reason for properties degradation with the ferroelectric film thickness decrease, including decreasing polarization, hysteresis slope, dielectric permittivity, etc. We perform dead layer analysis at the PZT-Pt interface for the films with different internal structure. The dead layer thickness δ was calculated from the hysteresis tips obtained at different voltages to exclude leakage influence. For comparison, the dead layer thickness was estimated from the dielectric permittivity-thickness dependencies and from hysteresis slope technique proposed by A.Tagantsev [1]. Capacitance and hysteresis tips techniques give a good correlation for dense polycrystalline films: δ ~ 2.5 Å. For porous PZT films, the dead layer thickness demonstrate higher values: δ = 12 Å for capacitance measurements, and δ = 5.8 Å for hysteresis measurements. The reason is higher leakage currents in porous PZT films causing shunting of dead layer capacitance. Tagantsev's technique gives twice-triple lower δ values, which does not correlate with low-field dielectric permittivity measurements.

[1] A. K. Tagantsev, M. Landivar, E. Colla, and N. Setter, J. Appl. Phys. 78, 2623 (1995).

Keywords: dead layer, metal-ferroelectric interface, ferroelectric films.

We-S-P-47

Effect of the rare earth ion substitution on structural, dielectric and magnetic properties of perovskite $Re_2Bi_2Fe_4O_{12}$ (Re = Eu, Sm, La) ceramics

Javier Alonso Cuervo Farfán [1], Diego Seiti Fukano Viana [2], Flávio Paulo Milton [2], Ducinei Garcia [2], David Arsenio Landínez Téllez [1], Jairo Roa Rojas [1]

[1] *Physics of Novel Materials Group, Physics department, National University of Colombia, A.A. 5997 Bogota DC, Colombia, Bogota, Colombia*

[2] *Ferroelectric Materials Group, Physics department, Sao Carlos Federal University, Rodovia Washington Luís, Km 235, Sao Carlos- Sao Paulo, Brazil, Sao Carlos, Brazil*

The conventional solid-state reaction method was applied for the processing of the perovskite $Re_2Bi_2Fe_4O_{12}$ (Re = Eu, Sm, La) compounds. Under optimized processing conditions, it make possible to obtain single-phase sintered bulks with relatively high apparent density. Complex impedance and magnetic measurements at low temperature showed dielectric relaxation processes, which occurs above Curie and Neel characteristic temperatures, influenced by the rare earth ion substitution. Furthermore, from the magnetization hysteresis loops, analyzed at 50 K, 200 K and 300 K, it was observed that magnetic state drastically changed upon the rare earth choice.

Keywords: magnetic properties, complex impedance, polycrystalline materials, perovskite,

---

We-S-P-48

NSMM Review – Part I: Scorecard of NSMM *versus* Goldschmidt's Factor formalism

Vignaswaran K. Veerapandiyan, YuHusn Liao, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven C. Tidrow

Alfred University, Alfred, United States

The new simple material model (NSMM) is discussed in context to the culmination of results of consecutive reports discussed in "NSMM Review" Parts: (II) - (IV). Here, through comparing the room temperature structure, lattice parameter and volume of roughly 100 Perovskite materials, we numerically reiterate the significant improvement in modeling performance that temperature dependent NSMM provides over Goldschmidt's tolerance factor formalism (GTFF) at room temperature. Additionally, NSMM maintains such enhanced performance over extended temperature ranges, from roughly 100 K to near the melting temperature of the material. Although NSMM is based on many of the same structural foundations as GTFF, inclusion of physical constraints within NSMM enhances predictive power versus GTFF which is simply a correlation relation. The physical constraints are used for development of temperature dependent ionic radii, which are used in conjunction with the Clausius – Mossotti relation for development of coordination and temperature ionic polarizability. When combined, the coordination and temperature dependent genome-like ion properties, radii and polarizability can be used to predict/model a wide range of temperature dependent material properties, including but not limited to crystal structure, lattice parameter and volume, relative permittivity, and polarization- and volume-induced structural phase transition temperatures. For example, the overall comparison scores of NSMM versus GTFF for the series $A^{1+}Nb^{5+}O_3$ and A^{1+} $Ta^{5+}O_3$ with A being Ag,

Cs, H, K, Li, Na, Rb, and $A^{2+}Ti^{4+}O_3$ with A being Ba, Ca, Eu, Pb, and Sr, NSMM out scores GTFF and provides additional information that GTFF is unable to address.

Keywords: Goldschmidt's tolerance factor, coordination and temperature dependent ionic properties, polarization induced structural phase transition, volume induced structural phase transition, Clausius - Mossotti relation

---

We-S-P-49

Ferroelectric property in nano-layered Hafnium oxide

Sita Dugu [1], Shojan Pavunny [1, 2], Rajesh Katiyar [1], Ram S Katiyar [1]

[1] *University of Puerto-Rico, Rio-piedras, San Juan, United States*
[2] *US Naval Research Laboratory, Washington DC, United States*

Ferroelectric materials have been progressively used in non-volatile memory applications. Multifunctional properties of ferroelectric and multiferroic complex oxides permit researchers to develop new approaches in the field of memory storage and optical devices. Both doped and undoped HfO_2 have attracted much attention from the viewpoints of ferroelectricity due to its CMOS compatibility. We found the ferroelectric behavior in HfO_2 thin film grown by plasma enhanced Atomic Layer Deposition (ALD). The ultra thick ~ 20 nm films showed a remnant polarization ~10 μC/cm^2. Further studies of the film that confirmed ferroelectric nature by observing phase hysteresis and butterfly amplitude loops through Piezoresponse Force Microscopy (PFM) techniques. The novel achievement can be used for future potential applications such as non-volatile FeRAM. Further characteristic of the film will be shown during presentation.

Keywords: Ferroelectricity, dielectric, memory, ALD

We-S-P-50

Dielectric behavior of functional Paint/PMN-PT nanocomposite films

Ashok Batra, Bir Bohara, Mohan Aggarwal, Ravi Lal

AL. A&M University, Huntsville, United States

This article presents, for the first time, the detailed functionality of 0-3 Paint/PMN-PT composite films concerning their dielectric and electric transport characteristics. Paint: Lead Magnesium Niobate-Lead Titanate (Paint/PMN-PT) composite films have been fabricated by the conventional cost effective paint brushing technique. The dielectric parameters of the composite films were calculated by the measurement of capacitance and dielectric loss. The properties investigated include, dielectric constants, ε' and ε'' as a function of temperature, frequency and composition. From the foregoing parameters, it is

indicated that the dielectric constants and A. C. conductivity (σAC) increase with increase of filler content, and temperature, implying functionality of the films. The results reveal that σ_{AC} obeys the relation $\sigma_{AC} = A\omega^s$, and exponent s, was found to decrease by increasing the temperature. It was found that, the correlated barrier hopping (C. B. H.) is the dominant conduction mechanism in nanocomposite films fabricated.

Keywords: Dielectric, Composites, PMN-PT, Paint

We-S-P-51

Investigation on the structural, dielectric, ferroelectric, and magnetic properties of BNTFCO ceramics

Margarita Correa [1], Claudia Zuluaga [1, 2], Ram Katiyar [2]

[1] *Universidad del Atlantico, Barranquilla, Colombia*
[2] *University of Puerto Rico, Puerto Rico, United States*

In this work we present the results of the investigation on the structural, dielectric, ferroelectric, and magnetic properties of $Bi_{4.15}Nd_{0.85}Ti_3Fe_{0.5}Co_{0.5}O_{15}$ (BNTFCO) ceramics. BNTFCO compounds were prepared by mechanical activation followed by heat treatments. The formation of the Aurivillius structure was confirmed by XRD. The unit cell was found to be orthorhombic with cell parameters a = 3.7996 Å, b = 3.6263 Å, c = 2.7217 Å and $\alpha = \beta = \gamma = 90°$. The magnetic measurements at room temperature showed well-behaved and saturated M-H hysteresis loop, typical of ferromagnetic behavior. On the other hand, the room temperature P-E hysteresis loop, although well-behaved, is not well saturated. Even though the sample clearly has ferroelectric property, this is poor in spite of Nd substitution. However, the M-H and P-E hysteresis loops, confirm that BNTFCO compounds is a RT single phase multiferroic.

Keywords: Aurivillius, multiferroics, ceramics.

We-S-P-52

NSMM Review – Part III: *Pm3m* coordination and temperature dependent *radii*

YuHusn Liao, Vignaswaran K. Veerapandiyan, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven C. Tidrow

Alfred University, Alfred, United States

Using geometric considerations within ionic radii space, from "NSMM Review – Part II", we report the genome-like ionic radii properties of twelve, twelve-fold coordinated A-site ions Ag^{1+}, Cs^{1+}, K^{1+}, Na^{1+}, Rb^{1+}, Ba^{2+}, Ca^{2+}, Eu^{2+}, Pb^{2+}, Sr^{2+}, Ce^{3+}, La^{3+} , twenty-two, six-fold coordinated B-site ions Ca^{2+}, Mg^{2+}, Mn^{2+}, Pb^{2+}, Al^{3+}, Ce^{4+}, Cr^{4+}, Hf^{4+}, Mo^{4+}, Os^{4+}, Pb^{4+}, Pr^{4+}, Ru^{4+}, Sn^{4+}, Ce^{4+}, Tb^{4+}, Tc^{4+}, Ti^{4+}, U^{4+}, Zr^{4+}, Nb^{5+}, Ta^{5+}, U^{5+}, and, four, six-fold coordinated C-site anions O^{2-}, F^{1-}, H^{1-}, I^{1-}. These genome-

like ionic radii properties are utilized to determine ionic polarizabilities as discussed in "NSMM Review – Part IV". The coordination and temperature dependent "effective" ionic radii, along with additional structural information, provide significant improvement in determining the temperature dependent position of atoms which provide improved seed positions for more sophisticated modeling approaches, including computationally intense algorithms. NSMM thus provides useful information by itself while also reducing the computation time necessary to yield a broader range of material properties not yet fully addressed using NSMM.

Keywords: *Coordination and temperature dependent ionic radii, Goldschmidt's factor, Shannon ionic radii, temperature dependent lattice parameter, temperature dependent lattice volume*

We-S-P-53

NSMM Review – Part IV: coordination and temperature dependent polarizabilities

Vignaswaran K. Veerapandiyan, YuHusn Liao, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven C. Tidrow

Alfred University, Alfred, United States

Using improved temperature dependent unit cell volume, from "NSMM Review – Part III", within the Clausius – Mossotti relation, we update the reported genome-like ion properties, polarizabilities, of ten, twelve-fold coordinated A-site ions Ag^{1+}, K^{1+}, Na^{1+}, Ba^{2+}, Ca^{2+}, Eu^{2+}, Pb^{2+}, Sr^{2+}, Ce^{3+}, La^{3+} , five, six-fold coordinated B-site ions, Al^{3+}, Sn^{4+}, Ti^{4+}, Nb^{5+}, Ta^{5+}, and the C-site anion O^{2-}, within materials possessing symmetry. In combination, the coordination and temperature dependent genome-like ion properties, radii, and polarizability can be used to predict/model a wide range of temperature dependent material properties, including but not limited to lattice parameter and volume, relative permittivity, polarization-induced structural phase transition temperature, and, volume-induced structural phase transition with both types of structural phase transitions discussed in "NSMM Review – Part V".

Keywords: coordination and temperature dependent polarizability, Shannon polarizability, polarizability, Clausius - Mossotti relation, polarization induced structural phase transitions

---

We-S-P-54

Growth and characteristics of the $CH_3NH_3PbBr_3$ perovskite crystal for optoelectronic applications

Raja Surabhi, Ashok Batra, Kamala Bhat, Samuel Uba, Ashwith Chilvery

AL. A&M University, Huntsville, United States

Organic and inorganic hybrid perovskites (e.g., $CH_3NH_3PbBr_3$), with advantages of simplistic processing techniques, tunable bandgaps, and superior charge-transfer properties, have emerged as a new class of innovatory optoelectronic semiconductors promising for various applications including

light-emitting diodes, photodetectors, and transistors. Perovskite solar cells fabricated with a variety of configurations have demonstrated unparalleled progress in efficiency in the recent past, reaching more than 20% from multiple research groups around the world. Both experimental and theoretical investigations on this hybrid perovskites have enabled some critical fundamental understandings of this hybrid system. There are major challenges for further research on halide perovskites including basic chemical and crystal structures, chemical synthesis of bulk/nanocrystals and thin films, device configurations, operation principles for various optoelectronic applications with a focus on solar cells. To broaden and boost their optoelectronic and photovoltaic performance, it is highly desirable and necessary to grow single crystal of organo-lead trihalide hybrid perovskites and investigate electronic and optical properties. Single crystals of hybrid perovskites should have long carrier diffusion lengths and remarkably low-trap densities than their polycrystalline thin film counterpart. There have been limited studies to comprehend the basic properties of resulting single crystals. Our present study presents the simple process of single crystal growth and offers a material platform for fundamental investigation of structural, electronic, and optical properties of perovskite materials such as methyl ammonium lead bromide ($CH_3NH_3PbBr_3$).

Keywords: Hybrid Perovskite, Crystal, Methyl Ammonium Lead Bromide

---

We-S-P-55

NSMM Review – Part V: Polarization and volume induced structural phase transitions

Vignaswaran K. Veerapandiyan, YuHusn Liao, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven Tidrow

Alfred University, Alfred, United States

Using temperature dependent genome-like ion properties, radii and polarizability, as discussed in "NSMM Review – Part III and Part IV, respectively, we demonstrate the ability of NSMM to identify and *a priori* predict both polarization- and volume-induced structural phase transitions of "simple" and "simply mixed" *Pm*3*m* Perovskites. In combination with geometric considerations, these results allow us to physically understand why the majority of "simple" and "simply mixed" Perovskites are not cubic *Pm*3*m* at room temperature and thus why so many of them undergo structural phase transitions from the prototypic cubic symmetry. Further, we demonstrate the ability of NSMM to predict the temperature dependent relative permittivity of some Perovskite materials.

Keywords: temperature dependent structural phase transitions; polarization-induced structural phase transitions; volume-induced structural phase transitions; polarization- and volume-induced structural phase transitions

---

We-S-P-56

NSMM Review – Part VI: Clausius – Mossotti relation incorporates Curie and Curie – Weiss laws

Vignaswaran K. Veerapandiyan, YuHusn Liao, Walter A. Schulze, Scott T. Misture, Steven M. Pilgrim, Steven C. Tidrow

Alfred University, Alfred, United States

The classical Clausius – Mossotti relation links relative permittivity to fundamental properties of the atom, e.g., *radii* and polarizability. The Clausius – Mossotti relation also incorporates the Lorentz – Lorenz relation which links index of refraction of materials to fundamental properties of the atom, radii and polarizability. Further, the Curie and Curie – Weiss Laws of ferroelectrics like their magnetic counterparts are correlation relations. Here, using the coordination and temperature dependent ion properties, radii and polarizability, as taken from "NSMM Review – Part III" and "NSMM Review – Part IV", respectively, we demonstrate that the fundamental Clausius – Mossotti relation effectively subsumes both the Curie and Curie – Weiss Laws. Further, we show that the linkage between the experimentally or empirically determined material parameters of Curie constant and Curie temperature are through fundamental ion properties. Such linkages are discussed in some detail with several examples provided that demonstrate that NSMM provides a method for *a priori* predicting or at least reasonably accurately modeling material Curie constants and Curie temperatures of materials.

Keywords: Clausius - Mossotti relation; Curie Law; Curie - Weiss Law; polarization induced structural phase transitions; relative permittivity catastrophe

---

We-S-P-57

First principles studies in $Bi_{1-x}Nd_xFeO_3$ compositions

Gabriel H. Perin [1], Gustavo S. Dias [1], Ivair A. Santos [1], Ruyan Guo [2], Amar Bhalla [2], Jose E. Padilha [3], Luiz F. Cotica [1]

[1] *Department of Physics - State university of Maringa, Maringa, Brazil*
[2] *Department of Electrical and Computer Engineering - University of Texas at San Antonio, San Antonio - TX, United States*
[3] *Federal University of Parana at Jandaia do Sul, Jandaia do Sul - PR, Brazil*

Due to technological development, there is more and more need for new materials, which provide new properties and functions; the multiferroic materials are among these materials, and a well-known and studied composition is the $BiFeO_3$. By modifying this material by substitution with different atoms, it is possible to change its electrical and magnetic properties. In this work, by means of first principles Density Functional Theory calculations, we investigated the structural, electronic and magnetic magnetic properties of $Bi_{1-x}Nd_xFeO_3$ compositions. To take into account the random distribution of Nd, we used the Special Quasirandom Structure procedure to obtain the structure for each concentration x, ranging from 0.0 to 1.0. The study of the electron density showed that the neodymium doping causes distortions in the structure, and consequently changes the electronic, electrical and magnetic properties. In the band structure and density of states analyses, it was possible to see that the neodymium doping

leads to a decrease in the energy gap, and the contribution to the magnetization of the $Bi_{1-x}Nd_xFeO_3$ ompositions is caused by the iron 3d and the oxygen 2p orbitals.

Keywords: BiFeO3, electronic structure

We-S-P-58

Probing the pore structure of a chiral periodic mesoporous organosilica using liquid crystals

jayalakshmi vallamkondu [1], P. Lemieux Robert [2]

[1] *NIT Warangal, India, Warangal, India*

[2] *Queen's University, Kingston, Ontario, Canada, Kingston, Canada*

Periodic mesoporous organosilicas (PMO) are prepared by the surfactant-templated condensation of bridged organosilsesquioxane monomers. By controlling the nature of the organic segment, the type of surfactant and the condensation conditions, one can control the physical and chemical properties of the resulting PMO and produce highly ordered porous structures with a periodicity on the nanometer scale. The development of chiral PMO materials has been of significant interest given their potential in heterogeneous asymmetric catalysis, chiral chromatography and non-linear optics. Characterization of the chirality of pore structures in these materials thus far has been achieved by indirect methods including polarimetry and solid-state circular dichroism. We report herein a general and convenient approach to probe directly the pore structure of chiral PMO materials based on their interactions with inexpensive liquid crystalline solvents, which result in the induction of measurable chiral properties in the nematic (N) and smectic A (SmA) phases of the liquid crystals. The templated co-condensation of a biphenylene organosilsesquioxane monomer and a chiral binaphthyl organosilsesquioxane monomer produced a new chiral PMO material that was investigated as dopant in two different liquid crystal hosts. Measurements of induced circular dichroism and helical pitch in the nematic phase of the cyanobiphenyl liquid crystal 5CB, and the measurement of an induced electroclinic effect in the SmA phase of the phenyl benzoate liquid crystal 9OO4 were carried out. The induced chiral properties measured in these experiments are consistent with chirality transfer taking place inside the pores, and suggest that the inner structure of the pores in the PMO material is indeed chiral.

Keywords: Liquid crystals, mesoporous, helix

We-S-P-59

Meso-kinetics of one time relaxation electrical processes in $BaTiO_3$ ceramics - Boltzmann-Poisson model

Vojislav V.Mitić [1, 2], Zoran B.Vosika [1], Goran Lazović [3], Vesna Paunović [1], Ljubiša Kocić [1]

[1] *University of Niš, Faculty of Electronic Engineering, Niš, Serbia*
[2] *Institute of Technical Sciences of SASA, Belgrade, Serbia*
[3] *University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia*

Positive temperature coefficient of resistivity (PTCR) materials are widely used in the electronics industry for applications including temperature sensors, overheat protection, time delay circuits and current limiters for overvoltage or overcurrent protection, current stabilisers etc. In this respect, doped barium-titanate ceramics has attracted a considerable attention for small size processing and designing. AC conductivity studies of various BaTiO3 or similar ceramics produced equivalent circuits used for the impedance spectra fitting within the framework of RCPE elements serial connection (CPE-constant phase element), as a generalization of the Cole element. They corresponds to details of the ceramics grains structure and its dynamics: grain interior boundary, grain boundary, free electrons concentration, etc. which is typical behavior of diffuse ferroelectric or relaxor materials. One of models that explains PTC effect is the Heywang model, in terms of grain boundaries potential barriers of the Shottky type. In order to consider quantum transport under the influence of an electron-electron interaction in a mesoscopic conductor, the Boltzmann-Poisson model is investigated jointly. In this presentation it will be considered an improved version of the existing model that corresponds to correct quadratic relation for varistor effect in the case of Heywang potential, in the approximation of one relaxation time for the Cole element. Validity conditions of this new model will be discussed.

Keywords: BaTiO3-ceramics, dielectrics, kinetics, Heywang model

---

We-S-P-60

Preparation and characterization of PAN-EC-PC-TPAI-I_2 gel polymer electrolytes for dye-sensitized solar cells

Faisal Chowdhury

1. Center for Ionics University of Malaya, Department of Physics, University of Malaya, 50603 Kuala Lumpur, Malaysia 2. Department of Chemistry, University of Chittagong, Chittagong-4331, Bangladesh, Kuala Lumpur, Malaysia

Gel polymer electrolytes (GPEs) consisting of polyacrylonitrile (PAN) polymer, ethylene carbonate (EC) and propylene carbonate (PC) plasticizers and different compositions of tetrapropylamonium iodide (TPAI) salt have been prepared and investigated for the application in dye-sensitized solar cells (DSSCs). The electrochemical impedance spectroscopy (EIS), linear sweep voltammetry (LSV), X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy techniques have been utilized to characterize the GPEs. From the EIS study lowest bulk impedance, R_b (17 Ω) and highest ionic conductivity (4.72×10^{-3} S.cm^{-1}) have been observed for the GPE containing 30 wt. % TPAI. The highest apparent diffusion coefficient of triiodide ion is 5.5×10^{-7}cm^2 s^{-1} at 0.051 (g) I_2 containing GPE with 30 wt. % of TPAI. Functional group interactions among PAN, EC, PC, and TPAI have been observed in FTIR spectra of the GPEs. An up-shift of XRD peak indicates the polymer-salt interaction and possible complexation of cation (TPA^+ ion) with lone pair electron containing site (-CºN) in the host polymer matrix at the N atom. The DSSC with this GPE (30% TPAI) shows highest

efficiency of 4.76% and short circuit current density of 19.74 mA.cm^2, open circuit voltage of 553.8 mV and fill factor 0.44.

Keywords: Gel Polymer Electrolyte; Electrochemical impedance spectroscopy (EIS); Linear sweep voltammetry (LSV); X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy techniques, Dye Sensitized Solar Cells (DSSC)

We-S--61

Keywords:

We-S-P-62

On the „inverted" phase transitions in ferroic crystals containing propylenediammonium cations

Janusz Przesławski [1], Matthew Crofton [1], Zbigniew Czapla [2]

[1] *Institute of Experimental Physics, University of Wroc?aw, Pl. M. Borna 9, 50-204 Wroc?aw, Poland, Wroc?aw, Poland*
[2] *Department of Physics, Opole University of Technology, Ozimska 75, 45-271 Opole, Poland, Opole, Poland*

In some hybrid crystals with a perovskite-like structure containing propylenediammonium cations ($NH_3(CH_2)_3NH_3$) and layered metal-halogen anionic sublattices, a "inverted" sequence of the symmetry change was observed. The change of symmetry from higher to lower one was detected during heating. Such reduction of the structure symmetry from orthorhombic to monoclinic was found for e.g. in $(NH_3(CH_2)_3NH_3CdBr_4$ and $[NH_3(CH_2)_3NH_3]CuCl_4$ crystals. The aim of the work is to give a more detailed description of the domain structure changes during the "inverted" transitions. It was shown that the orthorhombic mmm phase should be regarded as the prototype phase for the ferroelastic transition to the monoclinic phase. A critical index for the order parameter was determined from the temperature dependence of the linear birefringence at the continuous transition between orthorhombic phases.

Keywords: organic-inorganic compounds; phase transitions; linear birefringence; ferroelastic domains

---

We-S-P-63

The effect of fluorine doping on structural and dielectric properties of Diisopropylammonium bromide

Thirmal Chinthakuntla [1], Ratnamala Chatterjee [1], Simant Srivastav [1], Murugavel Pattukannu [2], Atalbihari Swain [2], Divyanshu Bhatnagar [1]

[1] *Indian Institute of Technology Delhi, New Delhi, India*
[2] *Indian Institute of Technology Madras, Chennai, India*

Organic molecular ferroelectrics are highly desirable due to their numerous advantages such as eco-friendly, light-weight, cost-effective, scalability, and low processing temperatures. The recent discovery of ferroelectricity in organic diisopropylammonium bromide - $C_6H_{16}NBr$ (DIPAB) single crystal renewed interest on this compound because of its large polarization (23 $\mu C/cm^2$) and good thermal stability (from 426 K down to liquid nitrogen temperature). In the present study, we have modified DIPAB with fluorine doping at bromine site. The resultant fluorine modified DIPAB polycrystalline samples are explored for their structural, thermal, dielectric properties. The Rietveld refinement has been done on the X-ray diffraction patterns to understand the structural properties whereas the dielectric and impedance spectroscopy are used to explore the dielectric relaxation in the samples. The different contributions for the dielectric relaxation and ac conductivity have been understood.

Keywords: DIPAB, dielectric, ferroelectric

We-S-P-64

Dielectric and impedance spectroscopic studies of pristine and lanthanum substituted $YBiO_3$

Divyanshu Bhatnagar, Thirmal Chinthakuntla, Ratnamala Chatterjee

Magnetics and Advanced Ceramics Laboratory, Physics Department, Indian Institute of Technology Delhi, New Delhi, India

YBiO3 has recently attracted the scientific community due to its novel properties such as high ionic conductivity, excellent photo-catalytic behavior and electrolyte material for solid oxide fuel cells. In this work, pristine and La doped YBiO3 (YBi1-xLaxO3 ($0.00 \leq x \leq 0.05$)) samples were successfully synthesized through co-precipitation. The phase purity of the synthesized samples has been confirmed by XRD measurements. All the samples were found in FCC structure; Rietveld refinements of the series YBi1-xLaxO3 ($0.00 \leq x \leq 0.05$) samples show that the lattice parameter varies from 5.42 Å to 5.46 Å as x changes from 0 to 0.05. The Raman spectrum of YBi1-xLaxO3 ($0.00 \leq x \leq 0.05$) samples revealed the existence of all five Raman active modes of fluorite structure, in agreement with XRD data. From the scanning electron micrographs it is evident that there is a continuous increase in grain size with increasing lanthanum concentration (from ~ 1 μm (for x = 0) to ~ 10 μm (for x = 0.05)). The temperature dependent dielectric spectra reveal a relaxation above 550 °C in YBO. The relaxation temperature reduces to ~400 °C for x = 0.05. Further, dielectric measurements show that the value of dielectric constant enhanced with lanthanum incorporation. The impedance spectroscopy measurements confirmed that the observed relaxation is of the non-Debye type and that the resistance increases with increase in temperature. The contribution of grains and grain boundary in resistance is also understood.

Keywords: YBiO3, Rietveld Refinement, Dielectric Studies, Impedance Spectroscopy, Nyquist Plots

---

We-S-P-65

Investigation of ferroelectric properties by using Monte Carlo simulations

Se-Hun Kim

Jeju National University, Jejusi, Korea, Republic of (South)

We carried out Monte Carlo simulations of the pseudo-spin Ising model in 2-dimensional ferroelectric structure. The Metropolis method was employed by studying the size dependence of the dielectric properties and the heat capacity of a two-dimensional ferroelectric system. The critical phenomena in the vicinity of the phase transition temperature was considered by the the values of critical exponents in view of the large-scale of lattice.

Keywords: Ferroelectrics, Ising model, Finite size scaling, Monte Carlo simulation

---

We-S-P-66

Multiple bandgaps of ferroelectric based two-dimensional phononic crystals slab with Archmedes and Fibonacci spiral holes

Amirullah Mamedov [1, 3], Selami Palaz [2], Oral Oltulu [2], Ekmel Ozbay [1]

[1] *Bilkent University, Nanotechnology Research Center, Ankara, Turkey*
[2] *Department of Physics, Harran University, URFA, Turkey*
[3] *International Research Center, Baku State University, Baku, Azerbaijan*

Phononic crystals (PCs) are media with periodically varying elastic properties and mass densities. In present paper we report the numerically investigations the spatio-spectral sound transmission properties and complete bandgaps of ferroelectric based 2D PCs slabs with Archimedes and Fibonacci spiral holes and present a discussion on the effects of negative refraction on the spatio-spectral selectivity of PCs. The transmission and reflection properties of periodic and quasi-periodic structures by using FDTD method were calculated. Also, the dominant mechanisms of acoustic losses in Archimedes and Fibonacci spiral structures are discussed. This study could be indispensable to practical applications of PCs slabs as band gap tuning.

Keywords: phononic crystals, elastic properties, bandgap

We-S-P-67

Electronic band structure and optical properties of $Gd_2(MoO_4)_3$: First Principle calculations

Amirullah Mamedov [1], Sevket Simsek [2], Gokay Ugur [3], Sule Ugur [3], Ekmel Ozbay [1]

[1] *Bilkent University, Nanotechnology Research Center, Ankara, Turkey*
[2] *Department of Material Sciences, Hakkari University, Hakkari, Turkey*
[3] *Department of Physics, Gazi University, Ankara, Turkey*

In the present work, the electronic band structure and optical properties of some $Gd_2(MoO_4)_3$ are investigated. The ground state energies and electronic structures were calculated using density functional theory (DFT) within the generalized-gradient approximation (GGA). The real and imaginary parts of dielectric functions and hence the optical functions such as energy-loss function, the effective number of valance electrons and the effective optical dielectric constant were also calculated. The presence of the MoO_4 tetrahedra in the lattice of $Gd_2(MoO_4)_3$, the similarity of the band structure and optical spectra of $Gd_2(MoO_4)_3$ to those other tetraoxyanions of molybdenium demonstrate an important role of the MoO_4 tetrahedra in the formation of the energy spectrum of $Gd_2(MoO_4)_3$ and other $RE_2(MoO_4)_3$ compounds. This means that the MoO_4 tetrahedra determine the lower edge of the conduction band and the upper edge of the valence band, and the conduction band is split into two subbands.

Keywords: ferroelastics, band structure, ab initio

We-S-P-68

High temperature thermoelectric properties of Sr-rich $Gd_{1-x}Sr_xMnO_3$ based manganites

Tanmoy Maiti, Ritwik Banerjee

Plasmonics and Perovskite Lab,Department of Materials Science and Engineering, IIT Kanpur, India, Kanpur, India

Manganites based oxides have shown promises recently for the applications as n-type thermoelectric materials. In the presnt work, Environment friendly, non-toxic perovskite $Gd_{1-x}Sr_xMnO_3$ (x = 0.5,0.6,0.7,0.8) ceramics were prepared by conventional solid state reaction route.The samples were then examined for their crystal structure (single phase) and morphology by XRD and SEM, respectively. Rietveld refinement of the XRD data of these manganites revealed orthorhombic crystal structure. Electrical conductivity(σ) and Seebeck coefficient (S) were measured in the wide range of temperature from room temperature to 900 K.Negative thermo-power (S) values obtained in these ceramics confirmed the n-type behavior of these manganites. Temerature dependent conductivity measurement showed the signature of metal to semiconductor (M-S) transitions in these samples. Furthermore,the conductivity mechanism of these manganites were explained using variable range hopping and small polaron hopping model.

Keywords: Perovskite,Manganites,Sr-rich,Thermopower,Metal to semiconductor(M-S) transitions

---

We-S-P-69

Structural and electrical properties of charge compensated dipole pairs substituted barium titanate

Vignaswaran Kaliyaperumal Veerapandiyan, Mackenzie Stevens, Steven Tidrow

Kazuo Inamori School of Engineering, Alfred University, Alfred, United States

Structural and electrical properties of $Ba[(Ga,Ta)_{0.05}Ti_{0.9}]O_3$ and $Ba_{0.8}Sr_{0.2}[(Ga_{0.05},Ta_{0.05})Ti_{0.9}]O_3$ have been characterized to determine the effects of charge compensated dipole pairs (Ga^{+3}, Ta^{+5}) on temperature-dependent material properties. XRD and Rietveld analysis have been used to determine lattice parameters, phase transition temperature(s), and coefficients of thermal expansion from RT to 1000 ^oC. Capacitance measurements have been conducted over the temperature range -180 ^oC to 200 ^oC and frequency range 100 Hz to 1 MHz to investigate the dielectric properties, including Curie temperature. $Ba[(Ga,Ta)_{0.05}Ti_{0.9}]O_3$ has a maxima in the relative permittivity curve that correspond to the tetragonal to cubic phase transition which is consistent with the Rietveld refinement of XRD data. The ε_r value for $Ba[(Ga_{0.05},Ta_{0.05})Ti_{0.9}]O_3$ is 600 at 100^oC and varies by ~ 25% over the temperature range [RT, 170]. Sr substitution for Ba in the A-site of dipole pair substituted ABO_3 is used to investigate the possibility of further increasing the relative permittivity value while maintaining the same trend of temperature insensitivity of relative permittivity. Experimental results are compared with several currently utilized models in an effort to better understand the effect of randomly dispersed charge compensated dipole pairs have on temperature-dependent material properties.

Keywords: Barium titanate, dipole-like substitution

We-S-P-70

First Principles study of piezoelectric properties and morphotropic phase boundary of $AgNbO_3$-based solid solutions

Sittichain Pramchu, Atchara Jaroenjittichai, Yongyut Laosiritaworn

Department of Physics and Materials Science, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand

Unique properties of piezoelectric materials in generating electrical voltage suggested to mechanical strain (and vice versa) grants the piezoelectric utilization over a wide range of applications. In general, superior piezoelectricity usually occurs at morphotropic phase boundary (MPB) of the considered compounds. However, to synthesis materials having compositions lying this MPB is not trivial. This work therefore theoretically concentrated on pursing how to arrive in MPB of some promising piezoelectric materials using density functional theory (DFT). DFT with plane-wave pseudopotential method was employed for the calculation. xKNbO$_3$−(1-x)NaNbO$_3$(KNN) with known MPB composition of x = 0.5 was used to validate the calculation. Then, $AgNbO_3$-based compounds, which inherits large polarization and high piezoelectric performance such as xAgNbO$_3$-(1-x)KNbO$_3$(ANKN), xAgNbO$_3$-(1-x)BaTiO$_3$(ANBT), and xAgNbO$_3$−(1-x)SrTiO$_3$(ANST), were chosen in this MPB compositional investigation. Form the results, MPB composition of KNN of x = 0.5 was computationally suggested, implying our calculation method for MPB is reliable. Further results indicate that ANKN exhibits structural phase transition between *Bmm*2 and *Pbma* crystal symmetry at $x \approx 0.2$ and 0.8. Also, there

occur two MPB compositions at $x = 0.125$ and 0.5 for ANBT (with phase transition between *P*4*mm* and *Pbma*), but no MPB for ANST. In addition, ANBT with $x \approx 0.5$ displays large polarization of about 44 $\mu C/cm^2$, suggesting ANBT-based compound a potential piezoelectric material for further development of piezoelectric-based device.

Keywords: piezoelectric materials, AgNbO3-based compounds, DFT, MPB

We-S-P-71

Thickness dependence of dynamic phase diagram in ferroelectric films: Monte Carlo and Neural Network investigation

Wimalin Laosiritaworn [1], Yongyut Laosiritaworn [2]

[1] *Department of Industrial Engineering, Faculty of Engineering, Chiang Mai University, Chiang Mai, Thailand*
[2] *Department of Physics and Materials Science, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand*

On moving to information technology era and the green-and-clean environment, high capacity, fast to access, and low power consumption digital media has gained great interest. The solid state drive consisting of ferroelectric layers has been chosen as promising candidate. However, due to the complexity of the ferroelectric structure, there are some incomplete pictures in describing/predicting ferroelectric phenomena especially in low dimensions. For instance, the generally considered Landau-Hamiltonian discards thermal fluctuation which is important close to the critical point, and the spin-Hamiltonian lacks of appropriate thermodynamic-limit description of ferroelectric phase transition. This work then combines both Hamiltonians and investigates using Monte Carlo simulation. With applied periodic electric field, the dynamic hysteresis behavior was investigated as functions of films' thickness, temperature, and field parameters. The dynamic critical point, separating the symmetric from the asymmetric hysteresis loop, was extracted as varying field parameter and films' thickness to draw dynamic phase diagrams. Artificial Neural Network was used to draw further details of hysteresis profiles among simulated conditions. The results show that dynamic critical point becomes higher with increasing field frequency as more thermal/electrical energy is required to compensate the faster field switching. Further, the critical point also increases with increasing the films' thicknesses due to the stronger ferroelectric interaction in thicker films. Different dipole interaction ranges show different critical magnitude but agree qualitatively. In addition, the results are in good qualitative agreement with experiments on ferroelectric films, where applicable.

Keywords: artificial Neural Network ferroelectric films, dynamic phase diagram

---

We-S-P-72

Low-frequency noise characteristics of $CuInP_2S_6$ lamellar crystal

Andrius Dziaugys [1], Ilona Zamaraite [1]

[1] *Faculty of Physics, Vilnius University, Vilnius, Lithuania*
[2] *Institute of Solid State Physics and Chemistry of Uzhgorod University, Uzhgorod, United States*

Low frequency noise with 1/*f*-type spectra has been observed in a wide variety of systems including fluctuations in resistors, various materials or even intensity fluctuations in music. Nevertheless, 1/f noise (or flicker noise) is a controversial phenomenon because the physical mechanism that gives rise to the manifestation of this noise type is still a point of debate. Thus, a considerably small number of papers have been dedicated to the investigation of noise in ferroelectrics [1,2]. In this work detailed investigation of low frequency noise characteristics of $CuInP_2S_6$ will be presented. To obtain a deeper insight into the phenomena of 1/*f* noise in $CuInP_2S_6$ crystal in the vicinity of phase transition, we investigated normalized voltage fluctuation density having a spectra of Lorentzian-type. In this study we tried to explain observed relaxational physical processes in the phase transition region based oneself on the carrier numbers fluctuation.

P. Jain et al.

[1] J. Banys, T. Ramoska, J. Matukas, S. Pralgauskaite, F. M. M. Alwaneh, V. V. Shvartsman and D.C. Lupascu. Ferroelectrics 417, 25-32 (2011).

[2] S. Pralgauskaitč, J. Matukas, R. Grigalaitis, J. Banys, I. Zamaraitč, M. M. Vitajovic Petrovic, J. D. Bobic, B. D. Stojanovic. Noise and Fluctuations (ICNF), International Conference on, Xian, 2015, 1-4 (2015).

Keywords: ferroelectrics, noise spectroscopy, dielectric spectroscopy

---

We-S-P-73

Effects of MnO_2 doping on the electrical properties of 0.99BCZT-0.01Seeds ceramic systems

Piewpan Parjansri [1], Sukum Eitssayeam [2]

[1] *Physics Division, Faculty of Science and Technology, Rajamangala University of Technology Krungthep, Bangkok, Thailand*
[2] *Department of Physics and Materials Science, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand*

This work investigated the electrical properties of BCZT-1.0 mol% BCZT-seeds ceramic systems doped with x mol% MnO_2. The BCZT seed was synthesized via molten-salt method. Then, the MnO_2 and 1.0 mol% BCZT were mixed with the starting materials of $Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O_3$ ceramics and prepared by mixed oxide method. The effect of MnO_2 on electrical properties of BCZT-BCZT seed ceramic was investigated. Results were found that the ceramics showed perovskite phase and no secondary phase for all samples. Density and grain size values were in the range of 5.45-5.57 g/cm^3 and 6.79-9.85 μm, respectively. The highest values of ε_r and P_r measured at room temperatures were 3900 and 8.22 μC/cm^2,

respectively which obtained at the sample of 1.0 mol% MnO_2. Tan δ of ceramic samples were lower than 0.02. In addition, d_{33} and g_{33} values were changed with MnO_2 content.

Keywords: electrical properties, perovskite, lead-free ceramics, seed-induced, BCZT ceramics

---

We-S-P-74

Phase relations in the Bi_2O_3-Mn_2O_3-M_2O_3 (M = Fe, Al, Ga) pseudo-ternary systems

Sreco Skapin [1], Amalija Golobic [2], Danilo Suvorov [1]

[1] *Jožef Stefan Institute, Ljubljana, Slovenia*
[2] *Faculty of Chemistry and Chemical Technology, Ljubljana, Slovenia*

Some Bi-based ceramics have been recently extensively studied due to their interesting ferroelectric, magnetic and multiferroic properties. In the present investigation a subsolidus high-temperature phase relations in air were determined in the systems: (1) Bi_2O_3-Mn_2O_3-Fe_2O_3, (2) Bi_2O_3-Mn_2O_3-Al_2O_3 and (3) Bi_2O_3-Mn_2O_3-Ga_2O_3. The samples were prepared by wet method from nitrates and/or acetate in order to obtain well homogenized starting powder, which were additionally fired at temperatures 760-790 °C until equilibrium was reached. Based on the X-ray powder diffraction data, relevant phase diagrams were constructed. Sillenite-like phases in all three systems form solid solution in entire compositional range, however, perovskite-related compounds $Bi_2M1_4O_{9+\delta}$ (M1 = Mn, Fe, Al, Ga) form solid solutions in limited range, and their extension depends on the system. Solid solubility regions and structural properties of the solid solutions were determined with detailed XRD analysis.

Keywords: Ferroelectrics, Phase Diagrams, Ternary Systems

We-S-P-75

Sintering behavior, phase structure and electric properties of KNNTS-BKNZ ceramics with excessive alkali metals

Rui Nie, Xing Xing, Jiagang Wu, Qiang Chen, Wen Zhang, Jianguo Zhu, Dingquan Xiao

College of Materials Science and Engineering, Sichuan University, China, Chengdu, China

$0.96(K_{0.48}Na_{0.52})_{1+x}Nb_{0.93}Sb_{0.02}Ta_{0.05}O_3$-$0.04Bi_{0.5}(K_{0.12}Na_{0.88})_{0.5}ZrO_3$ [$(KN)_x$NTS-BKNZ] lead-free piezoelectric ceramics were prepared by conventional solid-state reaction method. The effects of excessive alkali metals on the sintering character, phase structure, dielectric, piezoelectric, and ferroelectric properties were systematically explored. The sintering temperature of $(KN)_x$NTS-BKNZ ceramics gradually increases and the sintering temperature zone becomes narrow with the increasing x value. The coexistence of rhombohedral and tetragonal phases has been found in $(KN)_x$NTS-BKNZ ceramics when $0 \leq x \leq 0.03$. When $x \leq 0.03$, the ceramics show a continuous increasing of T_{R-T}, T_C, d_{33}, and εr with the increasing x. The maximal piezoelectric coefficient d_{33} of 415 pC/N was obtained at x = 0.03. In addition, these ceramics presented a good temperature stability in piezoelectricity. This study

exhibits that excessive alkali metals make a great impact on sintering character and electric properties on KNN ceramics. It was believed that this work would be helpful for further enhancing piezoelectric properties in KNN ceramics.

Keywords: Dielectrics, Ferroelectrics, Ceramics

We-S-P-76

Dielectric, Electrical Conduction, Piezoelectric and Impendence Analysis of Bi_3TiNbO_9 Piezoceramics with Ce-Modifications

Jing Yuan, Rui Nie, Jianguo Zhu

College of Materials Science and Engineering, Sichuan University, Chengdu, China

In the present work cerium substituted ceramics sample of compositions $Bi_{3-x}Ce_xTiNbO_9$ (x = 0.0 ~ 0.10) were synthesized by solid state reaction method. The crystal structure, dielectric, electrical conduction, piezoelectric and Impendence properties were systematically studied. Pure or modified Bi_3TiNbO_9 ceramics revealed the presence of only two-layer Aurivillius phase, indicating that Ce doping entered the A-site of pseudo-perovskite structure and formed solid solutions. Furthermore, Ce dopants act as a donor doping, increase the DC resistivity (1.5×10^6 Ω.cm at 500 ºC and 2.1×10^5 Ω·cm at 600 ºC)and piezoelectric properties. $Bi_{2.93}Ce_{0.07}TiNbO_9$ ceramics possess the optimum d 33 value (~17 pC/N) together with a high T C point (883 ºC). The d_{33} value of $Bi_{2.93}Ce_{0.07}TiNbO_9$ eramic remains ~ 13.3 pC/N after annealing at 500 ºC. These factors suggest that the Ce doping Bi_3TiNbO_9 ceramic is a promising candidate for ultra-high temperature sensor applications. The detailed electrical properties for Ce-doping Bi_3TiNbO_9 ceramics in the high temperature region were determined using electrochemical impedance spectra. It was found that oxygen vacancies make a major contribution of both electrical conduction and dielectric relaxation.

Keywords: Dielectric relaxation, electrical conduction, ferroelectrics

---

We-S-P-77

Stress dependence of structure, electronic and optical properties of $BaTiO_3$ from WC, VdW-DF-C09 and HSE Functional calculations

Eleicer Ching-Prado

Department of Natural Science, Faculty of Science and Technology, Technological University of Panama, Panama City, Panama

Optimization of $BaTiO_3$ crystal unit cell was realized with WC and VdW-DF-C09 exchange-correlation functional under different hydrostatic pressure from -100 to 100 GPa. Thus, changes in the crystal lattice parameters and volume are presented and discussed, as well as changes in the different Ba-O and Ti-O bond lengths. While the self-consistent calculations (scf) were realized using HSE functional in order

to obtain electronic band structure, density of state (DOS) and optical properties. Löwdin charge analysis, related to charge transfer of Ba, Ti, and O, shows the nature of the atomic bonds as function of the hydrostatic stress, including the contribution of empty orbits 6p, 5d and 4f from Ba atoms, 3d and 4f from Ti atoms and 3d and 4f from O atoms. Finally, the dielectric function imaginary part spectra, from 0 to 15 eV, are presented and discussed.

Keywords: Simulations, Functional Calculations, Optical Properties

---

We-S-P-78

Enhanced performance in AZO based transparent flexible TFTs due to oxygen vacancy in ZnO film with Zn-Al-O interface fabricated by atomic layer deposition

Yang Li, Huanhuan Wang, Jinzhu Wuand, Xiaohong Wu

Harbin Institute of Technology, Harbin, China

Highly conductive and optical transparent Al doped ZnO (AZO) thin film composing of ZnO with Zn-Al-O interface was fabricated by thermal atomic layer deposition (ALD) method. The as-prepared AZO thin film exhibits excellent electrical and optical properties, with high stability and compatibility with temperature-sensitive flexible photoelectronic devices: film resistivity is as low as 5.7×10^{-4} Ω·cm; the carrier concentration is high up to 2.2×10^{21} cm^{-3}; optical transparency is greater than 80 % in a visible range; the growth temperature is below 150 °C on the PEN substrate. Compared with the conventional AZO film containing by ZnO and Al_2O_3 interface, we propose that the underlying mechanism of the enhanced electrical conductivity for the current AZO thin film is attributed to the oxygen vacancies deficiency derived from the free competitive growth mode of Zn-O and Al-O bonds in Zn-Al-O interface. The flexible transparent transistor based on this AZO electrode exhibits the favorable threshold voltage and Ion/Ioff ratio, showing promising for use in high resolution, fully transparent and flexible display applications.

Keywords: ZnO, Films, Dielectrics

We-S-P-79

Anomalous dielectric behaviour in Cr^{3+} substituted $Ba_{0.90}Sr_{0.10}TiO_3$ ferroelectric ceramics

Parveen Kumar, Chandra Prakash, K.K. Raina

DIT University, India, Dhradun, India

Polycrystalline ferroelectric ceramic samples of Cr^{3+} substituted $Ba_{0.90}Sr_{0.10}TiO_3$ were prepared by the solid state reaction method. The samples were substituted with Cr^{3+} at Ti-site up to 2 mol%. X-ray diffraction analysis confirmed the formation of single phase perovskite tetragonal structure with space group *P*4*mm*. Dielectric properties were measured as a function of temperature at different frequencies. Dielectric peak for all the samples can be noticed which is a typical ferroelectric to paraelectric

transition. It was found that for the sample with 2% Cr^{3+} abnormal dielectric behaviour can be noticed within a small temperature range near transition temperature. The dielectric constant was found to increase with increase in frequency in this temperature range. Furthermore, the transition temperature shifts towards lower temperature as the frequency increases. The detailed study of structural and dielectric properties were done and discussed here.

Keywords: Dielectrics, ferroelectrics

We-S-P-80

Dielectric properties of HHTP-4H2O cold pressed pellets

Sergejus Balčiūnas [1], Anna Peterson [2], Maksim Ivanov [1], Jasper Adamson [2], Jūras Banys [1]

[1] *Vilnius University, Vilnius, Lithuania*

[2] *National Institute of Chemical Physics & Biophysics, Estonia, Estonia, Estonia*

The idea that water molecules can be translated into a polar form of ice was introduced in early 1933 in a paper written by J. D. Bernal and R. H. Fowler. More recent studies have shown that low-dimensional polar ice can be obtained through dimensionality reduction in confined phases like in water filled carbon and inorganic nanotubes. However, in those systems the switchable bulk dipolar alignment of polar ice is difficult. Therefore, this pursuit has shifted to exploiting polar ice confined in crystalline voids. In this poster presentation, dielectric properties of 2,3,6,7,10,11-hexahydroxytriphenylene tetrahydrate cold pressed ceramics will be presented. The measurements of dielectric permittivity was performed using HP 4284A precision LCR meter and P(E) curves were obtained using AixACCT TFAnalyzer 2000 E system. The dielectric spectra show an anomaly at 256 K temperature. Furthermore, it can be noted that the temperature dependence curves are close to following the Curie Weiss law which is typical for improper ferroelectrics. A field of up to 60 kV/cm was used for P(E) measurements. No hysteresis loops were observed below the phase transition.

Keywords: Dielectrics, ceramics, improper ferroelectrics

We-S-P-81

Dielectric and structural properties of PVDF-$NaNbO_3$ - based cold sintered composites

Deepankar S. Gyan, Parth Sharma, Yash Tamrakar, Akansha Dwivedi

Department of Ceramic Engineering, IIT-BHU, Varanasi, India, Varanasi, India

The objective of the present work is to apply cold sintering process (CSP) to synthesize ceramic-polymer nanocomposites of antiferrolectric ($NaNbO_3$) & related materials and investigate their dielectric and energy storage properties. Here, we have shown that CSP actually helps in achieving composites with better density when ceramics are used as matrix compared to polymer matrix composite. Dense samples of $NaNbO_3$-PVDF, (1-x)$NaNbO_3$-x$CaTiO_3$-PVDF, and (1-x)$NaNbO_3$-x$CdTiO_3$-PVDF nanocomposites

have been prepared at low temperature < 180^0C. XRD structure reveals that the β phase of the PVDF is formed along with the orthorhombic phases of their respective ceramic matrix for all the samples. High resolution SEM analysis confirms the formation of PVDF coated ceramic grains for all the samples. Enormous increase in the dielectric constant (from 1000 to 14000) is observed at 1 KHz in some of the composites. Qualitative analysis for the recoverable energy is performed from Polarization-Electric field loops, which predicts very high breakdown strength for these materials as compared with their ceramic counterparts.

Keywords: PVDF, Ferroelectric, Dielectric

We-S-P-82

Electrocaloric effects in the lead-free $Ba(Zr,Ti)O_3$ relaxor ferroelectric from atomistic simulations

Zhijun Jiang [1, 2], Sergei Prokhorenko [2], Sergey Prosandeev [2, 3], Yousra Nahas [2], Dawei Wang [1], Jorge Íñiguez [4], Emmanuel Defay [4], Laurent Bellaiche [2]

[1] School of Electronic and Information Engineering and State Key Laboratory for Mechanical Behaviour of Materials, Xi'an Jiaotong University, Xi'an 710049, China
[2] Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas 72701, United States
[3] Institute of Physics and Physics Department of Southern Federal University, Rostov-na-Donu 344090, Russia
[4] Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), 5 Avenue des Hauts-Fourneaux, L-4362 Esch/Alzette, Luxembourg

Atomistic effective Hamiltonian simulations are used to investigate electrocaloric (EC) effects in the lead-free $Ba(Zr_{0.5}Ti_{0.5})O_3$ (BZT) relaxor ferroelectric. We find that the EC coefficient varies non-monotonically with the field at any temperature, presenting a maximum that can be traced back to the behavior of BZT's polar nanoregions. Below the Burns temperature, this maximum of EC coefficient is demonstrated to be correlated to a very specific microscopic feature. We also introduce a simple Landau-based model that reproduces the EC behavior of BZT as a function of field and temperature, and which is directly applicable to other compounds. Finally, we confirm that, for low temperatures (i.e., in nonergodic conditions), the usual indirect approach to measure the EC response provides an estimate that differs quantitatively from a direct evaluation of the field-induced temperature change [1].

References

[1] Z. Jiang, S. Prokhorenko, S. Prosandeev, Y. Nahas, D. Wang, J. Íñiguez, E. Defay and L. Bellaiche, Phys. Rev. B **96**, 014114 (2017).

Acknowledgments

Z.J., S. Prokhorenko, and L.B. are grateful for DARPA Grant No. HR0011-15-2-0038 (MATRIX program) for support. Z.J. also acknowledges support from the NSFC, Grants No. 11574246, No. 1390472, and No. U1537210, National Basic Research Program of China, Grant No. 2015CB654903.

S. Prosandeev is supported by ONR Grant No. N00014-12-1-1034, and Grants No. 3.1649.2017/4.6 from RMES, and No. 16-52-0072 Bel_a from RFBR. Y.N. is supported by ARO Grant No. W911NF-16-1-0227. We also acknowledge funding from the LNRF (Grant No. 15/9890527 Greenox, J.Í. and L.B.) and Pearl (Grant No. P12/4853155 Cofermat, J.Í. and E.D.) programs.

Keywords: Electrocaloric effects, Relaxor ferroelectrics, Effective Hamiltonian

---

We-S-P-83

Direct imaging of the effect of screening of ferroic domains by means of UHV PFM

Cecile Saguy, Maya Barzilay, Itamar Holzman, Asaf Hershkovitz, Yachin Ivry

Technion - Israel Institute of Technology, Haifa, Israel

Ferroelectric domains give rise to macroscopic polarization. The polarization is typically stabilized with surface charge, which in turn is screened by mobile charges available from the ambient, e.g. carboxyl and hydroxyl groups as well as humidity. By imaging nano domains in thin PZT films under various environmental conditions we studied the effect of screening on ferroelectric domains and were able to characterize the ferroic-domain coherence length with and without surface screening.

Keywords: Ferroics, domains, PFM

Thursday, September 7th, 2017 - Plenary Room - 08:10 - 09:00

Plenary - PLENARY 03

Th-S-O-01

(INVITED) Guided materials design: Search for ferroelectrics with targeted properties

Turab Lookman

Los Alamos National Laboratory, Santa Fe, United States

Finding new materials with targeted properties with as few experiments as possible is a key goal of accelerated materials discovery. The enormous complexity due to the interplay of structural, chemical and microstructural degrees of freedom in materials makes the rational design of new materials with targeted properties rather difficult. Machine learning and statistical design, used in industry for solving complex problems, are increasingly being adapted for the design of new materials by learning from past data. However, the number of well characterized samples available as sources of data to learn from is typically small; as a result, uncertainties associated with the predictions from model fits, or even those from measurements, become large and important. The choice of the next experiment or calculation solely based on the machine model predictions is prone to be suboptimal. Thus, optimization schemes

are needed for decision making to guide experiments using uncertainties to explore the vast material descriptor space. I will discuss how an active learning framework that iteratively combines machine learning, optimization and experiments can lead to the discovery of piezoelectric solid-solutions with targeted properties.

Keywords: accelerated discovery, uncertainties, data-driven

Thursday, September 7th, 2017 - Plenary Room - 09:00 - 09:50

Plenary - PLENARY 04

Th-S-O-01

(INVITED) Domain dynamics in multiferroics

Manfred Fiebig

Department of Materials, ETH Zurich, Zurich, Switzerland

The functionality of any ferroic material depends on its domains. Consequently, their shape and manipulation in external fields are of major interest. In compounds uniting magnetic and electric order in the same phase, the magnetoelectric coupling on the level of the domains is, however, largely unexplored. For such so-called multiferroics it is therefore not known how exactly the electric or magnetic fields affect the multiferroic domains and their walls. In my talk I will discuss this issue. In particular, I will describe electric-field control of magnetic domains for compounds such as $TbMnO_3$ and $MnWO_4$ [1]. For compounds such as hexagonal $YMnO_3$ and epitaxial $SrMnO_3$ thin films [2], I will furthermore show that domain walls in multiferroics can be considered as new, mobile type of functional ferroic interface. Finally, I will present an example of all-optical control of a multiferroic state. The antiferromagnetic order parameter in multiferroic $TbMnO_3$ is reversed repeatedly, using light pulses of two different colours. Switching depends on a unique relation between the wavelength of the light, its optical absorption and the electric polarization field induced by the antiferromagnetic order of $TbMnO_3$ [3]. We access the multiferroic domains and their walls by nonlinear optics, here in the form of second harmonic generation — doubling of a laser frequency in a material.

References

[1] M. Matsubara et al., Science 348, 1112 (2015)
[2] C. Becher et al., Nature Nano. 10, 661 (2015)
[3] S. Manz et al., Nature Phot. 10, 653 (2016)

Keywords: multiferroic, domains, second harmonic generation, all-optical switching, oxide electronics

Thursday, September 7th, 2017 - Room1 - 10:20 - 10:50

keynote speaker - THEORY III

Th-S-O-01

(INVITED) Critical dynamics and formation of the intermediate ferroelectric phase in the Zr-rich $PZr_{1-x}Ti_xO_3$

Sergey Vakhrushev [1, 2], Daria Andronikova [1, 2], Alexey Bosak [3], Yurii Bronwald [1, 2], Roman Burkovsky [1, 2], Dmitry Chernyshov [4], Igor Leontiev [5]

[1] *Ioffe Institute, St. Petersburg, Russia*
[2] *Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia*
[3] *ESRF, Grenoble, France*
[4] *SNBL, ESRF, Grenoble, France*
[5] *Southern Federal University, Rostov-on-Don, Russia*

In the last decades, the interest to the PZT solid solution has grown sharply. The most contradictory is information about the structure of the PZT with Ti concentration below 6% [1]. In our combined inelastic and diffuse scattering study of PZT we have addressed the critical instability close to the Γ-point and to the BZ boundary. In the first case, in contrast to the Ref.1 we found lattice instability at q ≈ (0.2 0.2 0) in some cases resulting in the formation of the incommensurate structure. For the BZ vicinity, we found that the temperature dependent diffuse scattering is observed aside of the M-point. Also it is extinct at h = k (Q=(1.5 1.5 0)). Such extinction rule indicates that this component is related to the oxygen octahedra tilts. Our IXS measurements have revealed strong asymmetry of the scattering intensity in respect to the Brillouin zone boundary. Intensity of the central peal (CP) at Q1 = (1.55 0.45 0) is very low, while at Q2 = (1.45 0.55 0) it is high. This is similar to the results reported in the Ref. [3]. Observed scattering pattern can be tentatively described as the result of the coupling of the M3 and M2' modes. Interference term in this case can suppress the scattering at the one side of the zone boundary and enhancing it at the other side.

References

[1] J Ricote et al., Phys.: Condens. Matter 10, 1767–1786 (1998).

[2] A.K. Tagantsev et al., Nature Communications 4 2229 (2013).

[3] M. Paściak et al., Phase transitions 88, 273 (2015).

Keywords: Antiferroelectrics, mixed perovskites, critical scattering

Thursday, September 7th, 2017 - Room2 - 10:20 - 10:50

keynote speaker - DIELECTRICS III

Th-S-O-01

(INVITED) What determines a highly piezoelectric morphotropic phase boundary?

Xiaobing Ren

Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan Multi-disciplinary Materials Research Center, Frontier Institute of Science and Technology, Xi'an Jiaotong University, Xi'an, China., Xi'an, China

Large piezoelectricity is usually found at morphotropic phase boundary (MPB), a composition-induced phase boundary between two ferroelectric phases. However, only a small fraction of MPBs (e.g., in PZT, PMN-PT, BZT-BCT, etc) show large piezoelectricity. It remains a long-standing puzzle why not all MPBs yield large piezoelectricity. Here, by a comparative study of two MPB systems of $BaZr_{0.2}Ti_{0.8}O_3$-$PbTiO_3$ (BZT-PT) and $Bi_{0.5}Na_{0.5}TiO_3$-$PbTiO_3$ (BNT-PT), we found that the symmetry relation between the two ferroelectric phases at MPB plays a crucial role in piezoelectric activity. BZT-PT ceramic, having *R*3*m*/*P*4*mm* MPB, exhibits strong piezoelectricity of d_{33} = 500 pC/N, whereas BNT-PT ceramic, having *R*3*c*/*P*4*mm* MPB, exhibits much weaker piezoelectricity of d_{33} = 150 pC/N. The sharp difference between the two types of R/T MPBs is shown to arise from a significant difference in free energy barrier associated with oxygen octahedral tilting at MPB. An oxygen octahedral tilting/untilting transition at *R*3*c*/*P*4*mm* MPB leads to a high free energy barrier and results in low piezoelectric activity, whereas *R*3*m*/*P*4*mm* MPB with octahedral untilting produces large piezoelectricity due to low free energy barrier at such MPB. This feature appears quite general in most of known MPBs systems and may become a guideline for designing highly piezoelectric materials, in particular Pb-free materials.

Keywords: píezoelectrics, morphotropic phase boundary, lead free ferroelectrics

Thursday, September 7th, 2017 - Room3 - 10:20 - 10:50

keynote speaker - RELAXORS III

Th-S-O-01

(INVITED) On the paraelectric behavior of water at T = T* = 60 ºC as a polar liquid

Julio A. Gonzalo [2], Juan Carlos del Valle [1], Carmen Aragó [2], Manuel Marqués [2], Ginés Lifante [2], Daniel Jaque [2], José García Solé [2], Manuel Tello [3], Francisco Jaque [2]

[1] *Departamento Química Física C 02 Universidad Autónoma de Madrid 28049 Madrid, Madrid, Spain*
[2] *Departamento Física Materiales C 04 Universidad Autónoma de Madrid 28049 Madrid, Madrid, Spain*
[3] *Facultad de ciencia y Tecnología Universidad del País Vasco 48080, Bilbao, Spain*

Curie-Weiss like temperature dependence of the dielectric permitivity has been shown to take place in water. A bi-linear change at T*= 60 ºC has been reported recently. In this work an effective field statistical theory is developed for polar liquids such as water which describes well its behavior through

T*. It implies a change in dipole moment from a value close to that in ice to a value close to that in water vapor. The Lindemann relationship is used to estimate the fractional oscillation of the water molecule from melting temperature to T* and beyond in terms of the Debye temperature of water T_{Debye} = 224 K.

Keywords: Paraelctric Behavior, Temperature Dependence, Water, Thermal Anomalies

Thursday, September 7th, 2017 - Room4 - 10:20 - 10:50

keynote speaker - FERROICS/MULTIFERROICS III

Th-S-O-01

(INVITED) Static and dynamic magnetoelectric coupling in multiferroics: A review

Stanislav Kamba [1], Filip Kadlec [1], Christelle Kadlec [1], Jakub Vít [1], Stella Skiadopoulou [1], Fedir Borodavka [1], Yi Sheng Chai [2], Martha Greenblatt [3]

[1] *Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*
[2] *Institute of Physics, Chinese Academy of Sciences, Beijing, China*
[3] *Rutgers, The State University of New Jersey, Piscataway, United States*

The microscopic origin of the **static magneto-electric coupling**, i.e. the change of magnetization with electric field or of polarization with magnetic field, is already well understood. Depending on the specific magnetic structure of the investigated materials, the *exchange striction*, the *inverse Dzyaloshinskii-Moriya* (D-M) interaction or the spin-dependent covalency between the metal *d* state and ligand *p* state may play the key role. In contrast, due to the **dynamic magnetoelectric coupling**, magnons can be excited in THz spectra by the electric component of the electromagnetic radiation; therefore, these excitations are called **electromagnons** and contribute to permittivity. Interestingly, different coupling mechanisms can be responsible for the static and dynamic magnetoelectric couplings in the same material. For example, in $TbMnO_3$, the static polarization is induced along the crystallographic c axis by the inverse DM interaction due to a noncollinear spiral spin structure. Nevertheless, due to exchange striation, two broad electromagnons activate in the E||a polarized THz dielectric spectra. We investigated various materials with the Y- and Z-type hexaferrite structures. A small applied magnetic field induces a transverse conical ferrimagnetic structure where the inverse DM interaction is responsible for the appearance of a static polarization in the hexagonal plane. Electromagnons activate due to exchange striction in the E||c polarized THz spectra. Above 2-4 Tesla, the electromagnons and the static polarization disappear, because the magnetic structure transforms to a collinear one. During our talk we will also explain identical origin of static and dynamic magnetoelectric couplings in multiferroic Ni_3TeO_6.

Keywords: multiferroics, magnetoelectric coupling, electromagnons, phonons, THz spectroscopy

Thursday, September 7th, 2017 - Room1 - 10:50 - 11:15

Invited talk - THEORY III

Th-S-O-01

(INVITED) Hybrid improper ferroelectricity in Ruddlesden-Popper $A_3B_2O_7$ ceramics

Xiao Qiang Liu, Juan Juan Lu, Jing Wei Wu, Xiang Ming Chen

School of Materials Science and Engineering, Zhejiang University, Hangzhou, China

Improper ferroelectricity has been attracted many attentions because of its great potential application in creating room temperature multiferroicity with strong magnetoelectric coupling. Recently, the hybrid improper ferroelectricity (HIF) has been proposed by the first-principle calculation, and the ferroelectricity is induced by a complex distortion pattern consisting of two oxygen octahedron tilting modes, such as $a^-a^-c^0$ and $a^0a^0c^+$ (in Glazer's notation) in perovskite [1]. The HIF should widely exist in the perovskites and layered perovskites since the oxygen octahedron rotations are ubiquitous distortions in the perovksite-related materials. In the present talk, the experimental evidences of HIF in Ruddlesden-Poper $Ca_3(Ti,Mn)_2O_7$ and $(Sr,Ca)_3Sn_2O_7$ ceramics have been shown. The room temperature ferroelectric hysteresis loops are observed in these ceramics, and a polar orthorhombic structure with two oxygen tilting modes has been confirmed by the X-ray powder diffraction. A first-order phase transition around 1100 K in $Ca_3Ti_2O_7$ was evidenced, and the temperatures of phase transitions decrease linearly with increasing of the contents of Mn^{4+} and Sr^{2+} ions [2].

References

[1] N.A. Benedek, and C.J. Fennie, Phys. Rev. Lett., 106, 07204 (2011).

[2] X.Q. Liu, J.W. Wu, X.X. Shi, H.J. Zhao, H.Y. Zhou, R.H. Qiu, W.Q. Zhang, and X.M. Chen, Appl. Phys. Lett., 106, 202903 (2015) .

Keywords: Hybrid improper ferroelectricity; Ruddlesden-Poper structure; Oxygen octahedron tilting

Thursday, September 7th, 2017 - Room2 - 10:50 - 11:15

Invited talk - DIELECTRICS III

Th-S-O-01

(INVITED) Clausius – Mossotti relation fractal modification

Vojislav Mitic [1, 2], Vesna Paunovic [1], Ljubisa Kocic [1]

[1] *University of Niš, Faculty of Electronic Engineering, Nis, Serbia*

[2] *Institute of Technical Sciences of SASA, Belgrade, Serbia*

The microstructure characteristic and dielectric properties of doped $BaTiO_3$ ceramics were investigated in the light of Clausius – Mossotti relation (CMR) which incorporates both the Curie and Curie – Weiss Laws. The samples of rare earth doped $BaTiO_3$ were prepared using by conventional solid state procedure and sintered at 1320 ^oC. Microstructural and compositional studies were performed by SEM equipped with EDS system. The dielectric characteristic of doped $BaTiO_3$ ceramics like as dielectric constant have been done by using LCR-Metra Agilent 4284A in the frequency range 20 Hz - 1 MHz and temperature range 20-180 ^oC. The Clausius – Mossotti relation is used to clarify the influence of dopant on the dielectric properties and $BaTiO_3$ phase transformation. Curie parameters (*C*, *Tc*) and a critical exponent of nonlinearity (*g*) were calculated by using a Curie-Weiss law. Also, new approach on correlation between microstructure and dielectric properties of doped $BaTiO_3$ based on fractal geometry (grains shapes, pores and intergranular contacts) has been developed, using method of fractal modeling of a microstructure configurations reconstruction.

Keywords: Clausius – Mossotti relation, BaTiO3-ceramics, fractals

Thursday, September 7th, 2017 - Room3 - 10:50 - 11:15

Invited talk - RELAXORS III

Th-S-O-01

(INVITED) Defects and dielectric polarization in polar functional materials

Yun Liu

The Australian National University, Canberra, Australia

Ionic doping and/or substitution in polar functional materials provide opportunities to tune the polarization for the peak performance or to create new polarization behaviors. In the past, the research in this field mainly focuses on the development of the relationship between the macroscopic structures (e.g. average structure determined by X-ray powder diffraction) and properties. It is found, however, that in many cases, such a relationship becomes very complicated and cannot be properly built. This is because that in a strongly correlated solid-state system, these ions can be structurally and/or chemically accommodated differently in local region but do not change the average structure. The trend that such ionic doping and/or substitution influence the properties is often not straightforward. In this talk, I will use several examples to demonstrate the local consequence of ionic doping and/or substitution and their impact on polarization property, and thus drawing your attention on the material design for high performance and new functions.

Keywords: local structure, defect, ionic doping, ionic substitution, polar functional materials

Thursday, September 7th, 2017 - Room4 - 10:50 - 11:15

Invited talk - FERROICS/MULTIFERROICS III

Th-S-O-01

(INVITED) Polarization and spin order pattern of multiferroic RMn_2O_5 based on a magnetic space group

Yukio Noda [1, 2], Hiroyuki Kimura [1]

[1] *Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Japan*
[2] *High Energy Accelerator Research Organization (KEK), Tsukuba, Japan*

Simultaneous ordered phase of ferroelectric and magnetic order parameters is called "multiferroic" [1]. Cycloid spin order can induce ferroic polarization pattern, and many examples were found over the past decades. RMn_2O_5 is one of the examples, which has complicated magnetic and dielectric successive phase transitions. The spin order pattern was confirmed as cycloid structure [2], and two mechanisms, $\mathbf{S}\times\mathbf{S}$ and $\mathbf{S}\cdot\mathbf{S}$, were confirmed [3]. In this talk, we will show how the cycloid spin order pattern is induced based on a magnetic space group. One example is YMn_2O_5. YMn_2O_5 has $\mathbf{q}_M=(1/2,0,1/4)$ magnetic propagation vector, and then $\mathbf{q}_L = (0,0,1/2)$ lattice modulation vector. Thus, crystal space group is $Pb2_1m$ with $a_0 \times b_0 \times 2c_0$ unit cell, and magnetic space group is P_Bb2_1m with $2a_0 \times b_0 \times 4c_0$ unit cell. This magnetic space group naturally induces cycloid spin structure and then macroscopic ferroelectric polarization. Information of magnetic space group helps to reduce the number of fitting parameters tremendously for magnetic structure analysis and also to consider the spin structure change associated with polarization reverse.

References

[1] H. Katsura *et al*. Phys. Rev. Lett. 95, 057205 (2005).

[2] Y, Noda, *et al*, J. Phys. Condens. Matter 20, 434206 (2008).

[3] S. Wakimoto *et al*., Phys. Rev. B 88, 140403(R) (2013).

Keywords: multiferroic, spin-induced ferroelectricity, RMn2O5, magnetic space group

Thursday, September 7th, 2017 - Room1 - 11:15 - 12:30

Oral presentation - THEORY III

Th-S-O-01

Experimental and theoretical determination of anharmonic soft phonons in the improper ferroelectric $YMnO_3$

Dipanshu Bansal [1], Jennifer L. Niedziela [1], V. Ovidiu Garlea [2], Douglas L. Abernathy [2], Songxue Chi [2], Yang Ren [3], Haidong Zhou [4], Olivier Delaire [1, 5]

1 Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, United States
2 Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, United States
3 Advanced Photon Source, Argonne National Laboratory, Argonne, United States
4 Department of Physics and Astronomy, University of Tennessee, Knoxville, United States
5 Department of Mechanical Engineering and Materials Science, Duke University, Durham, United States

Ferroelectric materials display spontaneous and switchable electric polarization (*P*) emerging from breaking inversion symmetry upon cooling below the ferroelectric transition temperature, *T*FE. In proper geometric ferroelectrics, *P* is driven by a soft zone-center polar phonon mode, but in improper ferroelectrics the anharmonic coupling between a stable zone-center polar phonon mode and unstable zone-boundary non-polar modes triggers the ferroelectricity. While the soft mode transition in proper ferroelectrics has been thoroughly investigated using both experimental and theoretical techniques, the exact mechanism of the transition driven by non-polar modes in improper ferroelectrics remains less well understood. This knowledge gap results from limitations of experimental studies with Raman and infra-red spectroscopy, intrinsically limited to $q \simeq 0$ (Γ-point), as well as from the failure of the often-used quasi-harmonic approximation in lattice dynamics simulations using density functional theory, for strongly anharmonic systems. These difficulties have precluded the direct observation and realistic modeling of unstable zone-boundary q~=0 modes and their anharmonic coupling with the zone-center polar mode. To bridge this gap, we have performed comprehensive *T*-dependent, momentum-resolved phonon dispersion measurements in the archetypal improper ferroelectric, YMnO3, including the behavior across *T*FE, using inelastic neutron scattering, as well as single-crystal x-ray diffraction. In addition, we performed both 0 K and finite temperature first-principles lattice dynamics simulations, including anharmonic renormalization effects, directly revealing the zone-boundary soft-mode, which condenses at *T*FE. Our results are compared with proposed models of improper ferroelectric transitions and previous experimental observations.

Keywords: Improper ferroelectrics, finite temperature lattice dynamics simulations, single-crystal inelastic neutron scattering, single-crystal x-ray diffraction, calorimetry

---

Th-S-O-02

Pressure-induced transitions in ferroelectric single-crystal $PbZr_{0.54}Ti_{0.46}O_3$

Muhetaer Aihaiti [1], Maddury Somayazulu [1], Dmitry Popov [2], Yujuan Xie [3], Xifa Long [3], Zuo-Guang Ye [3], Ronald E. Cohen [1, 4], Russell J. Hemley [5]

1 Geophysical Laboratory, Carnegie Institution of Washington, Washington DC, United States
2 HPCAT, Geophysical Laboratory, Carnegie Institution of Washington,, Argonne, United States
3 Department of Chemistry and 4D LABS, Simon Fraser University,, Burnaby, Canada
4 Department of Earth and Environmental Sciences, Ludwig Maximilians Universität, Munich, Germany
5 Department of Civil and Environment Engineering, The George Washington University, Washington DC 20052, USA, Washington DC, United States

Pressure-induced phase transitions in single-crystal PbZr0.54Ti0.46O3 are investigated with high-pressure Raman scattering and x-ray single crystal and powder diffractions. Appearance of a Raman peak near 380 cm−1 indicates a structural transition at 3 GPa. A second transition, driven by an optical soft phonon, occurs at 9 GPa. A third transition occurs above 27 GPa, accompanied by a large changes in the Raman spectra and a concomitant splitting of the (pseudo-cubic) (111) and (220) diffraction lines. We identify the transitions as a monoclinic (*C*m) to rhombohedral transition (*R*3m) at 3 GPa, followed by a rhombohedral (*R*3m) to rhombohedral (*R*-3c) transition at 9 GPa, and a further symmetry-lowering transition at 27 GPa.

Keywords: PZT single crystal, structural transitions, high-pressure, Raman scattering, x-ray diffraction

---

Th-S-O-03

The symmetry-mode decomposition, structural refinement and ferroelectricity of (1-x)$AgNbO_3$-x$LiTaO_3$

Teng Lu [1], Ye Tian [1, 2], Andrew Studer [3], Ray Withers [1], Xiaoyong Wei [2], Yun Liu [1]

1 Research School of Chemistry, The Australian National University, Canberra, Australia
2 Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education & International Center for Dielectric Research, Xi'an Jiaotong University, Xi'an, China
3 Australian Centre for Neutron Scattering, The Australia Neutron Science and Technology Organisation, Lucas Height, Australia

The phase evolution of the (1-x)AgNbO3-xLiTaO3 solid solution is investigated by the neutron diffraction, dielectric and ferroelectric measurements. The symmetry-mode decomposition of the distorted AgNbO3 structure defined on the experimental space group, *Pmc21* has been conducted. The four main modes, T4+, H2, Λ3 and Γ4-, exhibit large distorted amplitude to stabilize the overall *Pmc21* structure. The mode refinement with referring to the *Pmc21* was adopted to this material system. The structural refinement results suggest that with the increasing LiTaO3, the structure will partially transfer from the orthorhombic to rhombohedral phase whose fraction grows up accordingly, along with a sudden drop in the mode amplitudes of the H2 and Λ3. The hidden structural correlation between H2 and Λ3 modes helps understand the improper nature of the antiferroelectricity observed in the AgNbO3. The variation of the main modes helps build the bridge between the *Pmc*21 and *R*3*c* phases, providing the mechanism underlying the phase transition between these two phases. Furthermore, the evolution of the *R*3*c* phase fraction and associate mode amplitude in both *Pmc*21 and *R*3*c* phases can well explain the additional peak observed in the temperature-dependent dielectric spectra and composition-dependent polarisation-electric field hysteresis loops.

Keywords: Antiferroelectric, Phase transition, Symmetry-mode decomposition

---

Th-S-O-04

(INVITED) The role of strain and surface charge in stabilizing ferroic domains and atomic-scale dipole moments

Yachin Ivry [1], Asaf Hershkovitz [1], Maya Barzilay [1], Florian Johann [2], Cecile Saguy [1], Itamar Holzman [1]

[1] *Technion - Israel Institute of Technology, Haifa, Israel*

[2] *Asylum Research, an Oxford Instruments company, Santa Barbara, United States*

The dynamics and reversibility of ferroelectric domains as a response to external excitations is attractive for a broad range of applications. Surface charge and strain play a significant role in affecting the domain dynamics, and hence has garnered much attention. Yet, the great experimental challenges associated with imaging the effect of these parameters on the domain dynamics have encumbered the understanding of the fundamental behavior of ferroelectricity at the atomic and nanometer scale. We have recently utilized a combination of experimental approaches to address the effects of surface charge and strain on the ferroic domain stability, including variable-temperature PFM and TEM as well as PFM in vacuum. Our preliminary results shade new light on the origin of ferroic domain stability.

Keywords: Ferroics, domains, domain walls

Th-S-O-05

Piezoelectric response induced phase transition in perovskite thin films

Hyeon Jun Lee [1], Chan-ho Yang [2], Hiroshi Funakubo [3], Ji Young Jo [1]

[1] *Gwnagju Institute of Science and Technology, Bukgu, Korea, Republic of (South)*

[2] *KAIST, Daejeon, Korea, Republic of (South)*

[3] *tokyo institute of technology, Tokyo, Japan*

Ferroelectric materials are critical components in a wide range of devices such as non-volatile memories, actuators, sensors, and electro-optic devices. For the practical applications in recent trend of miniaturization, it is essential to understand and enhance ferroelectricity of thin films including piezoelectricity and polarization switching. Recently, special attention has been given to ferroelectric materials due to the presence of morphotropic phase boundaries (MPB), or strain driven mixed phases of ferroelectric domain that enhanced electromechanical property. In the ferroelectric $BiFeO_3$ (BFO) thin films, for example, the film tends to form rhombohedral phase in the middle of tetragonal phase in order to relieve the stress from substrate. The existence of rhombohedral phase has been well predicted to enhance electromechanical properties of BFO thin films arising from the large lattice distortion under an applied electric field; however, its dynamic phenomena has not been clearly investigated yet partially due to the lack of experimental tools. Recently, time resolved micro X-ray diffraction under electric field allow us to resolve not only structural change but also electromechanical properties of thin films. Change of diffracted intensity and shift of diffracted peak position under electric field will provide information on ferroelectric switching and piezoelectric response, respectively. As results, we found nonlinear phase transition between simple cubic and super tetragonal structures. The simple cubic structure showed ferroelectric switching under electric field while super tetragonal only showed linear piezoelectric response indicating the origin of phase transition.

Keywords: time resolved x-ray diffraction, phase transition, individual ferroelectric switching in a film, dynamics

Thursday, September 7th, 2017 - Room2 - 11:15 - 12:30

Oral presentation - DIELECTRICS III

Th-S-O-01

A study of the multiferroic state under high pressure across the phase diagram of $Mn_{1-x}Co_xWO_4$ for 0.05 > x > 0.17

Melissa Gooch [1], Narayan Poudel [1], Bernd Lorenz [1], Feng Ye [2], Jinchen Wang [2], Jaime Fernandez-Baca [2, 3], Ching-Wu Chu [1, 4]

[1] *Texas Center for Superconductivity at the University of Houston, Houston, United States*
[2] *Quantum Condensed Matter Division, Oakridge National Laboratory, Oak Ridge, United States*
[3] *Department of Physics and Astronomy, The University of Tennessee, Knoxville, United States*
[4] *Lawrence Berkeley National Laboratory, Berkeley, United States*

While $Mn_{1-x}Co_xWO_4$ phase diagram has been extensively studied, it is also well known that systems with strong magnetic frustration can have increased sensitivity to small perturbations and these perturbations can result in new states. With the increased research efforts into device applications over the last years, understanding these complex systems will hopefully lead to new and interesting advancements in basic research as well as applications. Revisiting the $Mn_{1-x}Co_xWO_4$ phase diagram at x = 0.15, two multiferroic phase coexist and at this boundary on the phase diagram the conical spin extends to lower temperature, in addition to the a-c spiral spin structure forming below 7 K. On either side of the boundary we have a spiral spin structure for $x < 0.15$ and a conical spin for $x > 0.15$. To further explore the complex phase diagram of $Mn_{1-x}Co_xWO_4$, high pressure dielectric and polarization measurements were conducted at key dopings: x = 0.05, 0.012, 0.0135, 0.15, and 0.17. Our results are also supported by high pressure neutron results conducted by J. Wang *et. al*. The effect of external pressure on the $Mn_{1-x}Co_xWO_4$ system can be described as similar to Co doping for higher doping levels; however, for lower doping levels this may not be the case.

Keywords: polarization, high pressure

Th-S-O-02

Highly resistive nanostructured $BiFeO_3$ monoliths by Spark-Plasma Sintering: A re-oxidation study

Eduardo Volnistem [1], Diego Viana [2], Daniel Silva [1], Ducinei Garcia [2], José Eiras [2], Gustavo Dias [1], Ivair Santos [1]

[1] *State University of Maringá, Maringá, Brazil*
[2] *Federal University of São Carlos, São Carlos, Brazil*

$BiFeO_3$ is a multiferroic magnetoelectric material with a rhomboedrally distorted perovskite structure (R3c space group) presenting ferroelectric and antiferromagnetic (G-type) ordering at room temperature with elevated Curie (TC ~ 1103 K) and Néel (TN ~ 643 K) temperatures. However, the formation of undesired phases in polycrystalline $BiFeO_3$, mainly $Bi_{25}FeO_{39}$ and $Bi_2Fe_4O_9$ turns the preparation of high resistive single-phased BiFeO3 ceramics a challenge. In this work, high-energy ball milling allied to fast sintering were applied to achieve phase-pure nanostructured powders and Spark-Plasma Sintering (SPS) was used to synthesize nanostructured $BiFeO_3$ monolithic samples. Single-phased $BiFeO_3$ powder were obtained by the milling process and exhibited a mean size around 150 nm and SPS resulted in highly dense monoliths samples. However, X-Ray Diffraction (XRD) evidenced the presence of secondary phases after SPS process and electric measurements revealed low electrical resistivity. A thermal treatment under oxygen positive pressure (60 psi) were used to promote sample re-oxidation and impedance spectroscopy confirmed an enhanced resistivity after 96 h treatment. Vibrating Sample Magnetometry (VSM) measurement shows magnetization around 3,5 emu/g after oxygen annealing and microstructural analyses by electron scanning microscopy (SEM) reveals no grain growth after SPS as well as after oxygen annealing.

Keywords: Bismuth ferrite, Spark-Plasma Sintering, Dielectric Properties.

Th-S-O-03

Synthesis, structure and piezo-/ferroelectric properties of a novel bismuth-containing ternary complex perovskite solid solution

Zenghui Liu [1, 2], Alisa Paterson [2], Hua Wu [3, 2], Pan Gao [1], Wei Ren [1], Zuo-Guang Ye [2, 1]

[1] *Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education & International Center for Dielectric Research, Xi'an Jiaotong University, Xi'an, China*
[2] *Department of Chemistry and 4D LABS, Simon Fraser University, Burnaby, Canada*
[3] *Department of Applied Physics, Donghua University, Shanghai, China*

To develop high-performance piezo-/ferroelectric materials and to understand their underlying physical and chemical mechanisms, a novel ternary solid solution has been synthesized by solid state reaction method in the form of ceramics with compositions across the morphotropic phase boundary (MPB). This ternary system is formed by incorporating Bi-based complex perovskite $Bi(Zn_{2/3}Nb_{1/3})O_3$ (BZN) into the relaxor-based binary solid solution of $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT). X-ray diffraction analysis indicates that the (0.95-*x*)PMN-0.05BZN-*x*PT solid solution transforms from a rhombohedral phase to a tetragonal phase when the composition is varied across the MPB which is located at $x \sim 0.30$ to 0.33. Enhanced relaxor behavior is found in this system and the relaxor state transforms to a ferroelectric phase spontaneously upon cooling, or under application of an electric field. The incorporation of BZN into PMN-PT results in the suppression of the MPB-related depoling (at T_{RT}) and a significant enhancement of piezoelectric and ferroelectric properties compared with those of PMN-PT binary ceramics. This enhancement of properties is attributed to the beneficial effects of BZN which enhances the structural distortion due to the lone-pair electrons on Bi^{3+} and the ferroelectrically active

Zn^{2+} and Nb^{5+}, and to the enhanced relaxor behavior arising from the increase of the local disorder and nanodomains effect. With its strengthened properties, the (0.95-*x*)PMN-0.05BZN-*x*PT system becomes a promising electronic ceramic material for such devices as actuators, sensors, capacitors, and transducers for a wide range of applications.

Keywords: Complex perovskite solid solution, PMN-PT-BZN ternary system, Local polar structure, Relaxor-to-ferroelectric phase transformation, Piezoelectric and ferroelectric properties

---

Th-S-O-04

(INVITED) Large magnetoelectric couplings in lead-free nanocomposites

Aiping Chen [1], Ahmad Eshghinejad [2], Yaomin Dai [1], John Bowlan [1], Zhongchang Wang [3], Erik Enriquez [1], Erik Knall [1], Judith MacManus-Driscoll [4], Haiyan Wang [5], Antoinette Taylor [1], Rohit Prasankumar [1], Jiangyu Li [2], Dmitry Yarotski [1], Quanxi Jia [6]

[1] *Center for Integrated Nanotechnologies (CINT), Los Alamos National Laboratory, Los Alamos, United States*
[2] *University of Washington, Seattle, United States*
[3] *International Iberian Nanotechnology Laboratory, Braga, Portugal*
[4] *University of Cambridge, Cambridge, United Kingdom*
[5] *Purdue University, Purdue University, United States*
[6] *University at Buffalo - The State University of New York, Buffalo, United States*

The vertically aligned $BaTiO_3$:$CoFe_2O_4$ nanocomposites exhibit multiferroic properties above room temperature, which has been confirmed by the temperature dependent second harmonic generation (SHG) and magnetization measurements. Both magnetization and polarization were found aligned along the out-of-plane direction due to large out-of-plane lattice strain. The magnetic field dependent SHG has demonstrated the coupling between BTO and CFO components. The direct magnetoelectric (ME) coupling is investigated by using piezoresponse force microscopy (PFM) under different magnetic fields. A large longitudinal ME coefficient α_{31} of over 2000 mV/cm Oe is estimated by averaging the PFM amplitude change of BTO matrix upon applying magnetic fields. Phase field simulation found that the ME coupling strongly depends on the size of nanopillars. This work explored the mechanisms of magnetoelectric couplings and the coupling strength in vertically aligned metal-oxide nanocomposites.

Keywords: thin films, epitaxial, magnetoelectric coupling

Thursday, September 7th, 2017 - Room3 - 11:15 - 12:30

Oral presentation - RELAXORS III

Th-S-O-01

Empirical correlations and a phenomenological description for relaxor dielectric response

Ilya Grinberg

Department of Chemistry, Bar Ilan University, Ramat Gan, Israel

Since the first synthesis and characterizaiton of $Pb(Mg,Nb)O_3$, relaxor ferroelectrics have been a source of fascination for materials scientists due to their unusual properties and also due to their importance in technological applications. While they possess other unusual features, dielectric response has been the hallmark of relaxor behavior and has been the focus of most studies of relaxors. Relaxors exhibit a diffuse peak in the plot of dielectric constant versus temperature as well as a strong dependence of the dielectric constant on the frequency of the applied electric field (dispersion). Since the pioneering work of Setter and Cross, both of these properties have been shown many times to be highly sensitive to the cation arrangement in the perovskite and in our previous work we have demonstrated that a quantitative relationship exists between the B-cation disorder as expressed by the standard deviation (second moment) of the B-cation valence of the oxygen atoms and the $\Delta T_{\varepsilon,max}$ parameter that describes the dielectric dispersion. Nevertheless, several key question have remained unresolved. For example, it is unclear how the Vogel-Fulcher and quadratic Lorentzian expressions characterizing dispersion and diffusion emerge (are connected to) the relaxor structure and dynamics. In this work, use the recently discovered nanodomain structure of relaxors as a basis for deriving a simple and general theory of relaxor behavior and use theoretical arguments and empirical correlations to show how local structure and compositions control the relaxor dielectric response as characterized by dispersion ($\Delta T_{\varepsilon,max}$) and diffusion ($\sigma$) descriptors.

Keywords: relaxors

Th-S-O-02

$Ba\{[Ga_x,Ta_x]Ti_{(1-2x)}\}O_3$: Induced diffuse phase transitions using charge compensated dipole pairs (Ga-Ta) introduced in barium titanate parent matrix

Vignaswaran K. Veerapandiyan, Walter Schulze, Scott Misture, Steven Pilgrim, Steven Tidrow

Kazuo Inamori School of Engineering, Alfred University, Alfred, United States

$Ba\{[Ga_x,Ta_x]Ti_{(1-2x)}\}O_3$ with x equal to 0, 0.0025, 0.005, 0.01, 0.025, 0.05, 0.075 and 0.1 have been prepared by conventional solid-state reaction and sintered to > 95% density. Structural and dielectric characterization has been performed to investigate the effect of dipole-like concentration on the properties. Dielectrically, the $Ba\{[Ga_x,Ta_x]Ti_{(1-2x)}\}O_3$ phase transition evolves from a classic ferroelectric to a diffuse phase transition (DPTs) as *x* increases. The $Ba\{[Ga_{0.01},Ta_{0.01}]Ti_{0.98}\}O_3$ possesses diffuseness parameter comparable to $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT), yet it lacks the frequency and temperature dependence of T_m. For a given DC bias, $Ba\{[Ga_x,Ta_x]Ti_{(1-2x)}\}O_3$ possesses capacitance tunability exceeding that of PMN-PT. In comparison to $BaTiO_3$, $Ba\{[Ga_x,Ta_x]Ti_{(1-2x)}\}O_3$ possesses enhanced electrical resistivity and greater time constant at and above room temperature. The diffuseness of ε_r is found to increase linearly with the dipole concentration. *In-situ* XRD, including Rietveld refinement, has been performed to determine the lattice parameter, coefficient of thermal expansion and phase transition temperature of each composition within the temperature range [RT, 1000 ˚C]. The unusual properties of $Ba\{[Ga_x,Ta_x]Ti_{(1-2x)}\}O_3$ will be discussed in context with available models

describing donor and acceptor dopants spatially separated in the parent matrix that inter-relate lattice parameter, Curie temperature, and other properties.

Keywords: Barium titanate, diffuse phase transition, dipole-like substitutions

---

Th-S-O-03

Lattice dynamics, dielectric behaviour and acoustic waves in tetragonal tungsten-bronzes

Elena Buixaderas [1], Martin Kempa [1], Christelle Kadlec [1], Petr Ondrejkovic [1], Michal Landa [3], Jan Dec [2], Marek Pasciak [1], Jiri Hlinka [1], Maxim Savinov [1]

[1] *Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*
[2] *Institute of Materials Science, University of Silesia, Katowice, Poland*
[3] *Institute of Thermomechanics, Czech Academy of Sciences, Pregue, Czech Republic*

There are many tunable properties in the tetragonal tungsten-bronze (TTB) structure, and this is important in the quest for materials with new capabilities for electronics. After the flexible perovskite structure, the TTBs are, probably, the most versatile materials nowadays, because of the presence in their structure of different channels that can be filled with many different cations that tune dielectric, ferroelectric, piezoelectric or even magnetoelectric properties, and also due to their intrinsic structural anisotropy. Probably the most studied TTB is (Sr,Ba)Nb_2O6 (SBN), in which the amount of Sr in the structure, and the vacancies formed, can change its dielectric behavior from a regular ferroelectric to a relaxor ferroelectric. Similar change can be produced also using Ca instead of Sr, although in a minor scale. Precisely the role played by these two cations is the key to understand the origin of the ferroelectricity and the dielectric behavior in these compounds. Not only in the way they affect the lattice dynamical behavior (atomic vibrations), but also in the way microstructures and nanostructures are formed (micro and nananodomains, polar nanoregions, mesoscopic correlated clusters). In this work I will show results taken in these materials using broad-band spectroscopy (dielectric and coaxial spectroscopy together with THz spectroscopy and Far IR spectroscopy) to cover the frequency range 10-10^{14} Hz in the dielectric response, together with Raman, Brillouin and Resonant ultrasound spectroscopies.

Keywords: ferroelectric relaxors, tungsten-bronzes, dielectric response, phonons, broad-band spectroscopy

---

Th-S-O-04

The normal to diffuse phase transition crossover from thermal expansion analysis in calcium modified lead titanate

Flavia Estrada, Ducinei Garcia

Federal University of São Carlos, São Carlos, Brazil

For materials with diffuse phase transition, local polarization exists even above the temperature at which the dielectric permittivity reaches maximum (T_M). This net polarization only disappears above the Burns temperature (T_B). In this work, the polarization vs. temperature feature of $Pb_{1-x}Ca_xTiO_3$ (PCT) ceramics, x = 0.35 to x = 0.55, were determined from the thermal expansion data taking into account the strain and polarization relation. It was considered that the electrostriction is a constant and the same as that of the cubic phase for all compositions. The Burns temperature was determined and compared to T_M. For low calcium concentration, T_B-T_M is close to 50 K, but increases to 150 K at the highest Ca concentration. From these results and those found for the temperature dependence of the dielectric permittivity, in compositions between x = 0.45 and x = 0.475 it can be considered that occurs the normal to diffuse crossover of the PCT solid solutions.

The authors are grateful to Dr. Manuel H. Lente to the thermal expansion measurements facilities and to CAPES, FAPESP and CNPq Brazilian funding agencies for financial support.

Keywords: ferroelectric ceramic, negative thermal expansion, relaxor-like phase transition

---

Th-S-O-05

An exceptional hysteresis-strain-thermal stability combination of electrostrain via re-entrant relaxor-ferroelectric composite

Minxia Fang [1], Yuanchao Ji [1], Xiaobing Ren [1, 2]

[1] *Multi-Disciplinary Materials Research Center, Frontier Institute of Science and Technology, and State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China, Xi'an, China*

[2] *Ferroic Physics Group, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, 305-0047, Ibaraki, Japan, Tsukuba, Japan*

Electromechanical materials (mainly ferroelectric materials) can convert electrical energy to mechanical work and have been widely used in actuators, ultrasonic imagines and telecommunciations. However, the combination of low hystersis and large strain with good thermal stability has been hardly attained in ferroelectric materials since the discovery in 1920. Here we report an exceptional combination of low hysteresis (< 10%) and large electrostrain (0.16% at 6 kV/mm) over a broad temperature range (~80 K) in a lead-free $(Ba_{0.925}Bi_{0.05})(Ti_{1-x/100}Sn_{x/100})O_3$ (BT-5Bi-xSn) ceramic system. Moreover, it is against the conventional hysteresis-strain trade-off, i.e., both hysteresis and strain properties become better. In-situ transmission electron microscopy observations further reveal a "frozen" heterogeneous microstructure of isolated ferroelectric domains embedded into relaxor matrix over a broad temperature range, namely the re-entrant relaxor-ferroelectric composite (RRFC). This RRFC serves as the origin of the property anomalies: reversible non-180^o polarization rotation with negligible irreversible domain wall motion over a broad temperature range, which is different from previous well-known wisdoms of morphotropic phase boundaries in ferroelectrics or polar nanoregions in relaxors. Our work may open a new way to develop high-performance electromechanical materials.

Keywords: relaxor-ferroelectric composite, large electrostrain, low hysteresis, re-entrant

Thursday, September 7th, 2017 - Room4 - 11:15 - 12:30

Oral presentation - FERROICS/MULTIFERROICS III

Th-S-O-01

Effect of magnetic and electric fields on magnetization and polarization of $BiMnO_3$ multiferroic films

Ahmad M. A. Alrub Alrub

Ahmad Musleh Alrub, Ma'an, Jordan

Abstract— A symmetric standing film of a single crystal of $BiMnO_3$ multiferroics is investigated by using Landau theory. Different hysteresis loops are studied: magnetization versus magnetic field loop, magnetization versus electric field loop, polarization versus electric field loop, and polarization versus magnetic field loop. The effect of temperature on the remnant magnetization and polarization as well as the coercive fields is displayed. A comparison of these loops between film and bulk $BiMnO_3$ multiferroics is conducted.

Keywords: Thank you for organizing this conference

Th-S-O-02

Effects of cryomilling on ferroic properties of $BiFeO_3$ nanoparticles ceramics

Eduardo A. Volnistem [1], João M. P. Leonardo [1], Daniel M. Silva [1], Ducinei Garcia [2], José A. Eiras [2], Gustavo S. Dias [1], Luiz F. Cótica [1], Ivair A. Santos [1]

[1] *Maringá State University, Maringá, Brazil*
[2] *São Carlos Federal University, São Carlos, Brazil*

Bismuth ferrite, $BiFeO_3$ (BFO), is a multiferroic magnetoelectric compound with rhomboedrally distorted perovskite structure (ABO_3) and *R*3*c* space group exhibiting ferroelectric and antiferromagnetic ordering at room temperature with high Currie (~ 1103 K) and Neel (~ 643 K) temperatures. The BFO magnetic ordering is characterized by a canted spin structure that gives rise to a spiral modulation with a periodicity of 62 nm, leading to null macroscopic magnetization. In this sense, size dependent properties of BFO has attracted attention and many protocols for the synthesis of nanoparticles and nanostructured ceramics have been trying. Nonetheless, conventional synthesis as wet chemical rotes of nano-sized particles are not cost-effective for mass production. In this context, cryomill was proposed as a new technique consisting in a low temperature ball-milling process using liquid nitrogen for the fabrication of nanoparticles in large quantities. In this present work, a home-built setup for cryomill in a planetary ball mill was applied to obtain single-phased BFO nanoparticles and the powder properties were explored. In addition, bulk ceramics were made under low temperature by

different conditions and then structural, micro structural, dielectric and magnetic properties were investigated and its improvements were correlated to synthesis parameters.

Keywords: Multiferroic Magnetoelectric, BiFeO3, Cryomill

Th-S-O-03

Improved magnetic properties, dielectric and structural characterizations in Mn doped $0.9BiFeO_3$-$0.1BaTiO_3$ compositions

Ricardo Gotardo [1], Raquel Alonso [1], Jaciele Rosso [2], Guilherme Santos [2], Luiz Cótica [2], Ivair Santos [2], Klebson Silva [2], Ruyan Guo [3], Amar Bhala [3], Daniel Silva [2]

[1] *Department of Natural Sciences, Technological Federal University of Paraná, Cornélio Procópio, Brazil*
[2] *Department of Physics, State University of Maringá, Maringá, Brazil*
[3] *Department of Electrical and Computer Engineering, University of Texas at San Antonio, San Antonio, Brazil*

Bismuth ferrite ($BiFeO_3$; BFO) is one of the most studied multiferroic materials, mainly due to its reported magnetoelectric properties at room temperature, potential use in nonvolatile memory applications and developments in the fundamentals of solid state physics. BFO ferroelectric and antiferromagnetic phase transitions are found significantly above room temperature, i.e., it is a ferroelectric material below T_c ~1100 K, and an antiferromagnetic one below T_N ~650 K. The drawbacks of BFO for bulk practical applications are the low resistivity and the difficult to synthetize single-phased polycrystalline materials. To overcome these problems one solution is the synthesis of solid solutions with other perovskite materials, such as $BaTiO_3$ or $PbTiO_3$, and doping these materials with multiple valence ions like Mn. Therefore, in this work, we describe the structural, dielectric, magnetic and Mössbauer spectroscopy studies in $0.9BiFeO_3$–$0.1BaTiO_3$ solid solutions doped with Mn processed by high-energy ball milling. Especially for the Mn doped samples a structurally correlated magnetization enhancement is reported. X-ray diffraction and Rietveld refinement studies revealed a distorted perovskite structure with the coexistence of rhombohedral and monoclinic symmetries. Mössbauer spectroscopy results showed a magnetic spectral signature of ordered Fe^{3+} ions for the rhombohedral phase of the undoped sample, and for both rhombohedral and monoclinic phases of the Mn doped samples. A significant magnetization increase (reaching 0.50 emu/g), associated to the magnetic ordering of the *Cm* phase and to the retention of the Mn^{3+} valence state, was observed for Mn doped samples.

Keywords: Multiferroic, BiFeO3, Structural Properties,Dielectric properties, Magnetism

---

Th-S-O-04

The effect of time-dependent magnetic field on electrical polarization in bismuth ferrite

S. Omid Sayedaghaee [1, 2], Sergey Prosandeev [2, 3], Bin Xu [2, 3], Charles Paillard [2, 3], Laurent Bellaiche [1, 2, 3]

[1] *Microelectronics-Photonics Program, University of Arkansas, Fayetteville, AR, United States*
[2] *Physics Department, University of Arkansas, Fayetteville, AR, United States*
[3] *Institute for Nano Science and Engineering, University of Arkansas, Fayetteville, AR, United States*

The dynamical coupling of different order parameters in multiferroic $BiFeO_3$ (BFO) can result in new effects. In this study, the behavior of polarization under the application of an *AC* magnetic field superimposed on a *DC* field ($H=H_{dc}+h_{ac}Sin(\omega t)$) is studied by using an atomistic effective Hamiltonian scheme within a Molecular Dynamics (MD) technique. The dependence of the quadratic magnetoelectric coefficient, β, on the frequency of applied magnetic field is then extracted. It is first found that, when the frequency of applied magnetic field, ω, is within few GHz, the obtained value for β is in the order of 10^{-8} C/m^2T^2 which agrees with previously reported measurements. Moreover, the behavior of β significantly changes when the frequency of applied magnetic field becomes close to that of a magnon. Finally, at higher frequencies of applied magnetic field, an additional high frequency oscillation is observed in the behavior of polarization versus time, which is a result of the influence of the natural phonon frequency in addition to the frequency of the applied magnetic field.

Keywords: magnetoelectric coupling, atomistic simulations, dynamics, multiferroic

---

Th-S-O-05

Metaferroics: higher field effects in a multiferroic

Christopher E.r Wagner, Pradeep Kumar
University of Florida, Gainesville, United States

The multi order parameter systems and their cross responses are generally considered in linear response at low fields and are viewed as a continuous responses. Here we consider the cases when the responses for all order parameters, at higher fields and at temperature T = 0 are discontinuous. We report results for a model that incorporates metamagnetism as a magnetic response, metaelectricity as a dielectric response and the two fields interact in a bilinear term, representing the hidden field model. The results show a rich phase diagram, mutually dependent critical magnetic and electric fields and the evolution of all physical observables with temperature.

Keywords: Ferroics, Multiferroics, Metaferroics

Thursday, September 7th, 2017 - Room4 - 12:40 - 13:40

- WOMEN

Thursday, September 7th, 2017 - Room1 - 13:50 - 14:20

keynote speaker - DOMAINS III

Th-S-O-01

(INVITED) Emergent chirality in oxide superlattices

Ramamoorthy/ Pedriac Shafer Ramesh

UCBerkeley, Berkeley, United States

The complex interplay of spin, charge, orbital, and lattice degrees of freedom has provided for a plethora of exotic phase and physical phenomena. Among these, in recent years, topological states of matter and spin textures have emerged as fascinating consequences of the electronic band structure and the interplay between spin and spin-orbit coupling in materials. In this lecture, I will discuss work on oxide superlattices that leverage the competition between charge, orbital, and lattice degrees of freedom. I will particularly focus on superlattices of $PbTiO_3/SrTiO_3$ as a model system in which we can create complex, vortex-antivortex pairs (that exhibit smoothly varying ferroelectric polarization with a 10 nm periodicity) that are reminiscent of topological features such as skyrmions and merons. The key role of a combination of advanced layer-by-layer growth techniques, atomic-resolution mapping of structure and local polar distortions using scanning-transmission electron microscopy, xray spectromicroscopy and phase-field modeling approaches will be discussed. Finally, the implications of these observations are discussed as they pertain to producing new states of matter and emergent phenomena (such as chirality) in such superlattices. I will finish up by spending some time on the broader context of oxide superlattices.

Keywords: ferroelectric superlattices; vortex formation; emergent behavior;

Thursday, September 7th, 2017 - Room2 - 13:50 - 14:20

keynote speaker - THz/IR/RAMAN I

Th-S-O-01

(INVITED) Ultrafast polarization dynamics in ferroelectric thin films

Aaron Lindenberg

Stanford University / SLAC, Stanford, United States

I will present recent experimental studies of ultrafast optical and THz electric-field-driven responses in ferroelectric thin films and nanostructures. Using a combination of femtosecond x-ray, electron, and nonlinear optical probes, these studies enable us to elucidate fundamental time-scales governing the dynamics of the ferroelectric polarization and the associated atomic-scale response. These results show that one can drive large-scale reorientations of the polarization of a ferroelectric thin film on femtosecond time-scales. I will also describe, briefly, recent results probing optically-driven atomic-scale dynamics and structural reorganizations in the hybrid perovskites.

Keywords: ultrafast dynamics, second harmonic generation, x-ray scattering, THz

Thursday, September 7th, 2017 - Room3 - 13:50 - 14:20

keynote speaker - GROWTH & MATERIALS III

Th-S-O-01

(INVITED) Crystalline phase, micro-structure and electrical properties of lead-free piezoelectric KNN-based films

Wei Ren

Electronic Material Research Laboratory, Key Laboratory of Ministry of Education & International Center for Dielectric Research, Xi'an Jiaotong University,, Xi'an, China

Lead-free piezoelectric ceramics with the composition of $0.915K_{0.5}Na_{0.5}NbO_3$-$0.075BaZrO_3$ - $0.01Bi_{0.5}Na_{0.5}TiO_3$ (KNN-BZ-BNT) show excellent piezoelectric properties with a good thermal stability, as the formation of vertical morphotropic phase boundary. In this work, the films of KNN-BZ-BNT were grown on Nb-doped $SrTiO_3$ substrates with different orientations to investigate the crystal phase and further optimize the performances of films. The thin films show highly preferential orientations in accordance with the orientations of single crystalline substrates. Crystalline phase of the samples was determined to be rhombohedral, which has the spontaneous polarization along [111] direction. Thus the (100)-oriented film demonstrates the most superior piezoelectric properties. All the films exhibit a weak contrast and remarkable homogeneity in the local static out-of-plane piezo-response phase images, suggesting a strong self-polarization. Detailed TEM investigation indicates that the self-polarization in KNN-BZ-BNT films is attributed to the formation internal built-in electric field from the bottom electrode. The $La_{0.7}Sr_{0.3}MnO_3$ layer deposited on $SrTiO_3$ as the bottom electode is more favorible to formation the self-polariztion effect. The layered-redistribution of Ba and Zr ions in the films is one of the possible reasons. The lattice parameters in the Zr-rich and Ba-rich areas also show the difference, which this phenomenon might lead to formation of a super structure and be a reason for improvement of electrical properties of KNN films by Ba and Zr co-doping.

Keywords: lead-free piezoelectric, thin films, structures, MPB

Thursday, September 7th, 2017 - Room4 - 13:50 - 14:20

keynote speaker - ENERGY HARVESTING

Th-S-O-01

(INVITED) The bulk photovoltaic effect in polar oxides for robust and efficient solar energy harvesting

Andrew Rappe

University of Pennsylvania, Philadelphia, United States

Solar energy is the most promising source of renewable, clean energy to replace the current reliance on fossil fuels. Ferroelectric (FE) materials have recently attracted increased attention as a candidate class of materials for use in photovoltaic devices. Their strong inversion symmetry breaking due to spontaneous polarization allows for excited carrier separation by the bulk of the material and voltages higher than the band gap (E_g), which may allow efficiencies beyond the Shockley-Queisser limit. Ferroelectric oxides are also robust and can be fabricated using low cost methods such as sol-gel thin film deposition and sputtering. Recent work has shown how a decrease in ferroelectric layer thickness and judicious engineering of domain structures and FE-electrode interfaces can dramatically increase the current harvested from FE absorber materials. Further improvements have been blocked by the wide band gaps (E_g = 2.7 - 4 eV) of FE oxides, which allow the use of only 8 - 20% of the solar spectrum and drastically reduce the upper limit of photovoltaic efficiency. In this talk, I will discuss new insight into the bulk photovoltaic effect, and materials design to enhance the photovoltaic efficiency. We calculate from first principles the current arising from the "shift current" mechanism, and demonstrate that it quantitatively explains the observed current. Then, we analyze the electronic features that lead to strong photovoltaic effects. Finally, we present new oxides that are strongly polar yet have band gaps in the visible range, offering prospects for greatly enhanced bulk photovoltaic effects.

Keywords: ferroelectric, photovoltaic, shift, current, design

Thursday, September 7th, 2017 - Room1 - 14:20 - 15:00

Invited talk - DOMAINS III

Th-S-O-01

(INVITED) Atomic structure and dynamic behaviors of domain walls and polar vortices in multiferroic thin films

Xiaoqing Pan

Department of Chemical Engineering and Materials Science, University of California-Irvine, Irvine, CA, United States
Department of Physics and Astronomy, University of California-Irvine, Irvine, CA, United States

The applications of ferroelectric materials stem from the ordering of polarization and switching of the polarization states by applied bias. A fundamental understanding of the atomic scale mechanism underlying the domain formation and polarization switching is critical for the design of devices. In this talk, the atomic structure and dynamic behaviors of domain walls and polar voritices in multiferroic $BiFeO_3$ films will be reported. According to in-situ TEM studies, the charged domain walls can be created or erased by applying a bias, and the resistance of the local film strongly depends on the characteristics of these charged domain walls. Furthermore, by mapping the polarization distribution, it was found that a monolayer thick conducting oxide existing on the $BiFeO_3$ film surface causes a significant increase of local polarization and exotic high-density nano-domains with large strain

variations emerge. Finally, small defects in ferroelectric thin films can act as nano-building-blocks for the emergence of novel topological states of polarization ordering, namely, hedgehog/antihedgehog nanodomain arrays in $BiFeO_3$. The emergent polarization states such as hedgehog/antihedgehog and vortex/ antivortex topologies not only modify the local lattice symmetries and thus induce the coexistence of mixed-phases resembling the morphotropic phase boundary with high piezoelectricity, but also lead to flux-closure vortex structures. Phase-field simulations suggest that the observed novel polarization states are formed due to the coupling between the polarization ordering and the charged defects existing in the films. Thus, engineering of defects may provide a new route for developing ferroelectic/multiferroic-based nanodevices.

Keywords: in-situ TEM, domain walls, polar vortices

Th-S-O-02

(INVITED) Nanoscale domain structures in uniaxial ferroelectric single crystals

Vladimir Shur

School of Natural Science and Mathematics, Ural Federal University, Ekaterinburg, Russia

The main aspects of the nanodomain structure evolution in various uniaxial ferroelectrics have been reviewed. The most interesting scenarios of the domain kinetics important for micro- and nanodomain engineering and the variety of metastable nanodomain patterns appeared in highly non-equilibrium switching conditions have been classified and described systematically. All obtained results have been discussed in terms of the unified kinetic approach based on the analogy between domain structure evolution and the new phase growth during first-order phase transformation. In ferroelectrics the nucleation probabilities are determined by the local value of the sum of the external field produced by voltage applied to the electrodes, and partially screened depolarization field produced by bound charges. The bulk screening effect which allows stabilizing almost any tailored domain pattern is the basis of the domain engineering. The key role of the screening retardation in formation of self-assembled nanodomain structures has been demonstrated in various ferroelectrics. The experimental data obtained by modern experimental methods with high spatial and temporal resolution allowed studying the domain formation and growth with nanoscale resolution. The crucial role of screening effectiveness for domain shapes and scenarios of the sideways domain wall motion is demonstrated both experimentally and by computer simulation. It was demonstrated how the highly non-equilibrium switching conditions can be realized. The obtained fundamental results allowed to formulate the physical basis for rapidly developed modern fields of technology named micro- and nanodomain engineering and domain wall engineering. The recent achievements in creation of the short-pitch domain patterns have been reviewed.

Keywords: Nanodomains, nanodomain engineering, domain shape, nucleation, self-assemled structures

Thursday, September 7th, 2017 - Room2 - 14:20 - 15:00

keynote speaker - THz/IR/RAMAN I

Th-S-O-01

(INVITED) Using intense THz pulses to probe and control dynamics in multiferroics

Rohit Prasankumar, Pamela Bowlan, Stuart Trugman, Dmitry Yarotski, Antoinette Taylor

Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, United States

Multiferroic oxides have attracted much attention in recent years due to their potential for controlling magnetism with an electric field and ferroelectricity (FE) with a magnetic field. Most multiferroics, however, typically display relatively weak coupling between these parameters and rarely operate near room temperature. This has motivated researchers to design and fabricate layered oxide heterostructures, with the goal of enhancing the magnetoelectric (ME) coupling between individual ferroelectric and magnetic layers while also increasing their operating temperature. However, further progress in this area requires a deeper understanding of the underlying mechanisms and timescales limiting ME coupling in both bulk and heterostructured multiferroics. In the past few years, we have demonstrated that ultrafast optical and terahertz (THz) spectroscopy is a unique tool for probing the interplay between FE and magnetic ordering in canonical bulk multiferroics such as $HoMnO_3$ and $EuYMnO_3$ as well as in multiferroic oxide heterostructures. For example, these studies have revealed a long-lived, photoinduced enhancement of the FE polarization in a FE/ferromagnet (FM) heterostructure, and have also shown that femtosecond optical pulses can induce transient magnetoelectric coupling in a FE/FM heterostructure, with implications for high speed magnetoelectric devices. We have also used THz pulses to directly probe low energy modes in these materials, allowing us to determine the timescales governing energy transfer from electronic to magnetic degrees of freedom. Overall, our studies demonstrate that ultrashort optical pulses can help unravel the mechanisms underlying magnetoelectric coupling in multiferroic oxides, with the potential for all-optical control on femtosecond timescales.

Keywords: Ultrafast, optics, terahertz, multiferroics

Th-S-O-02

(INVITED) THz dielectric responses derived from dipole clusters of $BaTiO_3$-based ferroelectrics

Takuya Hoshina, Motoharu Sakurai, Hiroaki Takeda, Takaaki Tsurumi

School of Materials and Chemical Technology, Tokyo Institute of Technology, Tokyo, Japan

Barium titanate ($BaTiO_3$)-based system is the most widely used ferroelectrics and the most important dielectric material for multilayered ceramic capacitors. The excellent dielectric property of $BaTiO_3$-based system has attracted much attention not only in the electroceramic industry but also in fundamental research. In $BaTiO_3$-based system, ionic and dipole polarizations predominantly determine the dielectric property. The ionic polarization is related to lattice vibrations. On the other hand, the dipole polarization is governed by the ferroelectric domain-wall contributions in multi domain crystals and ceramics. Additionally, the dielectric relaxation related to order-disorder phenomena derived from dipole clusters have been reported even at a high temperature above Currie temperature (T_C). However, these polarization mechanisms are complicated and as yet unclarified. Thus, accurate dielectric spectra

in the THz region is highly desired in the analysis of the ionic polarization and order-disorder relaxation. In this study, we developed a far-infrared spectroscopic ellipsometer for measuring THz complex permittivity of high-permittivity materials, and measured the complex permittivity of $BaTiO_3$-based ferroelectrics in the frequency region of 30 – 700 cm^{-1} (0.75 – 21 THz). THz dielectric spectra of $BaTiO_3$ single crystal and $Ba_{0.6}Sr_{0.4}TiO_3$ ceramics could not be represented by a harmonic oscillator model, which suggested anharmonicity of ferroelectric phonon mode. Based on an eight-site order-disorder model, we analyzed the THz dielectric spectra of $BaTiO_3$-based ferroelectrics. It was found that the order-disorder mode coupled with the Slater mode greatly contributes the high permittivity of $BaTiO_3$-based ferroelectrics.

Keywords: THz ellipsometer, dipole cluster, order-disorder, barium titanate

Thursday, September 7th, 2017 - Room3 - 14:20 - 15:00

Invited talk - GROWTH & MATERIALS III

Th-S-O-01

(INVITED) PLD growth of ultra-thin $SrTiO_3$ films on Si(100): coverage and thermal budget effects

Danilo Suvorov, Daniel Diaz Fernandez, Matjaž Spreitzer, Tjaša Parkelj

Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia

The Pulsed Laser Deposition (PLD) technique offers several key advantages with respect to Molecular Beam Epitaxy (MBE) for the growth of epitaxial $SrTiO_3$ (STO) ultra-thin films on Si, but the research on PLD growth of these materials is scarce. A novel procedure, which uses a ½ ML buffer layer of Sr grown also by PLD, has been developed over the last two years at our group. It uses separate STO deposition, oxidation and crystallization stages for the growth of 10-12 ML samples, in order to minimize the interface reactions. In this work, the impact of the coverage deposited after the STO oxidation and crystallization stages, along with the crystallization method, is tested and optimized with in-situ and real-time RHEED, and ex-situ XPS, AFM and XRR measurements. It has been found that a combination of oxidation and crystallization every 2 ML improves the surface crystallinity and minimizes the crystallization starting temperature. The minimization of the thermal budget improves the interface quality, but decreases the STO density, while the composition and morphology of the samples stay close to that from stoichiometric STO. These results can be explained as a result of the balance between the critical thickness, minimum energy and proper Sr/Si coverage, and they improve the general knowledge about this growth and interface, allowing for the growth of high-quality templates for the epitaxial overgrowth of other complex oxides in a more efficient way.

Keywords: PLD, Sr-titanate, Si-substrate, epitaxy, interfaces

Th-S-O-02

(INVITED) Transmission electron microscopy of multifunctional hard coatings

Jiechao Jiang [1], Minghui Zhang [1], Yi Sheng [1], Jaroslav Vlček [2], Efstathios Meletis1 [1]

[1] *Materials Science and Engineering Department University of Texas at Arlington, Arlington, United States*
[2] *Department of Physics University of West Bohemia,, Plze?, Czech Republic*

Multifunctional coatings of ultra-high temperature ceramics consisting of transition metal based borides (ZrB_2, HfB_2, TaB_2), carbides (TiC, TaC, ZrC, HfC), and nitrides (ZrN, HfN, TaN) exhibit high melting temperature, high hardness, outstanding oxidation and corrosion resistance, thermal shock resistance and high thermal stability. Such coatings have high potential for a much wider industry-specific applications, such as, surface protection of high-speed cutting tools, turbine blades and vanes, hypersonic vehicles (to construct sharp wing leading edges and nose tips for thermal protection), atmospheric re-entry and rocket propulsion systems. The coatings with such desirable properties possess unique microstructures. In this talk, we present transmission electron microscopy (TEM) of selected multifunctional hard coatings with unique structures: (1) Si-B-C-N and Hf-B-Si-C-N coatings with extraordinary high temperature stability, high hardness and high oxidation resistance. The coatings remain amorphous when annealed > 1500 °C in air and exhibit an extraordinary oxidation resistance due to formation of finely distributed h-BN or HfO_2 nano-crystals embedded in an amorphous SiO_2 matrix at very high temperatures. (2) Zr-B-C-N coatings with a high hardness of 37 GPa and a modulus of 317 GPa, possess an unique nano-needle structure with ZrN and/or Zr(B,N) nano-domain structures (~2 nm) that are semi-coherently joined via Zr-N monolayer interfaces. (3) Hf-B-Si-C coatings which with only a slight variation in Si content exhibit entirely different microstructures and thus, mechanical and oxidation resistance properties.

This work was supported by the U.S. NSF under Award NSF/CMMI DMREF-1335502.

Keywords: TEM , hard coating, microstructure

Thursday, September 7th, 2017 - Room4 - 14:20 - 15:00

Invited talk - ENERGY HARVESTING

Th-S-O-01

Defect engineered complex oxide thin films with anomalous multifunctionalities

Chonglin Chen

University of Texas at San Antonio, San Antonio, United States

Complex oxides have demonstrated various important physical properties such as various dielectric and unusual magnetic properties. These extraordinary phenomena are highly dependent upon the degrees of the freedom of the charge distribution, spin and orbital status, and the lattice structures. Among the

perovskite cobalt oxide system, the complex cobalt oxide can exhibit different cobalt and oxygen coordination from tetrahedral, pyramidal to octahedral dependent on the oxygen contents, leading to various crystal structures with a great flexibility of the oxygen frameworks. Thus, oxygen nonstoichiometry becomes a very crucial parameter for tuning their atomic structure and physical properties. For instance, $LnBaCo_2O_{5+d}$ (LnBCO, Ln= rare transition metal elements) systems exhibit various unique physical properties not only due to the presence of A-site disordered and A-site ordered structures (the close ionic sizes of Ln and Ba), but also the degree of ordered oxygen vacancy structures. These defect engineered structures induce the formation of various double perovskite structures and the strong couplings of multifunctionalities from ferroelectricity, ferromagnetism, optic/magnetoelectric response in a single phase double perovskite thin films. These findings open a new avenue for material genetic design and synthesis by tailoring the atomic defect structures to facilitate the strong correlated multifunctionalities for novel device development. Details will be discussed in the talk.

Keywords: thin films, oxides

Th-S-O-02

(INVITED) Room-temperature aerosol deposition of ferroelectric ceramic films for power inverters in electric drive vehicles

U. Balu Balachandran, B. Ma, T. H. Lee, S. E. Dorris

Argonne National Lab, Argonne, United States

Future availability of high-temperature power inverters will advance the market share for highly fuel-efficient, environmentally friendly electric drive vehicles (EDVs). An integral part of vehicle power inverters is the DC buss capacitor, which has a significant influence on inverter lifetime, reliability, cost, and temperature of operation. Funded by the U.S. Department of Energy's Vehicle Technologies Program, Argonne is developing lead lanthanum zirconium titanate (PLZT)-based film capacitors for vehicular applications. A high-rate aerosol deposition (AD) process is being developed at Argonne to produce PLZT films with desirable properties. The AD process can produce dense films at room temperature; thus making the process amenable for depositing PLZT films on a variety of substrates such as polymer, glass, and metal foils. Recently we demonstrated that a ≈8-μm-thick PLZT film on aluminum-metallized polyimide substrate can be deposited in less than 10 minutes by the AD process. Films deposited by the AD process exhibited dielectric constant of ≈ 80 at 300 V bias, dielectric loss < 2%, mean breakdown voltage of ≈ 1000 V, and temperature-dependent properties suitable for advanced power inverters. Our results show that the AD process has great potential in reducing the manufacturing cost of high-temperature capacitors. Recently we produced ≈ 30 cm long and ≈ 2.5 cm wide PLZT films on aluminum-metallized thin polymer substrates. These PLZT films were wound into capacitors with terminations. The dielectric properties of the long-length PLZT films and the wound capacitors will be presented in this talk.

Work supported by the U.S. Department of Energy, Vehicle Technologies Program, under Contract DE-AC02-06CH11357.

Keywords: Ferroelectrics, Thin Films, Ceramics

Thursday, September 7th, 2017 - Room1 - 15:00 - 16:15

Oral presentation - DOMAINS III

Th-S-O-01

Direct observation of charged domain walls in hybrid improper ferroelectric $(Ca,Sr)_3Ti_2O_7$

Kousuke Kurushima [1, 2], Hirofumi Tsukasaki [1], Yui Ishii [1], Sang-Wook Cheong [3], Shigeo Mori [1]

1 Department of Materials Science, Osaka Prefecture University, Sakai, Osaka, Japan
2 Toray Research Center, Ohtsu, Shiga, Japan
3 Rutgers Center of Emergent Materials, Rutgers University, Piscataway, New Jersey, United States

Recently a large number of functional materials have been proposed based on first-principles calculations. For example, hybrid improper ferroelectric compounds such as double layered Ca3Ti2O7, Ca3Mn2O7 and (Ca/Sr/Ba)3(Sn/Zr/Ge)2O7 with the Ruddlesden-Popper structure were predicted to show ferroelectricity from first-principles calculations [1]. Recently Oh et al. succeeded in preparing single crystals of hybrid improper ferroelectric (Ca,Sr)3Ti2O7 and found the intriguing ferroelectric domain structure consisting of abundant charged domain walls with conducting head-to-head and insulating tail-to-tail configurations, even though they usually accompany a large electrostatic energy cost. In this work, using state-of-the-art aberration-corrected high-angle annular-dark-field (HAADF) scanning transmission electron microscopy (STEM), we investigated ferroelectric domain wall structures in (Ca,Sr)3Ti2O7 crystals at the atomic scale. We succeeded in observing directly three distinct types of ferroelectric domain walls at the sub-atomic scale, i.e., 180° domain walls, head-to-head type and tail-to-tail type charged domain walls. The FE 180° domain wall is atomically sharp between two adjacent FE domains with antiparallel ferroelectric polarization. On the other hand, it is revealed that charged domain walls are stably and abundantly present and they have unique domain wall structures.

References

[1] N. A. Benedek and C. J. Fennie, Phys. Rev. Lett. 106, 107204 (2011).

[2] Y-S. Oh et al., Nature Mater. 14, 407 (2015).

[3] F-T. Haung et al., Nat. Commun. 7, 11602 (2016).

Keywords: Charged domain walls, HAADF-STEM

Th-S-O-02

Electrical control and temperature tuning of chiral phases in electrotoroidic nanocomposites

Raymond Walter [1, 2], Sergei Prokhorenko [1], Zhigang Gui [3], Yousra Nahas [1], Lin-Wang Wang [4], Laurent Bellaiche [1]

[1] *Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, United States*
[2] *Department of Mathematical Sciences, University of Arkansas, Fayetteville, United States*
[3] *Department of Materials Science and Engineering, University of Delaware, Newark, United States*
[4] *Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, United States*

Electrotoroidic systems can exhibit optical activity if the electrical toroidal moment **G** of their electrical vortices couples to a spontaneous electrical polarization **P** [1]. Here we use large-scale atomistic simulations to explore electric field and temperature control of optical activity and related properties in chiral phases of an electrotoroidic nanocomposite. Specifically, we consider a $BaTiO_3$ nanowire in a $SrTiO_3$ matrix exhibiting electrical vortices with both axial G and P. Molecular dynamics for a second-principles effective Hamiltonian (Heff) finds the gyrotropic coefficient measuring optical activity is maximized at room temperature for some critical bias field. A temperature-electric field phase diagram of chiral and non-chiral phases is obtained from Monte Carlo simulations. We then follow the recipe of [2] in a low-temperature regime: we apply an electric field anti-parallel to the polarization to switch from the chiral vortex to a chiral, Bloch-like electrical skyrmion. However, this skyrmion exhibits insignificant optical activity, so we probe other optoelectronic properties. To this end, we extend work of [3] that used the Heff method to obtain equilibrium relaxed atomic configurations as input for the linear-scaling 3D fragment (LS3DF) method, a first-principles method for calculating electronic structure in >10,000 atom systems. Band gap and alignment change more significantly under temperature control of the vortex than under electric field control of the skyrmion, suggesting the former regime is superior for novel optoelectronic applications.

References

[1] Prosandeev et al., PRB 87, 195111 (2013)

[2] Nahas et al., Nat. Comm. 6, 8542 (2015).

[3] Gui et al., NanoLett 15, 3224 (2015).

Keywords: chirality, topological defects, vortex, skyrmion, large-scale atomistic calculations

---

Th-S-O-03

Towards functional polar domain walls in ferroelastic $CaTiO_3$

Guillaume Nataf [1, 2, 3], Mael Guennou [1], Jens Kreisel [2, 4], Patrick Hicher [5], Raphaël Haumont [5], Oktay Aktas [6, 7], Ekhart Salje [6], Ludovic Tortech [8], Dominique Martinotti [1], Claire Mathieu [1], Nick Barrett [1]

1 SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, Gif-sur-Yvette, France
2 Materials Science and Technology department, Luxembourg Institute of Technology, Belvaux, Luxembourg
3 Department of Materials Science, University of Cambridge, Cambridge, United Kingdom
4 Physics and Materials Science Research Unit, University of Luxembourg, Belvaux, Luxembourg
5 Laboratoire de Physico-Chimie de l'Etat Solide, ICMMO, CNRS-UMR 8182, Orsay, France
6 Department of Earth Sciences, University of Cambridge, Cambridge, United Kingdom
7 Department of Materials, ETH Zürich, Zürich, Switzerland
8 8IPCM, UMR CNRS 7201, UPMC, Université Pierre et Marie Curie, Paris, France

There is a growing interest for structural and electric properties of ferroelectric and ferroelastic domain walls. The emerging field of domain boundary engineering holds the promise of using the distinct functional properties of domain walls in and as devices. Here, we report a study of ferroelastic domain walls in paraelectric, non-polar CaTiO3. We report the observation of a strong signal in piezoelectric resonance spectroscopy (RPS), which we argue is due to the polar character of the walls. We also use a low energy electron microscope (LEEM) to observe twin walls in CaTiO3. As expected, adjacent domains present the same surface potential because the material is non-polar. However, the twin walls show clear surface potential contrast with respect to the domains. The same contrast is observed on a work function map. This provides direct in-situ evidence of the polar nature of ferroelastic twin walls in CaTiO3. In a second step, we study the manipulation of the surface charge at twin walls upon electron injection, realized by increasing the energy of the incoming electron beam of the LEEM. We show that the contrast between domain and domain walls vanishes upon electron irradiation with a characteristic time of 10 - 15 minutes. It is possible to recover the initial state, i.e. before charge injection, by annealing above 250 °C. The ability to observe polarity at the nanoscale and to tune the surface charge at twin walls gives perspectives toward functionalization of polar twin walls in CaTiO3.

Keywords: Domain walls, CaTiO3

Th-S-O-04

Probing ferroelectric domains with X-ray nanodiffraction

Marios Hadjimichael [1], Edoardo Zatterin [1, 2], Steven Leake [2], Pavlo Zubko [1]

[1] London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, 17–19 Gordon Street, WC1H 0HA, London, United Kingdom
[2] ESRF – The European Synchrotron, 71 Avenue des Martyrs, 38000, Grenoble, France

Domains in ferroelectric materials have been the subject of many years of research. Originally considered detrimental for ferroelectric thin films and undesirable for applications which require polarisation stability, the novel properties of domains and their boundaries, domain walls, have sparked scientific interest in their functionality and possible applications. Domain walls have been shown to enhance the properties of ferroelectrics and exhibit symmetry different to the bulk material, making multidomain ferroelectrics a pathway towards novel device implementations through domain wall nanoelectronics. Here we present results of synchrotron X-ray diffraction studies on $PbTiO_3/SrTiO_3$

superlattices. We look at the behaviour of ferroelectric domains in these materials across the ferroelectric phase transition. We discover a transition during which the domain walls change their orientation, from walls aligned along the <100> crystallographic axes at room temperature, to walls oriented along the <110> axes at higher temperatures and study this reorientation for different domain periods. Using a nanofocused beam, we map the real space distributions of these domains, providing the first non-invasive real space observations of buried domains in ferroelectric/dielectric superlattices. By mapping the domain orientations in the vicinity of a defect, we show that domain walls align along the edges of features in the topography of the thin film. We map the distribution of film lattice parameters around one of these features and we show that this alignment is associated with strain and large strain gradients. These findings offer a greater insight on how to control the orientations of domain walls in multidomain ferroelectric materials.

Keywords: ferroelectric, domains, superlattice, diffraction, oxides

---

Th-S-O-05

Effect of electric field on local structure probed by angular dependence of Raman scattering

Md Al Helal [1], Md Aftabuzzaman [1], Šarūnas Svirskas [3], Shinya Tsukada [2], Jūras Banys [3], Seiji Kojima [1]

[1] *Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, Japan*
[2] *Faculty of Education, Shimane University, Matsue, Japan*
[3] *Faculty of Physics, Vilnius University, Sauletekio av. 9, Vilnius, Lithuania*

$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) is one of the most widely studied relaxor ferroelectric materials with perovskite structure due to its outstanding physical properties. In the present study, the temperature, electric field, and angular dependences of Raman scattering were performed to clarify the physical origin of local structures in PMN-17PT single crystals. Upon cooling, the Raman active modes within the range between 500-900 cm^{-1} show significant changes at around 343 K, suggesting the change of paraelectric cubic to ferroelectric rhombohedral phase ($T_{C\text{-}R}$). The intensity variations of Raman active modes with the rotation angle in a paraelectric cubic phase at fixed temperature were observed clearly. Periodic functions, representing these intensity variations, were calculated theoretically by considering the local *F*m-3m and *R*3m symmetries, respectively. Theoretical calculations were then compared with the experimental data and a discussion was provided. Under the electric field along the [100] direction just above the $T_{C\text{-}R}$, the sudden changes in the intensities of the Raman peaks at around 740 and 780 cm^{-1} indicated the field induced phase transition from cubic to tetragonal structure. The applied electric field in a paraelectric cubic phase suppressed the random fields (RFs) and therefore, the change of Raman tensor ratio and phase differential were observed compared with the zero field results. In addition, at sufficiently higher electric field, the RFs were diminished and the angular variation changes perfectly from its zero field behavior.

Keywords: Raman scattering, Phase transition, Electric field, Polar nanoregions.

Thursday, September 7th, 2017 - Room2 - 15:00 - 16:15

Th-S-O-01

Terahertz dynamics of soft and central modes in ferroelectric superlattices

Anna Razumnaya [1, 2], Yury Tikhonov [1], Yury Yuzyuk [1], Nora Ortega [3], Ashok Kumar [3], Ram S. Katiyar [3]

[1] *Southern Federal University, Rostov-on-Don, Russia*
[2] *Université de Picardie Jules Verne, Amiens, France*
[3] *University of Puerto Rico, San Juan, United States*

Elastic strains in thin films and artificial superlattices composed of alternating layers of ferroelectric compounds provide a new route to enhance the properties of known ferroelectrics and create materials with superior properties for device applications. The series of ferroelectric $BaTiO_3/Ba_{1-x}Sr_xTiO_3$ (BT/BST-x) superlattices deposited on (001)MgO substrate using a PLD technique. The structural parameters of the layers were determined by X-ray diffraction. Near- and sub-Terahertz dynamics of soft and Debye-type central modes was studied by the polarized Raman spectroscopy of the BT/BST-x superlattices in the temperature range of 80-500 K. Due to the stress gradients in these BT/BST-x superlattices the phase transitions in BT and BST-x layers occur at different temperatures and depend on chemical composition of the BST-x layers. It was shown that temperature evolution of the low-frequency Raman spectra can be described within the model of coexisting damped harmonic oscillator and Debye relaxator. The occurrence of the pronounced central mode can explain the recently observed relaxor-like dielectric anomalies in BT/BST-x superlattices. We demonstrate that variation of chemical composition of the BST-x layers allows to tune distortions in alternating layers and to modify the shape of the dielectric permittivity as a function of temperature.

We acknowledge financial support from the RSF (grant N 14-12-00258) and FP7-ITN-NOTEDEV.

Keywords: Superlattice, Ferroelectrics, Raman Spectroscopy, Soft Mode, Debye Relaxator

---

Th-S-O-02

Electric-field tuning of a planar terahertz metamaterial based on strained $SrTiO_3$ layers

Christelle Kadlec [1], Volodymyr Skoromets [1], Filip Kadlec [1], Hynek Nemec [1], Hou-Tong Chen [2], Vlastimil Jurka [1], Karel Hruska [1], Petr Kuzel [1]

[1] *Institute of Physics Czech Academy of Sciences, Prague, Czech Republic*
[2] *Center for Integrated Nanotechnologies Los Alamos National Laboratory, Los Alamos, United States*

The development of tunable devices is still a significant challenge for the evolving terahertz (THz) technology. Components allowing for agile manipulation of THz radiation, together with efficient low-cost emitters and sensitive detectors, are expected to greatly enhance the versatility of future applications. The development of metamaterials represents a promising opportunity allowing efficient control of THz radiation. In this work, we demonstrate a metamaterial exhibiting a tunable response in the terahertz domain, controlled by a bias electric field. The active part of the metamaterial consists of

a periodic metallic pattern deposited on a thin epitaxially strained $SrTiO_3$ film. The role of the metallic structure is two-fold: it gives rise to the metamaterial resonance and it enables applying a bias to the $SrTiO_3$ film. The strained film exhibits a pronounced dependence of its permittivity on the bias, which exerts a strong influence on the resonance. Specifically, the resonance of our structure occurs near 0.5 THz and, upon applying a bias voltage of 55 V, a relative tunability of the resonance frequency of 19% was achieved at room temperature.

This work has been submitted to publication in Applied Physics Letters.

Keywords: ferroelectric thin film, tunability, metamaterial, metasurface

---

Th-S-O-03

Tunable terahertz range dielectric spectra of in domain-engineered ferroelectric nanostructures

Jiri Hlinka

Institute of Physics, Czech Acad. Sci., Prague, Czech Republic

The contribution of the ferroelectric soft mode to dielectric permittivity gives rise to the possibility of tuning the properties of material by means of an electric field when the soft mode has low enough frequency, and this has been used in many applications, where a strong static permittivity is required. In this contribution, conditions for observation of tunable terahertz-range dielectric resonances, associated with the presence of nanoscale ferroelectric domains, will be discussed. The starting point will be dielectric characterization of ferroelectric $BiFeO_3$ thin films and ceramic samples[1], and the very recent theoretical prediction of an occurrence of a peculiar terahertz resonance in $BiFeO_3$ [2].

This work was supported by the Czech Science Foundation (Project GACR 13-15110S) and by European Union funding under the 7th Framework Programme (Project NOTEDEV).

References

[1] S. Skiadopoulou, V. Goian, C. Kadlec, F. Kadlec, X. F. Bai, I. C. Infante, B. Dkhil, C. Adamo, D. G. Schlom, and S. Kamba, Phys. Rev. **B** 91, 174108 (2015).

[2] J. Hlinka, M. Pasciak, S. Korbel and P. Marton, In press (2017).

Keywords: THz, soft mode, BiFeO3

Th-S-O-04

Phonon-polariton dispersion relation of ferroelectric $LiTaO_3$ crystals

Seiji Kojima [1], Miroslaw Maczka [2]

[1] *Division of Materials Science, University of Tsukuba, Tsukuba, Japan*
[2] *Institute of Low Temperature and Structure Research, Wroclaw, Poland*

The broadband dispersion relation of active phonon-polaritons was studied in a ferroelectric lithium tantalate crystal. The reflectivity in the far- and mid-IR regions was measured by the reflection FT-IR measurement. The real and imaginary parts of a reflective index were calculated in the broadband frequency range between 3 and 36 THz. Using these values the dispersion relation of phonon-polariton including damping of polariton was determined using real and imaginary parts of a polariton wave vector. These phonon-polaritons with A1(z) and E(x,y) symmetry are infrared and Raman active. The observed polariton dispersion relation is in agreement within the experimental uncertainty with the phonon-polariton dispersion determined by the previous forward Raman scattering measurements.

Keywords: phonon-polariton, dispersion relation, ferroelectric, LiTaO3, FTIR, forward Raman scattering

---

Th-S-O-05

Resonance damping of the THz-frequency transverse acoustic phonon in the relaxor ferroelectric $KTa_{1-x}Nb_xO_3$

Eugene Iolin [1], Jean Toulouse [1], Daniel Petitgrand [2], Bernard Hennion [2], Ross Erwin [3]

1 Physics Department, Lehigh University, ,, Bethlehem, PA, United States
2 Laboratoire Leon Brillouin, CEA, Saclay, United States
3 National Center for Neutron Research, NIST, , Gaithersburg, MD, United States

Damping of the transverse acoustic (TA) phonon in single crystals of the homovalent relaxor KTa1-xNbxO3 with x = 0.15-0.17 was studied by means of inelastic cold neutron scattering near the (200) B.Z. point where diffuse scattering is absent, although it is present near (110). In a wide range of temperatures centered on the phase transition, T = 195 K ÷ 108 K, the TA phonon damping exhibits a step increase around the wavevector q = 0.07, a shallow maximum at q = 0.09 - 0.12 and remains high up to the highest wavevector studied of q = 0.16 (Phys. Rev. B 94, 214116). These results are explained in terms of a resonant interaction between the TA phonon and the tunneling reorientation of the off-center Nb+5 ions. The observed TA damping is successfully reproduced in a simple model that includes an interaction between the TA phonon and a dispersionless localized mode with frequency ωL and damping ΓL (ΓL<ωL). The values of ωL and ΓL are moderately dependent on temperature but the oscillator strength, M2, of the resonant damping exhibits a strong maximum in the range T ~120 K ÷ 150 K in which neutron diffuse scattering near the (110) B.Z. point is also maximum and the dielectric susceptibility exhibits the relaxor behavior.

Keywords: phonon, resonance, damping, off-center, ion

Thursday, September 7th, 2017 - Room3 - 15:00 - 16:15

Oral presentation - GROWTH & MATERIALS III

Th-S-O-01

Compressively strained lead titanate films

Yaqi Li, Ben Putland, Marios Hadjimichael, Pavlo Zubko

Department of Physics and Astronomy and London Centre for Nanotechnology, University College London, London, United Kingdom

Over the last decade, the concept of strain engineering has proven to be extremely fruitful in generating new polar phases and tuning the functional properties of ferroelectric oxides. The temperature-strain phase diagrams of a number of ferroelectrics have been extensively studied, both experimentally and theoretically. Lead titanate based ferroelectrics in particular have received a large share of the attention, especially in the tensile strain region where polarisation rotation and complex ferroelastic domain patterns have been predicted and observed. The compressive regime, however, is less well explored. We have studied thin films of lead titanate deep in the compressive strain region of the phase diagram and report on a complex evolution of the structure and surface morphology observed with increasing film thickness as the material attempts to accommodate or relax the substrate-imposed epitaxial strain.

Keywords: Strain engineering, PbTiO3

Th-S-O-02

Long-range stripe nanodomains in epitaxial (110)-$BiFeO_3$ thin films on (100)-$NdGaO_3$ substrate

yogesh sharma [1, 2, 3], Radhe Agarwal [2], Charudatta Phatak [3], Ram S. Katiyar [2], Seungbum Hong [3, 4]

[1] *Oak Ridge National Laboratory, Knoxville, United States*
[2] *University of Puerto Rico, San Juan, United States*
[3] *Argonne National Laboratory, Lemont, United States*
[4] *KAIST, Daejeon, Korea, Republic of (South)*

We have observed ferroelectric and ferroelastic nanodomains in (110)-oriented $BiFeO_3$ (BFO) thin films epitaxially grown on low symmetric (100) $NdGaO_3$ (NGO) substrate. We observed long range ordering of ferroelectric 109° stripe nanodomains separated by periodic vertical domain walls in as-grown 130 nm thick BFO films. The effect of $La_{0.67}Sr_{0.33}CoO_3$ (LSCO) conducting interlayer on domain configurations in BFO/NGO film was also observed with relatively short range-ordering of stripe domains due to the modified electrostatic boundary conditions in BFO/LSCO/NGO film. Additional studies on B-site doping of Nb ions in BFO films showed change in the domain structures due to doping induced change in lattice anisotropy while maintaining the stripe domain morphology with 109° domain

wall. This long-range array of ferroelectric and ferroelastic domains can be useful for optoelectronic devices and ferroelastic templates for strain coupled artificial magnetoelectric heterostructures.

Keywords: BiFeO3 thin films, Ferroelastic nanodomains, Scanning Probe Microscopy, Ferroelectricity, Doping effect

---

Th-S-O-03

Microstructural development of hard Hf-B-Si-C-N coating at high temperatures

Yi Shen [1], Minghui Zhang [1], Jiechao Jiang [1], Jaroslav Vlček [2], Efstathios Meletis [1]

[1] *Department of Materials Science and Engineering, University of Texas at Arlington, Arlington, United States*
[2] *Department of Physics, University of West Bohemia, Univerzitní 22, 306 14 Pilsen, Pilsen, Czech Republic*

Hf-B-Si-C-N films fabricated using reactive pulsed dc magnetron co-sputtering are hard, optically transparent, and exhibit superior high-temperature oxidation resistance. In this work, we have conducted a systematic and detailed microstructural analysis of the as-deposited $Hf_7B_{23}Si_{22}C_6N_{40}$ and $Hf_6B_{21}Si_{19}C_4N_{47}$ films and the annealed films up to various temperatures from 1100 °C to 1600 °C in air and in helium using HRTEM. The motivation for this research was to understand the behavior of the high temperature oxidation resistance by studying their microstructure evolution as a function of their exposure to high temperatures in view of their slight change in composition. The overall objective is to respond to the need for thin-film materials for severe environment applications which can resist corrosion and oxidation at elevated temperatures. All as-deposited films have a homogenous amorphous structure, while all annealed films were found to have a two-layered structure composed of a nanocomposite oxidized surface layer of HfO_2 particles embedded in a SiO_x matrix and an interlayer underneath. As the annealing temperature increased from 1100 □ to 1600 □, the interlayer structure gradually changes from a homogenous amorphous structure to a nanocomposite structure with nanocrystals embedded in an amorphous matrix. It is also found that a slight change in film composition results a significant change in the microstructure of the interlayer.

This work was supported by the U.S. NSF under Award NSF/CMMI DMREF-1335502.

Keywords: thin films, TEM, high-temperature oxidation resistance, microstructure

---

Th-S-O-04

Charged defects in ferroelectric oxides: investigation of doped $BaTiO_3$ thin films

Christopher Castro Chavarria [1, 2], Andreas Klein [2], Mario Maglione [1], Sandrine Payan [1], Quentin Simon [1], Andreas Hubmann [2], Hans Wardenga [2]

[1] *Institute for Condensed Matter Chemistry Bordeaux, UPR 9048 ICMCB-CNRS, University of Bordeaux, 33608 Pessac Cedex, France, Pessac, France*

[2] *Darmstadt University of Technology, Institute of Materials Science, Petersenstraße 23, D-64287 Darmstadt, Germany, Darmstadt, Germany*

BTO thin films are chemically substituted and processed as to generate and control point defects. Mn and Nb-doped BTO thin films were deposited by RF-sputtering. Their chemical, structural, optical, dielectric and electric properties were analyzed by Impedance spectroscopy in dependence on temperature, frequency and static electric field, X-Ray Diffraction, ex-situ and in-situ XPS, Ellipsometry and leakage currents measurements. At 100 kHz and 20 °C, Mn-doped films exhibit low dielectric losses around 1% and low relative permittivity around 300; whereas Nb-doped films exhibit higher values, 7% and 700 correspondingly. We observed the effect of doping in the Fermi level position (E_F). In fact, there is a difference of 0.6 eV between the E_F of Nb and Mn-doped BTO thin films. Moreover, we observed that the E_F in BTO: Mn thin films (300nm) is around 2.2 ± 0.1eV instead of 1eV, leading to the conclusion that the E_F in BTO is pinned by the $Mn^{3+/2+}$ defect level transition rather than that of $Mn^{4+/3+}$.The E_F observed by XPS correlates well with electrical measurements where BTO:Mn showed low current density whereas BTO:Nb showed higher current density at E_{bias}=100 kV/cm. In addition to this, we performed an interface experiment between STO: Nb single crystal and BTO: Mn thin film. We observed the evolution of the valence band maximum and the core levels of Sr, Ba, Ti and O in function of the film thickness, showing that E_F varies from 3.2 eV to 2.8 eV within few nanometers up to 120 nm.

Keywords: BaTiO3, leakage currents, Impedance spectroscopy, in-situ XPS, point defects

---

Th-S-O-05

(INVITED) Direct synthesis of tetragonal $BaTiO_3$ nanoparticles by sonochemical and surface active etching method

Thitirat Charoonsuk [1, 2], Wanwilai Vittayakorn [1, 5], Rangson Muanghua [3], Naratip Vittayakorn [1, 2, 5]

[1] *Electroceramic Research Laboratory, College of Nanotechnology, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*

[2] *Advanced Material Research Unit, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*

[3] *Department of Electronics Engineering, Faculty of Engineering, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*

[4] *Department of Chemistry, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*

[5] *Nano-KMITL Center of Excellence on Nanoelectronic Devices, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*

In this work, two direct synthesis methods; sonochemical and surface active etching method, are proposed as a simple way to achieved $BaTiO_3$ nanoparticles. In the sonochemical process, the oxides of perovskite $BaTiO_3$ were synthesized successfully without a calcination step. Synthesis parameters detailed exploration considering the role of sodium hydroxide (NaOH) concentration, synthesis atmosphere, ultrasonic reaction time and precursor concentration on the perovskite phase formation and particle size was presented. It was found that nanocrystals were formed directly before being oriented

and aggregated into large particles in aqueous solution under ultrasonic irradiation. The nucleation in the sonocrystallization process was accelerated by the implosive collapse of bubbles, while the crystal growth process was inhibited or delayed by shock waves and turbulent flow created by ultrasonic radiation. A pure complex perovskite phase of spherical shape was formed completely in a short irradiation time without the calcination process. In the surface active etching process, the micrometer-sized $BaTiO_3$ precursor was converted successfully to nanometer-sized particles, and its irregular shape changes to nearly uniform spheres, with accurate stoichiometric control. The effects of temperature and time on surface active etching process is provided deeper insights into the mechanism and offers an important role to control the particle sizes more precisely. Experimental procedures revealed a possible process mechanism observed within the etched surface and Oriented-attachment growth models, and this demonstrated approach could be used as an excellent platform for preparing ceramic nanoparticles. Both methods are highly recommended for the preparation of other functional materials with controlled morphology, size, size distribution, and composition.

Keywords: BaTiO3, nanoparticles, surface active etching, sonochemical

Thursday, September 7th, 2017 - Room4 - 15:00 - 16:15

Oral presentation - ENERGY HARVESTING

Th-S-O-01

Study of electrocaloric effect, recoverable energy storage density, dielectric and piezoelectric properties in modified barium titanate

Nasima Khatun, Somaditya Sen

Indian Institute of Technology Indore, Indore, India

The electrocaloric effect (ECE) in ferroelectric and anti-ferroelectric materials is gaining great attraction in several fields of research due to its potential application in replacing the environmentally harmful conventional refrigeration by realizing solid-state cooling with compact size and high efficiency, which are highly desirable for a broad range of applications. In this work keeping three facts (environmentally friendly material, ECE near room temperature and better entropy change) we have prepared modified $BaTiO_3$. The samples are prepared by sol-gel synthesis followed by calcination at 800 ^oC and sintering at 1350 ^oC. Phase confirmation is done by X-ray diffraction. Scanning electron microscopy is carried out for microstructure and morphological analysis. Dielectric measurements are done at different temperatures up to 250 ^oC for a frequency range of 100 Hz to 10 MHz. The piezoelectric constant (d_{33}) is measured at room temperature. The piezo voltage constant (g_{33}) is derived from d_{33} and relative dielectric constant ε_{33}. The Cuire temperature (T_C) is found to be decreased with increasing La concentration, and this is satisfactory with the aim. The ECE is calculated around the T_C by following the indirect method in which hysteresis loops are measured at different temperature and change in entropy is calculated using thermo-dynamical relations including Maxwell's relation. The observed change in ECE for these modified $BaTiO_3$ is found to have a good correlation with the amount of La

doping. The recoverable energy storage density calculated from the hysteresis loops also shows the similar correlation with La-doping concentration.

Keywords: Ferroelectric, Electrocaloric effect, Dielectric, Piezoelectric

---

Th-S-O-02

Phase transitions in doped hafnia thin films for pyroelectric applications

Min Hyuk Park [1], Tony Schenk [1], Michael Hoffmann [1], Steve Knebel [1], Jan Gaertner [1], Thomas Mikolajick [1, 2], Uwe Schroeder [1]

[1] *NaMLab gGmbH, Dresden, Germany*
[2] *Chair of Nanoelectronic Materials, TU Dresden, Dresden, Germany*

Fluorite ferroelectrics have been gaining increasing attention since their first report in 2011 [1]. This unexpected ferroelectricity was proven to originate from the formation of a non-centrosymmetric orthorhombic phase with space group of $Pca2_1$ [2]. A temperature dependent phase transition involved with this new polar phase was suggested to be promising for various applications based on pyroelectricity [3,4]. However, phase transitions in hafnia thin films doped with various dopants have not been comprehensively studied to date. Although the valence number, size, spatial distribution of dopants, the grain size distribution, and the distribution oxygen vacancies are expected to influence the phase transition, their effect has not been investigated in depth. In this presentation, therefore, the effects of aforementioned factors on the phase transition are systematically examined. The temperature dependent phase transitions in hafnia thin films were strongly affected by the valence number of dopants. Doping tri-valent ions increases the oxygen vacancy concentration, and it is believed that the spatial inhomogeneity of these oxygen vacancies can potentially broaden the phase transition in hafnia thin films.

References

[1] T. S. Boescke et al. Appl. Phys. Lett. 99, 102903 (2011).

[2] X. Sang et al. Appl. Phys. Lett. 106, 162905 (2015).

[3] M. H. Park et al. Nano Energy 12, 131 (2015).

[4] M. Hoffmann et al. Nano Energy 18, 154 (2015).

Keywords: Pyroelectricity, Phase transition, Fluorite, Hafnia, Lead-free ferroelectric

---

Th-S-O-03

Flexible ferroelectric oxide films for mechanical energy harvesting

JongHoon Jung [1], TaeKwon Lee [1], JaeWoong Kim [1], ChangWon Ahn [2], Seung-Hyun Kim [3]

[1] *Department of Physics, Inha University, Incheon, Korea, Republic of (South)*
[2] *Department of Physics, University of Ulsan, Ulsan, Korea, Republic of (South)*
[3] *School of Engineering, Brown University, Providence, United States*

In contrast to the ferroelectric polymers, inorganic ferroelectric oxide films are strong for thermal shocks and have extremely large piezoelectric as well as pyroelectric coefficients. However, that they have been limitedly used in flexible energy due to their rigidity. In this talk, we will report the development of an inorganic PZT, BFO film based mechanical energy harvesting devices. By adopting a newly developed flexible Ni−Cr metal foil substrate and a perovskite-structure-compatible $LaNiO_3$ (LNO) bottom electrode, we successfully grow a flexible PZT, BFO films with a high remanent electric polarization, high piezoelectric coefficient, and high pyroelectric coefficient. The ferroelectric inorganic film-based devices have been proven to stably generate electric power even in harsh environments including high humidity, strong base environment, and elevated temperatures.

Keywords: Flexible Ferroelectric Films, Mechanical Energy Harvesting, Electric Power, Harsh Environments

---

Th-S-O-04

Improved energy storage density and dielectric properties in La substituted $Ba(Ti_{0.95}Sn_{0.05})O_3$

R. Kumar [1, 3], K. Asokan [2], S. Patnaik [1], Balaji Birajdar [3]

1 School of Physical Sciences, Jawaharlal Nehru University, Delhi-110067, India
2 Materials Science Division, Inter-University Accelerator Centre, Delhi-110067, India
3 Special Centre for Nano Sciences, Jawaharlal Nehru University, Delhi-110067, India

(Ba1-zLaz)(Ti0.95Sn0.05)O3 (z = 0.0-0.035) ceramics were synthesized via the conventional solid state reaction method and characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) and Raman spectroscopy. Further their dielectric and ferroelectric properties were investigated. XRD measurements indicate the formation of a single and highly crystalline phase for all ceramic samples. The microstructural investigation from SEM indicates that a low La-doping of 1.5 and 2.5 atomic% inhibits the grain growth, while higher amounts of La-doping of 3.5 atomic % in barium stannate titanate (BTS) yielded the larger leafy grains. Raman spectroscopy suggests the substitution of La3+ ions at an A-site sublattice. Dielectric properties measurement revealed an enhanced dielectric permittivity constant with peak broadening. The discharge energy density obtained from the polarization versus electric field (P-E) hysteresis loops. The value of discharge energy density (Jd) ~ 0.21 J/cm3 was obtained for 2.5 atomic % of the La-doped sample, which is almost ~ 2.3 times higher than that of pure BTS sample (~ 0.09 J/cm3). Thus, the present study could lead to a new dimension in designing and application of the energy storage capacitors.

Keywords: Ferroelectrics; Diffuse phase transition; Micro-structural features; Discharge energy density.

Thursday, September 7th, 2017 - - 17:30 - 21:30

- Banquet

Friday, September 8th, 2017 - Plenary Room - 09:00 - 09:50

Plenary - PLENARY 05

Fr-S-O-01

(INVITED) Coupled multiple order parameters and their domain switching in magnetoelectrics

Tsuyoshi Kimura

University of Tokyo, Kashiwa, Japan
Osaka University, Toyonaka, Japan

One of the most important concepts in condensed matter physics is the spontaneous breakdown of symmetry in a solid, which bears the ordered phase and domains in its consequence. In magnetoelectric multiferroics, multiple order parameters coexist in a system, sometimes couple with each other, and exhibit nontrivial crossed phenomena. In this presentation, we deal with magnetoelectric multiferroics in which a symmetry breaking due to the orderings of various order parameters such as electric dipole, magnetic dipole, and magnetic quadrupole moments as well as chirality originating from these multipole moments. We show our recent research activity on exploration for new magnetoelectrics and manipulations of their multiple order parameters as well as domains.

Keywords: magnetoelectric effect, multiferroics, magnetic multipole moment, conical spiral magnetic order

Friday, September 8th, 2017 - Room1 - 10:20 - 10:50

keynote speaker - THEORY IV

Fr-S-O-01

NSMM Versus Goldschmidt's Factor Formalism a Scorecard

Steven Tidrow

Alfred University, NYSCC, Kazuo Inamori School of Engineering, Alfred, United States

Through comparing the room temperature structure, lattice parameter and volume of roughly 100 Perovskite materials, we numerically reiterate the significant improvement in modeling performance that the temperature dependent new simple material model (NSMM) provides over Goldschmidt's tolerance factor formalism (GTFF). Further, NSMM maintains such enhanced performance over extended temperature ranges, roughly 100 K to near the melting temperature of the material. Although NSMM is based on many of the same historical constructs as GTFF, physical constraints of NSMM overcome Goldschmidt's tolerance factor, a correlation relation. The physical constraints are used for development of temperature dependent ionic radii which are used in conjunction with the Clausius - Mossotti relation for development of coordination and temperature ionic polarizability. Combined, coordination and temperature dependent genome-like ion properties, radii and polarizability, can be used to determine a wide range of temperature dependent material properties, including but not limited to crystal structure, lattice parameter and volume, relative permittivity, polarization induced structural phase transition temperature, and, volume induced structural phase transition temperature. For example, the overall comparison scores of NSMM versus GTFF for the series $A^{1+}Nb^{5+}O_3$ and A^{1+} $Ta^{5+}O_3$ with A^{1+} being Ag, Cs, H, K, Li, Na, Rb, and $A^{2+}Ti^{4+}O_3$ with A^{2+} being Ba, Ca, Eu, Pb, and Sr, are shown. NSMM out scores GTFF and provides additional information that GTFF is unable to address.

Keywords: Simple Material Model, Goldshimdt's Tolerance Factor Formalism, Perovskite

Friday, September 8th, 2017 - Room2 - 10:20 - 10:50

keynote speaker - DIELECTRICS IV

Fr-S-O-01

(INVITED) The macro- and nanoscale phenomena in $BaTiO_3$ single crystal

Krzysztof Szot [1], Daniel Rytz [2], Iwona Lazar [1], Dariusz Kajewski [1], Krystian Roleder [1]

[1] *Institute of Physics, University of Silesia, 40-007 Katowice, Poland*
[2] *Forschungsinstitut für mineralische und metallische Werkstoffe, Edelsteine/Edelmetalle (FEE) GmbH, D-55743 Idar-Oberstein, Germany*

In spite of the fact that single crystals of $BaTiO_3$ of high quality can be grown since long time the properties of $BaTiO_3$ and the mechanism of its main phase transition at T_C are still intensively investigated. Complex physical mechanisms leading to the ferroelectric transition at T_C have been investigated through the structural, thermal, optical, lattice dynamics, dielectric, elastic, domain structure and electromechanical properties. The representative results of these investigations will be summarised, and new data of the piezoelectric properties of single crystal $BaTiO_3$ will be presented. The memristive behaviour - as promising effect for applications in micro-electronics and connected with the reversible transformation from a non-conducting to a metallic state - has opened another wide range of investigations. It was found that such a transformation cannot be described in terms of point defect chemistry only. We will explain that highly conducting extended defects play dominant role in the case of the memristive behaviour, and can help to understand such phenomena as self-polarization effects, aging phenomena, fractal shape of ferroelectric domains, screening effects, leakage currents and/or

electrically induced chemical transformations in the surface region. We believe that understanding the physical and chemical properties of the extended defects at the nanoscale may allow to accept an hypothesis that *true* barium titanate crystals are a kind of *a natural composite*. That is why the statement that *"... a clean, free ferroelectric surface in $BaTiO_3$ /.../ may be regarded as a ferroelectric metal*" is in our opinion an oxymoron.

Keywords: phase transition, extended defects, memristor

Friday, September 8th, 2017 - Room3 - 10:20 - 10:50

keynote speaker - NOVEL MATERIALS

Fr-S-O-01

(INVITED) Developing novel multiferroic materials

Naresh Dalal

Department of Chemistry and Biochemistry, and NHMFL Florida State University, Tallahassee, Florida 32306, USA, Tallahassee, United States

Multiferroic materials are lattices that simultaneously display two complementary properties, such as ferroelectricity and ferromagnetism. Developing such materials is synthetically quite challenging because most magnetic materials are inherently metallic, hence generally not expected to exhibit dielectric polarization under an externally applied electric field, a prerequisite for a ferroelectric lattice. Recently we have developed a systematic protocol for developing multiferroic systems, starting with either a well characterized magnetic lattice and adding an electrically polarizable ligand; or starting with a highly electrically polar compound and adding magnetic ions with matching ionic charge and radius. This presentation will discuss examples of both types; based in part on our recent reports [1-3].

References

[1] P. Jain et al., J. Am. Chem. Soc. 131, 13625 (2009).

[2] P. Jain et al., Quantum Materials 1, 16012 (2016).

[3] J.S. Kinyon et al.; Phys. Rev. B92, 144103 (2015).

Keywords: multiferroic, magnetoelectric, perovslites

Friday, September 8th, 2017 - Room4 - 10:20 - 10:50

keynote speaker - FERROICS/MULTIFERROICS IV

Fr-S-O-01

(INVITED) The structure and phase transitions of $Na_{1/2}Bi_{1/2}TiO_3$ – $ATiO_3$ solid solutions

Andris Sternberg

Institute of Solid State Physics, University of Latvia, Riga, Latvia

Recently the mixed phase-state of the rhombohedral and the other – presumably the nonpolar orthorhombic – phases, has been shown to exist in unpoled $Na_{1/2}Bi_{1/2}TiO_3$ (NBT) over a wide temperature range including the room temperature instead of the pure rhombohedral phase while only the rhombohedral phase is observed in the poled state. The finding raises the question about the characterisation of the structure of NBT solid solutions approaching the morphotropic phase boundary (MPB) frequently being assumed as rhombohedral even in the unpoled state. $CaTiO_3$ is found to stabilise the orthorhombic *Pnma* crystallographic structure. Clear stabilisation of the rhombohedral phase is found in NBT-$PbTiO_3$ solid solutions upon approaching the MPB. Even if some indications about stabilisation of the rhombohedral phase in NBT-$BaTiO_3$ solid solutions exist, there is no clearly increasing concentration of the rhombohedral phase found in all the concentration range of $BaTiO_3$ below the MPB. In difference from $CaTiO_3$, the NBT solid solutions with structurally similar $CdTiO_3$ have a complicated phase diagram. The solid solutions at low concentrations of $CdTiO_3$ have nonpolar symmetry group with $a^+a^+a^+$ octahedral rotations according to the Glazer notation, transforming to the $a^+b^+c^+$ polar symmetry group upon increasing the $CdTiO_3$ concentration. Such kind of tilting so far has never been found in real crystallographic structures.

Keywords: sodium bismuth titanate, structure, phase transitions

Friday, September 8th, 2017 - Room1 - 10:50 - 11:30

Invited talk - THEORY IV

Fr-S-O-01

(INVITED) Possibility of ferroelectricity in wurtzite-structured zinc oxide thin films

Hiroki MORIWAKE

Japan Fine Ceramics Center, Nagoya, Japan
National Institute for Materials Science, Tsukuba, Japan

The properties of a potentially new class of ferroelectric materials based on wurtzite-structured ZnO thin films are examined using first-principles calculations. Theoretical *P-E* hysteresis loops were calculated using the fixed-*D* method for both unstrained and (biaxially) strained single crystals. Ferroelectric polarization switching in ZnO (S.G. $P6_3mc$) is shown to occur via an intermediate non-polar structure with centrosymmetric $P6_3/mmc$ symmetry by displacement of cations relative to anions

in the long-axis direction. The calculated coercive electric field (E_c) for polarization switching was estimated to be 7.2 MV/cm for defect-free monocrystalline ZnO. During switching, the short- and long-axis lattice parameters expand and contract, respectively. The large structural distortion required for switching may explain why ferroelectricity in this compound has not been reported experimentally for pure ZnO. Applying an epitaxial tensile strain parallel to the basal plane is shown to be effective in lowering E_c during polarization, with a 5% biaxial expansion resulting in a decrease of E_c to 3.5 MV/cm. Comparison with calculated values for conventional ferroelectric materials suggests that ferroelectric polarization switching of wurtzite-structured ZnO may be achievable by preparing high-quality ZnO thin films with suitable strain levels and low defect concentrations.

Keywords: first-principles calculations. wurtzite-structure. ZnO.

Fr-S-O-02

(INVITED) Ferroelectricity in *κ*-Al_2O_3-type (A,Fe)$_2O_3$ (A=Al, Ga, Fe, Rh, In, Sc, and In) multiferroic oxides

Mitsuru Itoh

Laboratory for Materials and Structures, Tokyo Institute of Technology, Yokohama, Japan

κ-Al_2O_3-type structure ($Pna2_1$) is composed of close-packed oxygen layers with a sequence of ABACABAC…… , and has alternative stacking of spinel and corundum layers along c-axis. Cations in the mid-oxygen layers have four sites of one tetrahedral and three octahedral sites. Under the electric field applied along c-axis, oxygen layers in the corundum layer shift along ±a-axis to yield a shear in the spinel layer, subsequently, coordination of cations in octahedral/tetrahedral sites in the spinal layer change to tetrahedral/octahedral ones to cause a polarization switching [1]. In the present study, thin films of κ-Al_2O_3-type (A,Fe)$_2O_3$ (A =Al, Ga, Fe, Rh, Sc, and In) were prepared and their crystal structures, domain structures, ferroelectric and magnetic properties were systematically investigated experimentally and theoretically. Ferroelectricity was confirmed for all the films; however, the magnitude was found to be 10 ~ 20 % of the theoretical values [1], being correlated with the domain structures. Detailed polarization switching behavior and magnitudes of P_s, P_r, M_s, and T_N for (A,Fe)$_2O_3$ will be discussed in the presentation.

[1] A. Konishi *et al.*, unpublished

Keywords: κ-Al2O3-type structure, ferroelectricity, ferrimagnetism, domain structure, thin film

Friday, September 8th, 2017 - Room2 - 10:50 - 11:30

Invited talk - DIELECTRICS IV

Fr-S-O-01

(INVITED) Remarkable ferroelectric properties in ultrafine $BaTiO_3$ nanocrystals

Xiaohui Wang

Tsinghua University, Beijing, China

Ferroelectric properties of $BaTiO_3$ (BTO) nano-materials, especially the possible existence of ferroelectric critical size, are extensively studied for the use in devices of nanoscale memory storage and integrated microelectronics. Approaching the estimated ferroelectric critical size (2.5–3.6 nm), we first report the presence of ferroelectricity on BTO nanocrystal assemblies with an average crystal size of from 4.5 nm down to 2.8 nm. Crystal structure analyses based on atomic distribution function (PDF) revealed good structural coherence and confirmed the non-centrosymmetric phase structure of these nanocrystals at room temperature. With increase of the temperature, declined ferroelectric features and responses are observed by Raman scattering and second harmonic generation (SGH), indicating a quite diffuse phase transition of the nanocrystals. After self-assembled into a compact thin film, selectively written and read electric polarization of the nanocrystals shows direct evidence for the presence of ferroelectricity, which provides theoretical supports for the high-density ferroelectric memories. Owing to the remarkable ferroelectric properties, these nanocrystals are prospective to be used in various devices and offer promising candidates for the future printing electronic applications.

Keywords: BaTiO3 , Ferroelectricity, size effect,nanocrystal

Fr-S-O-02

(INVITED) Influences of nanogold addition on microchemical composition, domain structure and electrical properties of perovskite $BaTiO_3$-based ceramics

Supon Ananta

Department of Physics and Materials Science, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand, Chiang Mai, Thailand

Barium titanate ($BaTiO_3$) BT-based ceramics are of interest as the promising smart materials in commercial electrical components. However, they suffer from high sintering temperature requirement, low dielectric constant and high dielectric loss, causing a limitation for their practical utilizations. Thus, several solutions have been proposed to overcome these limitations including an approach of reinforcing the ferroelectric matrix phase with high electrical conducting phases. In this work, small amount of gold nanoparticles reinforced BT composites were developed by employing a solid-state sintering techniques without any binders. Apart from their environmental friendly, gold nanoparticles are thought to be reasonable candidate used for shortening the electrode distance in the nanometal/BT ceramics. These nanocomposites are expected to synergistically combine the properties of both the ferroelectric BT and the conductive gold nanoparticle, which could exhibit dielectric properties that are better than those of the monolithic BT ceramics. By employing a combination of several characterization techniques, the obtained results indicate that using different sintering temperature or gold nanoparticle amounts to produce the composites greatly affect the perovskite phase formation, densification, microstructure and dielectric properties of the materials. This work also addresses the domain evolution processes in BT-based ceramics containing various amounts of gold nanoparticles (AuNPs) as an additive by using

piezoresponse force microscopy (PFM). The obtained PFM images of the ceramics revealing the change of one spontaneously polarized state to another under various applied direct current voltage are discussed in terms of their domain topology, PFM phase shift and PFM amplitude.

Keywords: ferroelectric perovskite, barium titanate ceramics, gold nanoparticles

Friday, September 8th, 2017 - Room3 - 10:50 - 11:30

Invited talk - NOVEL MATERIALS

Fr-S-O-01

(INVITED) Inducing ferroelectricity into the M_3CuCl_3 ($M = Tl^+, K^+$) family of quantum antiferromagnets

Jared Kinyon, Naresh Dalal

Florida State University, Department of Chemistry, Tallahassee, United States

We report on the discovery of ferroelectricity in the well-studied, gapless quantum antiferromagnet NH_4CuCl_3. The ferroelectric transition temperature was found to be 69 K using specific heat and dielectric measurements [1]. NH_4CuCl_3 has been well studied because of its novel magnetization plateaus. It is also unique because it possesses a gapless ground state, in contrast with the isostructural $KCuCl_3$. In particular, EPR and neutron scattering techniques has shown that the potassium variant has weak interdimer coupling [2,3]. This feature was also thought to be true of the ammonium variant, with symmetry arguments playing a large role. Recent ^{14}NMR measurements have suggested that interdimer coupling may play a larger role than believed [4]. However, their possible multiferroicity, as both magnets and ferroelectrics, have not been reported. Such a finding would add a new dimension to their utility as memory storage elements. Here we report the discovery of ferroelectricity in NH_4CuCl_3, and several of its mixed lattices with K^+. Fields of up to 60 T were applied to study the magnetization behavior at 1.3 K, in addition to orientation and temperature dependent high-frequency EPR measurements. In this talk, we present details of our crystal growth and x-ray diffraction studies of lattice authenticity and purity, dielectric with and without applied magnetic fields, specific heat, magnetic susceptibility, pulsed fields, and EPR characterization of these novel materials.

Keywords: NH4CuCl3, multiferroic, specific heat, EPR, magnetization

---

Fr-S-O-02

(INVITED) Phonon mode links ferroicities in multiferroic $[(CH_3)_2NH_2]Mn(HCOO)_3$

Jan Musfeldt[1], Kendall Hughey [1], Amanda Clune [1], Michael Yokosuk [1], Amal al-Wahish [1], Ken O'Neal [1], Shiyu Fan [1], Nandita Abhyankar [2], Hongjun Xiang [3], Zhiquiang Li [4], John Singleton [5]

[1] *University of Tennessee, Knoxville, United States*
[2] *Florida State University, Tallahassee, United States*
[3] *Fudan University, Shanghai, China*
[4] *National High Magnetic Field Laboratory, Tallahassee, United States*
[5] *National High Magnetic Field Laboratory, Los Alamos, United States*

Magneto-infrared spectroscopy, magnetization, and lattice dynamics calculations were used to explore the phase transitions in multiferroic $[(CH_3)_2NH_2]Mn(HCOO)_3$. Both the 185 K ferroelectric transition and the magnetically-driven transition to the fully saturated state at 15. 3 T involve the formate bending mode, direct evidence of a common connection between the two types of ferroicities in this system that is much simpler than the coupling in rare earth manganites.

Keywords: molecule-based multiferroics, vibrational spectroscopy, phase diagrams, phonon behavior at low temperature and high magnetic field

Friday, September 8th, 2017 - Room4 - 10:50 - 11:30

Invited talk - FERROICS/MULTIFERROICS IV

Fr-S-O-01

(INVITED) Atomic control of ferroelectricity in oxide thin films and heterostructures

Tae Won Noh

Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul, Korea, Republic of (South)
Department of Physics and Astronomy, Seoul National University, Seoul, Korea, Republic of (South)

Perovskite structured oxides have been intensively investigated over 50 years due to the discoveries of exotic physical phenomena as well as abundant functionalities for practical applications. In the past decades, the rapid advancements in heteroepitaxy growth techniques further enable controls of structure, composition, and functionality of oxide heterostructures. In this talk, I will discuss the atomic scale control of oxide thin films/surfaces and the resulting ferroelectric properties. By controlling thermodynamic variables, we were able to engineer the atomic termination sequences of ferroelectric $BaTiO_3$ films. With the capacitor devices with symmetric and uniform interfacial termination sequences, we showed that the ferroelectric critical thickness can reach the theoretical limit value of 3.5 unit-cells [1]. With uniform TiO_2 surface termination, we found an unexpected high tunneling conductance near the one-unit-cell-high terrace edges. Spatially-resolved current-voltage spectroscopies and first-principles calculations suggest that local electronic reconstruction near the terrace edge can reduce the effective tunneling barrier width and thus enhance the tunneling conductance [2]. We also fabricated high quality ferroelectric tunnel junction (FTJ) devices with a single $BaTiO_3$ layer. We show that performance of such single layer FTJ devices can have two fundamental limits. To overcome such limits, we put extra $SrTiO_3$ barrier and effectively modulate the barrier potential [3]. Our work

demonstrates that atomic scale control of constituting layers is very important to control numerous functionalities of ferroelectric devices.

References

[1] Yeong Jae Shin, *et al*, Advanced Materials (10.1002/adma.201602795) (2017).

[2] Lingfei Wang, *et al*, *submitted*.

[3] Lingfei Wang, *et al*, Nano Letters 16, 3911 (2016).

Keywords: BaTiO3 thin film, interface, termination, ferroelectric critical thickness, ferroelectric tunnel junction

---

Fr-S-O-02

(INVITED) Modulation of Magnetoelectric Coupling in $BiFeO_3$ Mutiferroic Ceramics

Xiang Ming Chen, Xin Xin Shi, Xiao Qiang Liu

School of Materials Science and Engineering, Zhejiang University, Hangzhou, China

$BiFeO_3$ is the most promising single-phase multiferroic material due to its large polarization and high operating temperature and draws many attentions. As a typical type-I multiferroic material, the magnetoelectric coupling in $BiFeO_3$ is deemed to be weak due to the different origins of its ferroelectricity and magnetism. Here, the magnetoelectric effect in bulk $BiFeO_3$ is readdressed both theoretically and experimentally. Based on the DM interaction scenario, the magnetoelectric effect in $BiFeO_3$ is actually strong, with a coupling energy of about 1.25 meV and a magnetism-coupled parasitic polarization comparable to that of the type-II multiferroics. However, such strong magnetoelectric coupling also causes the cycloidal spin structure, which inhibits the observation of linear magnetoelectric coupling in bulk $BiFeO_3$. To resolve this contradiction, Sm-substitution is utilized to suppress the magnetoelectric effect and unlocks the weak ferromagnetism. At an optimized composition, such weak ferromagnetic state can be switched back to the cycloidal state by electric field, thus realizing electrically controlling of the magnetism. It has been argued that field-controlled phase transition is a promising path to colossal magnetoelectric effect.

Keywords: Multiferroic; BiFeO3; magnetoelectric coupling; ferroelectric; ferromagnetism

Friday, September 8th, 2017 - Room1 - 11:30 - 12:30

Oral presentation - THEORY IV

Fr-S-O-01

Critical scattering and incommensurate phase transition in antiferroelectric $PbZrO_3$ under pressure

Roman Burkovsky [1, 2], Sergey Vakhrushev [1, 2], Daria Andronikova [1, 2], Iurii Bronwald [1, 2], Alexey Filimonov [1], Alexander Tagantsev [3]

[1] *Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia*
[2] *Ioffe Physical-Technical Institute, St. Petersburg, Russia*
[3] *Swiss Federal Institute of Technology, Lausanne, Switzerland*

Antiferroelectric lead zirconate is the key ingredient in modern ferroelectric and piezoelectric functional solid solutions. By itself it offers opportunities in new-type non-volatile memory and energy storage applications. A highly useful and scientifically puzzling feature of this material is the competition between the ferro- and antiferroelectric phases due to their energetic proximity. It leads to a challenge in understanding of the critical phenomena driving the formation of the antiferroelectric structure. We report on the new picture of pre-transitional dynamics and phase diagram of $PbZrO_3$ in pressure-temperature space obtained by diffuse and inelastic scattering of synchrotron radiation. We show that application of hydrostatic pressure drastically changes the character of critical lattice dynamics and enables the soft-mode-driven incommensurate phase transition sequence in this material. In addition to the long known cubic and antiferroelectric phases we identify the new non-modulated phase serving as a bridge between the cubic and the incommensurate phases. The pressure effect on ferroelectric and incommensurate critical dynamics shows that lead zirconate is not a single-instability-driven system.

Keywords: Antiferroelectric, incommensurate phases, critical phenomena, high pressure

---

Fr-S-O-02

Lattice dynamics and dielectric relaxation in $PbMg_{1/3}Nb_{2/3}O_3$ relaxor from atomistic simulations

Alexei Bokov [1], Sergey Prosandeev [2], Dawei Wang [3], Zuo-Guang Ye [1, 3], Laurent Bellaiche [2]

[1] *Department of Chemistry and 4D LABS, Simon Fraser University, Burnaby, Canada*
[2] *2Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, United States*
[3] *Electronic Materials Research Laboratory, Key Laboratory of the Ministry of Education and International Center for Dielectric Research, Xi'an Jiaotong University, Xi'an, China*

Remarkable properties of relaxor ferroelectrics are related, first of all, to the complicated dipolar dynamics observed in these materials. Dynamical characteristics of relaxors and, in particular, the classical lead oxide perovskite relaxors have been studied in numerous works using different experimental techniques including dielectric spectroscopy, inelastic neutron, x-ray and light scattering, infrared spectroscopy, etc. Many unusual effects have been observed such as extremely large electric permittivity characterized by the diffuse maximum in the temperature dependence and dielectric relaxation arising from several polarization mechanisms, softening of several lattice vibration modes with temperature, mysterious “waterfall” effect associated with one of the modes, etc. However, none of the existing experimental techniques is able to explore the full desirable range of temperatures,

energies, eigenvectors and amplitudes. Therefore, different dipolar excitations are often to be studied by different methods and both the relation between these excitations and their role in the formation of relaxor behaviour remain controversial. This is the primary reason why the basic mechanisms of relaxor ferroelectricity are still unknown. Here we report the first successful atomistic simulation of the dipolar dynamics in lead oxide perovskite relaxor crystal which reproduces quantitatively the known experimental results obtained by different methods. The first-principles-based molecular dynamics simulations applied to the prototypical relaxor $PbMg_{1/3}Nb_{2/3}O_3$ allowed, in particular, to reveal the soft transverse optic phonon mode responsible for the ferroelectric phase transition, analyze the subterahertz relaxation dynamics and relate the empirically known characteristic temperatures to structural and dynamical features.

Keywords: Ferroelectric phase transitions, dielectric relaxations, phonons, relaxors, molecular dynamics simulations

---

Fr-S-O-03

Second order phase transitions in uniaxial ferroelectrics

James Scott [2], Stephen Rowley [2], Jason Lashley [1, 2]

[1] *1. Los Alamos National Laboratory, Los Alamos, United States*
[2] *The University of Cambridge, Cambridge, United Kingdom*

Quantum phase transitions occur in the halide salts of trissarcosine. Substitution of bromine or iodine for chlorine in $(CH_3NHCH_2COOH)_3CaCl_2$, (TSCC), suppresses the Curie temperature, T_C, from 130 K to 0 K at which point a zero temperature phase transition occurs between a ferroelectric and a paraelectric state as the doping level is varied.The ferroelectric transition in TSCC is observed to be second order in all experiments carried out so far, an uncommon feature among ferroelectrics, which implies that the zero temperature transition is likely to be a quantum critical point (QCP) with quantum fluctuations persisting over a range of temperatures and doping levels.

Keywords: Uniaxial, Second-Order

Fr-S-O-04

Structure, bandgap modulation, and magnetic switching in Fe_2O_3-doped ferroelectric ceramics

Jun Li, Yang Hong, Wenjing Wu, You Wu, Han Bai, Kouzhong Shia, Zhongxiang Zhou

Harbin Institute of Technology, Harbin, China

$(K_{0.5}Na_{0.5})NbO_3$-xFe_2O_3 perovskite ferroelectric ceramics (x = 0, 0.01, and 0.05) were prepared using a conventional solid-state reaction method. Structural and dielectric features of the as-prepared ceramics show the phases of the materials changed from orthorhombic to tetragonal with an increase in x, in

particular the coexistence of the orthorhombic and tetragonal phases gives rise to the enhanced ferroelectric properties for x = 0.01. Bandgap (E_g) modulation was achieved in the Fe_2O_3 doped KNN ceramics, the E_g exhibiting a drastic decrease as the doping content increases in experiment that the E_g = 2.886, 2.232 and 2.061 eV when x = 0, 0.01 and 0.05, and the CASTEP calculation shown the similar trend, indicating that the materials exhibit a higher performance with the absorption in visible light. Moreover, magnetic switching corresponding to a diamagnetic-ferromagnetic transformation was observed.

Keywords: band gap, ferroelectric ceramics, dielectric properties

Friday, September 8th, 2017 - Room2 - 11:30 - 12:30

Oral presentation - DIELECTRICS IV

Fr-S-O-01

Evolution of surface charge through the ferroelectric-paraelectric phase transition in $BaTiO_3$(001)

Claire MATHIEU [1], Christophe LUBIN [1], Gabrielle LE DOUEFF [1], Mattia CATTELAN [2], Nick BARRETT [1]

[1] *SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191, Gif-sur-Yvette, France*
[2] *Bristol Centre for NSQI, University of Bristol, Tyndall Avenue, BS8 1FD, Bristol, United Kingdom*

The perovskite $BaTiO_3$, which presents a tetragonal structure at room temperature, has its bulk polarization along the c-axis or the a-axes. For out-of-plane (perpendicular to the surface) polarized domains, the surface discontinuity leads to fixed polarization charge which in turn modifies the electrostatic surface potential. Charge-screening can alter the magnitude and sign of the surface potential. For example, unscreened and fully screened surfaces show opposite surface potential for the same underlying polarization. The surface potential may be further modulated at the surface where the atomic distortions associated with the ferroelectric (FE) state can be considerably altered. One recent report suggests that in $BaTiO_3$ the signature of surface domain ordering may persist well above the Curie temperature (T_C). The aim of the present study is to improve our understanding of how surface charge and polar adsorbates interact to influence domain order below, during and above the FE-PE phase transition. We have used PhotoElectron Emission Microscopy to study the evolution of the surface charge and domain structure in $BaTiO_3$(001) during the ferroelectric-paraelectric phase transition. At room temperature, in- and out-of-plane polarized domains are observed with ferroelectric and ferroelastic domain walls. Strong adsorbate screening is present resulting in inversion of the electrostatic surface potential contrast. Domain-related surface charge above T_C is still observable. Ferroelectric memory effects persist up to at least 550°C. The domain-like surface structures above T_C may be due to a combination of atomic relaxation, residual adsorbates and oxygen vacancies near domain walls.

Keywords: Phase transition, BaTiO3, Domain, Screening, PEEM

Fr-S-O-02

Phase transition behavior and defect chemistry of the $BaTi_{0.94}Sn_{0.06}O_3$ Ceramic investigated via in-situ extended X-ray absorption fine structure technique

Usa Sukkha [1, 3], Narong Chanlek [1], Rattikorn Yimnurun [2], Manoon Sutapun [3], Rangson Muanghlua [4], Naratip Vittayakorn [3, 5, 6], Pinit Kidkhunthod [1]

[1] *Synchrotron Light Research Institute (Public Organization), 111 University Avenue, Muang District, Nakhon Ratchasima, Thailand*
[2] *School of Physics, Institute of Science, and NANOTEC-SUT COE on Advanced Functional Nanomaterials, Suranaree University of Technology, Nakhon Ratchasima, Thailand*
[3] *Advanced Materials Research Unit, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*
[4] *Department of Electronics Engineering, Faculty of Engineering, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*
[5] *Department of Chemistry, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*
[6] *Nano-KMITL Center of Excellence on Nanoelectronic Devices, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand*

In this study, ferroelectric phase transitions in $BaTi_{0.94}Sn_{0.06}O_3$ (BTS) ceramic as a function of temperature are characterized with synchrotron X-ray absorption spectroscopy (XAS) technique, dielectric and ferroelectric measurements. Dense BTS ceramic exhibits orthorhombic symmetry confirmed by Rietveld refinement and Raman spectroscopy. The rhombohedral-orthorhombic (R-O), orthorhombic-tetragonal (O-T) and tetragonal-cubic (T-C) ferroelectric phase transitions were clearly observed in the dielectric results. Furthermore, anomalous dielectric relaxation around 90-105 K which far below the R-O phase transition was evidently founded. In order to investigate the local structure, In-situ extended X-ray absorption fine structure (EXAFS) was used especially at the ferroelectric phase transition region. The EXAFS results indicated a change in local structure around the Ti absorbing atom when the temperature increased. Evident of the O-T and T-O phase transitions is clearly seen in EXAFS results. Based on chemical analysis of bulk and surface of BTS ceramic by using X-ray photoelectron spectroscopy (XPS), anomalous dielectric relaxation should be attributed to mixed oxidation states of Sn.

Keywords: Dielectric, Ferroelectric, Phase transition, BaTiO3, Local structure

---

Fr-S-O-03

Mechanism of ferroelectric aging in donor&acceptor doped $BaTiO_3$ ceramics

Chao Zhou [1], Dingyue Hu [1], Lixue Zhang [1], Xiaobing Ren [2]

[1] *Xi'an Jiaotong University, Xi'an City, China*
[2] *National Institute for Materials Science, Ibaraki, Japan*

Physical properties of ferroelectric materials are usually tailored through introduction of acceptor and donor dopants that may cause different aging phenomena. Thus, it is of great interest to understand the aging behavior in the presence of both acceptors and donors. In this work, we report the aging effect in donor&acceptor doped BaTiO3 ceramics, reflected by the time-dependent change of polarization (P)-electric field (E) hysteresis loops in these cases with different dopant combinations of acceptors (Mn^{3+}, Fe^{3}+, Co^{3+}) and donors (Nb^{5+}, La^{3+}). The results indicate that the electronegativity and the ionic radius of acceptors, rather than the substitution site of the donors, play the key role in the formation of defect pairs which dominates the aging effect in donor&acceptor doped ferroelectrics. Finally, we propose a unified microscopic mechanism for the observed aging phenomena, and it provides direct instructions for manipulating the aging effect in ferroelectric materials.

Keywords: ferroelectric aging, defects, donor, acceptor

Fr-S-O-04

Rare-earth modified $BaTiO_3$ ferroelectric ceramics – Abnormal PTCR response

Marco Aurélio de Oliveira [1, 2], Jean Claude M'Peko [3], Antonio Carlos Hernandes [3], Ruyan Guo [4], Amar S. Bhalla [4], José de los Santos Guerra [1]

[1] *Grupo de Ferroelétricos e Materiais Multifuncionais, Instituto de Física, Universidade Federal de Uberlândia, Uberlândia – MG, Brazil*
[2] *Departamento de Física e Química, Universidade Estadual Paulista, Campus de Ilha Solteira, Ilha Solteira – SP, Brazil*
[3] *Grupo Crescimento de Cristais de Materiais Cerâmicos, Instituto de Física de São Carlos (IFSC), Universidade de São Paulo, São Carlos – SP, Brazil*
[4] *Multifunctional Electronic Materials and Devices Research Lab., Department of Electrical and Computer Engineering, The University of Texas at San Antonio, San Antonio – TX, United States*

Since the discovery of the ferroelectric and piezoelectric properties of Rochelle salt in 1920, the ferroelectric system, which has perhaps been one ot the most studied is the barium titanate ($BaTiO_3$). The $BaTiO_3$ presents a simple perovskite structure with excellent physical properties, such as high dielectric permittivity, high piezoelectric and pyroelectric coefficients, high mechanical stability and others. When modified with some donor and/or acceptor ions it also shows excellent semiconducting properties. In this work, the physical properties of the rare-earth modified $BaTiO_3$ system have been investigated. High-density ceramic samples were obtained from the polymeric precursors method (PPM), well known in the current literature for its efficiency, when compared to conventional methods commonly used for obtaining ceramic materials. Structural properties were carefully analyzed from x-ray diffraction (DRX) technique and Rietveld's refinement. The dielectric and electric properties were investigated focusing on the semiconducting properties promoted by the dopant ion. The Positive Temperature Coefficient of Resistivity (PTCR) response have been also investigated as a function of the doping element concentration. An abnormal behavior in the PTCR coefficient, suggests the amphoteric characteristics of such doping ion, which have not been reported in the current literature.

The authors would like to thank to FAPEMIG, FAPESP and CNPq Brazilian agencies for financial support. M. A. Oliveira also thanks the Materials Science Post-Graduation Program(PPGCM), UNESP, Ilha Solteira, Brazil.

Keywords: Ferroelectrics, BaTiO3, Semiconducting properties, PTCR effect

Friday, September 8th, 2017 - Room3 - 11:30 - 12:30

Oral presentation - NOVEL MATERIALS

Fr-S-O-01

Nanoscale tailoring of oxygen vacancy distribution by mechanically loaded scanning probe

Bo Wang [1], Saikat Das [2], Ye Cao [3], Sergei Kalinin [3], Tae Won Noh [2], Long-Qing Chen [1]

[1] Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, United States

[2] Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 08826, Korea, Republic of (South)

[3] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, United States

The intriguing behaviors of ferroic oxides in response to external stimuli at the nanoscale have attracted extensive interest in the recent decade. In particular, mechanically-induced phenomena enabled by a scanning probe, such as ferroic ordering reversal, domain wall movement, and local phase transition, offer new possibilities for the mechanical control of oxide-based multifunctional devices. Here we demonstrate a controlled modulation of the oxygen vacancy distribution by a mechanically loaded scanning probe in a homoepitaxial $SrTiO_3$ thin film. The Kelvin probe force microscopy imaging illustrates distinct motions of oxygen vacancies in lateral and vertical directions under the applied mechanical pressure, suggesting a strong coupling between chemical orderings and electromechanical fields at the nanoscale. To understand the mechanism involved, we extended the phase field model of ferroelectrics to incorporate the transport theory of semiconductors, the flexoelectric effect, and the Vegard effect. The simulations reveal that under mechanical stress, localized nonuniform electric dipoles are generated in otherwise paraelectric $SrTiO_3$ due to flexoelectricity, alters local electrostatics and thus redistributes the oxygen vacancy. Moreover, the Vegard's strain also interplays with the flexoelectric effect under specific circumstances and results in a downward depletion and a circumferential accumulation of vacancies under the probe tip. Tailoring oxygen vacancies distribution at the nanoscale in a controlled fashion may yield far-reaching implications for exploring defect-mediated emergent properties in multiferroic oxides.

Keywords: flexoelectric effect, oxygen vacancy, phase field modeling, Kelvin probe force microscope

Fr-S-O-02

Electronic structure of lead-free organic-inorganic hybrid $CH_3NH_3XI_3$ perovskite materials

Jintara Padchasri, Rattikorn Yimnirun

School of Physics, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand, Muang, Thailand

The importance of $CH_3NH_3XI_3$ or $MAXI_3$ (X=Pb and Ba) organic-inorganic hybrid materials has increased dramatically because of their potential use in solar cells. However, the basic structural characterization of these interesting materials remains sparse. In particular, advanced techniques, such as X-ray photoemission (XPS) and photoelectron emission spectroscopy (PES), could be employed to examine electronic structure and formation mechanism of these important perovskite materials. Here, systematic XPS and PES studies are employed to determine the electronic structure and chemical compositions of $MAXI_3$ powders. The results from this study help in explaining the possible electronic structure of the materials. The finding also leads to an awareness of the reactions, which in turn allow us to perform post synthetic reactions to form the organic-inorganic metal iodide perovskites.

Keywords: hybrid materials, electronic structure, X-ray photoemission, photoelectron emission spectroscopy

---

Fr-S-O-03

Coplanar waveguide resonator using pzt thin film coplanar waveguide resonator using pzt thin film

Reema Gupta [1], Lokesh Rana [1], Anjali Sharma [2], Monika Tomar [3], Vinay Gupta [1]

[1] *Department of Physics & Astrophysics, University of Delhi, Delhi, India, New Delhi., India*
[2] *Physics Department, Atma Ram Sanatan Dharma College, University of Delhi, Delhi, India, Delhi, India*
[3] *Physics Department, Miranda House, University of Delhi, Delhi, India, Delhi, India*

Microwave and RF filters play an important role in communication systems. Due to the proliferation of radar, satellite, and mobile wireless systems, there is a need for design methods that can satisfy the ever-increasing demand for accuracy, reliability, and fast development time. The demand of nanotechnology has gathered the major attention of researchers and scientists towards the miniaturization of microwave filters for wireless communication. Many materials have been explored for microwave device applications but very few reports are available on the fabrication of these devices in higher frequency range. Recent research in ferroelectric thin film based tunable devices and circuits has yield promising results for high frequency electronics. In the present study, a coplanar microwave resonator has been designed and fabricated using ferroelectric Lead Zirconium Titanate (PLZT) thin film. PZT was deposited using Pulsed Lased Deposition (PLD) technique under the optimized deposition parameters of substrate temperature, growth pressure and thickness. The PZT thin film was found to be polycrystalline with relatively high dielectric constant. The coplanar waveguide design was patterned using the conventional photolithography technique having PZT as the dielectric layer. Gold metal was

used as an electrode for coplanar waveguide resonator. The fabricated microwave resonator devices were diced and packaged for the microwave frequency measurements using Network Analyzer. The resonator response at 14.3 GHz has been recorded for the devices without PZT thin film. The Δ significant shift in frequency response has been observed towards lower side when the PZT layer (200 nm) was introduced in the prepared resonator.

Keywords: microwave resonators, coplanar waveguide, ferroelectric

---

Fr-S-O-04

Novel approach to mitigate the trade-offs between fast programming and long retention times in polymer ferroelectric memory

Vasileia Georgiou [2, 1], Dmitry Veksler [1], Jason Campbell [1], Pragya Shrestha [3, 1], Jason Ryan [1], Dimitris Ioannou [2], Kin Cheung [1]

[1] *National Institute of Standards and Technology, Gaithersburg, United States*
[2] *George Mason University, Fairfax, United States*
[3] *Theiss Research, La Jolla, United States*

The ferroelectric phenomenon involves physically rotating dipoles with an applied electric field. For memory devices, the need to program/erase at high-speed means that a polymer must have a glass transition temperature (T_g) below operation temperature such that the dipoles are not locked in place. Here, we demonstrate a radically new ferroelectric memory device concept based on polar polymers with T_g well above operation temperature. To realize fast operation, program/erase is done with a transient applied electric field and a transient elevated temperature well above T_g. After the program/erase operation, the device returns to operation temperature rapidly. Once cooled, the dipoles are locked in place ensuring long retention. We fabricated a thin-film ferroelectric field effect transistor (FeFET) using a polar polymer, CP1 polyimide (T_g ~ 265 ºC), as the gate dielectric (15nm) and polysilicon (15nm) channel. The fabricated FeFETs were programmed at ± 4V at 275 ºC. The device was cooled to room temperature while maintaining the applied electric field. The flat-band voltage shifts significantly and its direction depends on the sign of the applied field during programming. This flat band shift is found to be stable much longer than reported in the literature. Our dual-condition programming (temperature and electrical field) can lead to memory with extremely long retention times while using low cost processing materials that are CMOS compatible and highly scalable.

Keywords: polymer, memory, retention, FeFET, CP1

Friday, September 8th, 2017 - Room4 - 11:30 - 12:30

Oral presentation - FERROICS/MULTIFERROICS IV

Fr-S-O-01

Multiferroicity in Haldane spin-chain compound Sm_2BaNiO_5

Sanjay Kumar Upadhyay, Kartik Iyer, E. V. Sampathkumaran

Tata Institute of Fundamental Research,, Mumbai, India

We report the magnetic, dielectric, ferroelectric and magneto-electric behaviour of the Haldane spin-chain (S=1) insulating compound, Sm2BaNiO5. It has been reported in the literature that Sm2BaNiO5 orders antiferromagnetically around (TN=) 50 K through optical spectroscopic studies [1]. It is worthwhile to note that no anomaly was reported in the temperature (T) dependent magnetization (M) data at this temperature. M(T) data however reveal a broad peak around 22 K, which was attributed to of crystal-field effect of Sm+3. Very little literature exists to understand its electrical behaviour and the possible coupling with the magnetic field. The present dielectric data shows a broad peak around 22 K, which suggests possible correlation between electric dipoles and magnetism interestingly triggered by crystal-field effect. Conventional pyroelectric measurement reveals a peak near TN, which is found to arise from thermally stimulated depolarisation current However, the bias pyroelectric measurement reveals a weak peak around 22 K, reversing its sign for the opposite polarity of electric field, indicating the onset of ferroelectricity at this temperature. This is an intriguing observation, bringing out close correlation between the magneto-electric effect and the crystal-field splitting of the rare earth ion.

References

[1] A. S. Galkin and S. A. Klimin, J. Low Temp. Phys., 185 531 (2016).

Keywords: Multiferroic, Haldane spin-chain, pyroelectric

Fr-S-O-02

Spin excitations in the *Z*-type hexaferrites $(Ba_xSr_{1-x})_3Co_2Fe_{24}O_{41}$

Filip Kadlec [1], Christelle Kadlec [1], Jakub Vít [1], Fedir Borodavka [1], Martin Kempa [1], Jan Prokleška [2], Josef Buršík [3], Róbert Uhrecký [3], Jan Drahokoupil [1], Veronica Goian [1], Stanislav Kamba [1]

1 Institute of Physics, Czech Academy of Sciences, Prague 8, Czech Republic
2 Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic
3 Institute of Inorganic Chemistry, Czech Academy of Sciences, Rez, Czech Republic
4 Institut Laue-Langevin, Grenoble, France

Materials with the *Z*-type hexaferrite structure belong to the rare cases of room-temperature magneto-electric multiferroics, featuring a high resistivity, low permittivity and a low loss tangent. They exhibit a transverse conically ordered magnetic state up to ca. 400 K. Their particular feature is the absence of ferroelectric polarization at zero magnetization. However, a polar state can be magnetically induced via the inverse Dzyaloshinski-Moriya interaction; it arises at very weak intensities of external magnetic field and persists up to ca. 1.5 T. The dynamical magnetic properties of *Z*-type hexaferrites are still largely unknown; they present a great interest both from the fundamental point of view and with respect

to potential applications in memories, spintronics and magnonics. We have measured THz transmittance and far-infrared reflectivity of ceramics at temperatures from 5 to 900 K. Further, we carried out measurements of their magnetic susceptibility, magnetization and magneto-electric effect. For THz measurements, a magnetic field of up to 7 T was applied in the Faraday geometry. We observed a sharp resonance, whose position and damping depend strongly on temperature and applied magnetic field; we attribute it to an electromagnon, i.e. a magnon excited by electric field of the THz radiation. For field intensities above 2 T, another narrow resonance appears in the low-frequency part of the spectrum. At H = 7 T, its absorption peaks near 0.22 THz, a value which is temperature-independent within 5–250 K. This is probably a ferromagnetic resonance, whose frequency linearly increases with magnetic field.

Keywords: hexaferrite, electromagnon, THz spectroscopy, ferromagnetic resonance

---

Fr-S-O-03

Poly methyl methacrylate/ magnetite nano-composites

Salwa Abe- El- Messieh [2, 3], Doris Ramzy [1, 3], Nabih Tawfik [1, 3], Amira Nassar [1, 3], Azza Ward [2, 3], Yehia Badr [3, 3], Mohammed Hafez [3, 3]

[1] *National Research Center,solid state Department Dokki Cairo Egypt, Cairo, Egypt*
[2] *National Research Center,Microwave and dielectrics Department Dokki Cairo Egypt, Cairo, Egypt*
[3] *National Institute of Laser Enhancement Sciences (NILES), Cairo University, Cairo, Egypt;, Cairo, Egypt*

Magnetite nanoparticles were prepared by wet chemical precipitation technique. The particle size was examined by using transmission electron microscopy and found to be in the order of ~100 nm. Poly methyl methacrylate/ magnetite (PMMA/MG) nanocomposites with different concentrations of magnetite were prepared by casting method. The distribution of MG inside PMMA matrix was examined by scanning electron microscopy which indicate fine distribution of the MG particles inside PMMA matrix uptill 10% after which some aggregation was obtained. The magnetic properties of the studied composites revealed ferromagnetic and super paramagnetic. The X-ray diffraction reveals an increase in the degree of crystalinity by increasing MG content. The microhardness of composites was found to increase by the increase in MG content. The dielectric properties of the composites were investigated through the measurements of the permittivity ε' and dielectric loss ε". The measurements were carried out over a wide range of frequency (0.1 Hz and 1 MHz.) and temperature (30-90 ^{o}C). e' and e" were found to increase gradually by increasing MG content uptill 10% after which a dramatic increase was noticed. Also it is found that both values increase dramatically by increasing the applied temperature showing positive temperature coefficient. The electrical conductivity σ at 30 ^{o}C was found to be in the order of 10^{-9} S.cm^{-1} which recommends such composites to be used as antistatic materials. On the other hand, the values of s at 90 ^{o}C was found to be in the order of 10^{-3} S.cm^{-1} which behave like semiconductor at such high temperature.

Keywords: Poly methyl methacrylate magnetite nano-composites magnetic properties

dielectric properties
Electrical conductivity

Fr-S-O-04

Synthesis and properties of nanostructured BiFeO3-based ceramics

Ivair Santos [1, 2], Amar Bhalla [2]

[1] *State University of Maringá, Maringá, Brazil*
[2] *University of Texas at San Antonio, San Antonio, United States*

$BiFeO_3$ is a multiferroic magnetoelectric material with a rhomboedrally distorted perovskite structure (*R*3*c* space group) that presents ferroelectric and antiferromagnetic ordering at room temperature with elevated Curie (T_C ~ 1103 K) and Néel (T_N ~ 643 K) temperatures. However, the formation of undesired phases in polycrystalline $BiFeO_3$, mainly $Bi_{25}FeO_{39}$ and $Bi_2Fe_4O_9$, inhibits the electric, magnetic and magnetoelectric characterizations. In this context, alternative protocols for synthesize single-phased $BiFeO_3$ have been intensively studied in the last years. In this work, high-energy ball milling allied to fast sintering were applied to achieve nanostructured powders and Spark-Plasma Sintering (SPS) was used to synthesize nanostructured monolithic $BiFeO_3$ samples. The structural, microstructural and electric properties of the processed samples were investigated and correlated to the synthesis protocol. However, the formation of undesired phases in polycrystalline $BiFeO_3$, mainly $Bi_{25}FeO_{39}$ and $Bi_2Fe_4O_9$, inhibits the electric, magnetic and magnetoelectric characterizations. In this context, alternative protocols for synthesize single-phased $BiFeO_3$ have been intensively studied in the last years. In this work, high-energy ball milling allied to fast sintering were applied to achieve nanostructured powders and Spark-Plasma Sintering (SPS) was used to synthesize nanostructured monolithic $BiFeO_3$ samples.

Keywords: Multiferroic

Friday, September 8th, 2017 - Room1 - 13:50 - 14:20

keynote speaker - PROBE (NANOSCALE)

Fr-S-O-01

(INVITED) In-Situ transmission electron microscopy investigation of ferroelectric domain switching induced by external stimulation

Zibin Chen, Xiaozhou Liao

The University of Sydney, Sydney, Australia

Ferroelectrics results from the displacement of ions that leads to spontaneous polarization with the internal electric field pointing towards a specific direction in materials. A region with the same polarization direction is called a ferroelectric domain. Understanding ferroelectric domain switching behaviour under external stimuli is extremely important for the applications of ferroelectrics in memories, actuators and nanoelectronic devices. In this presentation, I will present our recent in-situ transmission electron microscopy investigation results on how separate and combined mechanical and electrical loadings affect ferroelectric domain structures [1] and how a high-energy electron beam can lead to local accumulation of trapped charges that determine local domain configurations [2]. Our results show that mechanical confinement during electrical loading adds one more degree of freedom for domain manipulation, which would provide an appealing possibility for significantly improving ferroelectric device performance, and that a high-energy electron beam can be used to precisely and reversibly control ferroelectric nano-domain morphology for memory storage devices.

References

[1] Z.B. Chen, L. Hong, F.F. Wang, S.P. Ringer, L.Q. Chen, H.S. Luo, X.Z. Liao, Phys. Rev. Lett. 118, 017601 (2017).

[2] Z.B. Chen, X.L. Wang, S.P. Ringer, X.Z. Liao, Phys. Rev. Lett. 117, 027601 (2016).

Keywords: ferroelectric, domain switching, in-situ transmission electron microscopy.

Friday, September 8th, 2017 - Room2 - 13:50 - 14:20

keynote speaker - THz/IR/RAMAN II

Fr-S-O-01

(INVITED) Driving structural dynamics in mutiferroics and ferroelectrics with THz light

Steven Johnson

Eigenössiche Technische Hochschule (ETH) Zürich, Zurich, Switzerland

Recent developments in the generation of highly intense few-cycle coherent pulses of THz-frequency electromagnetic pulses have suggested the possibility to use such pulses to drive structural changes in multiferroic and ferroelectric materials. According to some theoretical models, such pulses could be used to rapidly reorient domains on time scales of only a few picoseconds [1,2]. Here I discuss some recent experiments that use time-resovled x-ray diffraction to quantitatively track the motions of both spins in mutliferoic $TbMnO_3$ [3] and atoms in the ferroelectric $Sn_2P_2S_6$ [4] as they are driven coherently by a THz pulse with a significant spectral overlap to excitations that are thought to mediate such domain reorientations. The experiments observe large-scale motions that make it possible to estimate the

conditions that would be needed to realize switching of ferroic orientaitons in these mateirals on a time scale of less than 10 ps.

References

[1] M. Mochizuki and N. Nagaosa, Phys. Rev. Lett. 105, 147202 (2010).

[2] T. Qi et al., Phys. Rev. Lett. 102, 247603 (2009).

[3] T. Kubacka et al., Science 343, 1333 (2014).

[4] S. Grübel et al. arXiv:1602.05435.

Keywords: THz, x-ray, diffraction, ultrafast, time-resolved

Friday, September 8th, 2017 - Room3 - 13:50 - 14:20

keynote speaker - APPLICATIONS

Fr-S-O-01

(INVITED) Magnetoelectric gyrators for I-V conversion

Jiefang Li, Chung Ming Leung, Xin Zhuang, Dwight Viehland

Virginia Tech, Blacksburg, VA, United States

Many years ago a missing fundamental electrical element, the gyrator, was proposed based on transduction of magnetic flux and electric charge by Tellegen of Philips Research Laboratory. In fact, he conjectured the importance of magnetoelectric (ME) interactions in the gyrator's realization. However, the gyrator characteristics were never found in a single electrical element, until recently by our research group. It is a 4-wire element that has important key characteristics that the other four fundamental circuit elements (capacitor, resistor, inductor, and transformer) do not have, which includes: (i) the ability to convert current directly into voltage, and vice versa, without power loss; and (ii) the ability to reflect the other network elements as their duals (capacitor to inductor, resistor to admittance, voltage source into current source, and vice versa). Here, we show the realization of some of the potential of this missing electrical element using ME heterostructures, with regards to applications as energy efficient I-V conversion.

Keywords: piezoelectric, ferroelectric, magnetoelectric.

Friday, September 8th, 2017 - Room1 - 14:20 - 15:00

Fr-S-O-01

(INVITED) Magnetic resonance probing of ferroelectricity and magnetism in metal-organic frameworks

Nandita Abhyankar [3], Sylvain Bertaina [1], Maylis Orio [2], Naresh Dalal [3, 4]

[1] *Aix-Marseille University, CNRS, IM2NP UMR 7334, Marseille, France*
[2] *Aix Marseille University, CNRS, iSm2, Marseille, France*
[3] *Department of Chemistry & Biochemistry, Florida State University,, Tallahassee, United States*
[4] *National High Magnetic Field Laboratory (NHMFL), Tallahassee, United States*

We employ electron paramagnetic resonance (EPR) of Mn^{2+} as a spin probe to study the paraelectric−ferroelectric transition in $[(CH_3)_2NH_2]Mn(CHCO_2)_3$, (DMAMnF) and $[(CH_3)_2NH_2]Zn(CHCO_2)_3$ (DMAZnF dopped Mn^{2+}) , which are considered a model metal−organic framework (MOF) with a Pb-free perovskite architecture. In DMAMnF, we study the variation of the Mn^{2+} EPR line shape and intensity at the X-band (~9.5 GHz) over 80 to 300 K. The peaks are essentially Lorentzian, implying electron spin exchange at frequencies greater than 9.5 GHz. On cooling, an anomalous increase in the peak width is noted at the ferroelectric transition temperature Tc=185 K but no anomalous change in the normalized, double-integrated EPR signal intensity around the T_c , indicating that DMAMnF is transparent to microwave electric fields with a clear lack of magnetoelectric coupling, in contrast to an earlier report. In DMAZnF, the multifrequency EPR of the Mn^{2+} probe shows the motional dynamics of the DMA+ cation during the cooling down process. We show that depending on the time scale of the measure, the DMA+ is considered moving or frozen. We show that the sudden change of the EPR linewidth when crossing the ferroelectric transition is not due to the freezing of the DMA+ cation but to a ferroelastic transition.

Keywords: electron paramagnetic resonance, ferroelastic transition, ferroelectric transition

---

Fr-S-O-02

Surface acoustic wave devices for gas and biosensing applications

Monika Tomar Chowdhuri [1], Lokesh Rana [2], Reema Gupta [2], Vinay Gupta [2]

[1] *Physics Department, Miranda House, University of Delhi, Delhi, India*
[2] *Department of Physics and Astrophysics, University of Delhi, Delhi, India*

Surface Acoustic Waves (SAW) devices support the acoustic waves propagation on the surface and hence, any disturbance can be easily monitored making them suitable for sensing applications. On interaction of external stimuli with the acoustic wave, the velocity of the wave gets modified because of the mass loading, elastic loading or electric loading. Change in velocity results in the change in resonance frequency which can be transmitted and received easily with appropriate electronics, making them ideal for wireless applications. Rayleigh SAW devices show limited sensitivity in the presence of liquids due to damping. Some specific piezoelectric crystals with specific cuts can be used which support

Shear horizontal SAW for liquid measurements. These waves (Love waves) can be further trapped on the surface of the device by coating a suitable layer of lower acoustic velocity over the device. In the present work, low cost Rayleigh SAW devices have been fabricated on corning glass substrates with sputtered Zinc oxide film. A suitable sensing layer is deposited over the IDT's for gas sensing. The fabricated device is exploited detection of NO_2 gas efficiently. For the realization of biosensors, IDT's have been patterned over 36°YX lithium tantalate. The fabricated devices were coated with ZnO thin film as a guiding layer. Microchannels of PDMS have been prepared using SU8 mould. The microchannels have been pasted over the love wave SAW device and have been used for detection of uric acid efficiently. The results clearly demonstrate the application of SAW devices for biosensing and gas sensing.

Keywords: SAW, ZnO, Biosensor; Gas sensor

Friday, September 8th, 2017 - Room2 - 14:20 - 15:00

Invited talk - THz/IR/RAMAN II

Fr-S-O-01

(INVITED) Surface plasmon resonance based electro-optic and magneto-optic modulators

Vinay Gupta

Department of Physics and Astrophysics, University of Delhi, Delhi, India

Surface Plasmon Resonance (SPR) technique has been widely accepted as a standard tool for the optical characterisation of interfaces and thin films. An indigenously developed multipurpose table top SPR measurement setup has been exploitedto fabricate optical magnetic field sensors using magneto-optic kerr effect (MOKE). Otto ATR configuration in SPR is a very rapid and sensitive technique to examine the multilayered interfaces also. Ferroelectric materials have proved their potential in the fabrication of electro-optic (EO) modulators due to the high value of dielectric constants and electro-optic properties. SPR technology when combined with an EO material leads to the development of highly efficient optical light modulators due to high sensitivity towards the change in refractive index at the interface, This electro-optically modulated SPR detection process possess interesting features such as potentially reduced noise level and more immune to power drifts.Experimental results and theoretical simulations on the study of EO and MO properties using SPR technique are prevented.

Keywords: MOKE, Surface Plasmon Resonance, Electro-optics, Magneto-optics

---

Fr-S-O-02

(INVITED) Micro-Raman spectroscopy of doped-ZnO ferromagnetic and ferroelectric nano-materials with multiple-excitation wavelengths

Shiv Sharma

University of Hawaii, Hawaii Institute of Geophysics & Planetology, Honolulu, United States

Advances in micro-Raman spectroscopy with multiple-wavelength excitations are allowing nondestructive and in situ measurements of chemistry and structures of materials with molecular level sensitivity. A key parameter of a Raman system is excitation wavelength, which affects both depth of penetration into the sample (which is proportional to the laser wavelength) and Raman scattering intensity (inversely proportional to the fourth power of laser wavelength). UV (325 nm) laser excitation Raman spectroscopy has been used successfully to investigate lattice dynamics and phase transitions in thin films and superlattices of Sr- and Ba-titanates. In this presentation, micro-Raman investigations of chemically synthesized nanocrystalline cobalt-substituted (up to 10 atomic%) ZnO samples exhibiting room temperature ferromagnetism are discussed. These studies were carried out using multiple laser excitation wavelengths − 457.9, 532 and 785 nm. The Raman spectra of the samples excited with 457.9 nm show predominantly lattice modes of ZnO because of pre-resonance enhancement. In the Raman spectra of cobalt-doped ZnO samples excited with 532 and 785 nm, clear evidence is found for the presence of Co_3O_4 (an impurity phase not detectable in XRD) in the samples with cobalt exceeding 3%. Results of micro-Raman measurements on ferroelectric Li-doped and Li-implanted ZnO, and (Co, Li) co-implanted ZnO films, which show simultaneous ferromagnetic and ferroelectric properties at room temperature, will be discussed.

Keywords: micro-Raman spectroscopy, multiple-laser excitation, nanocrystalline doped ZnO, ferromagnetic, ferroelectric

Friday, September 8th, 2017 - Room3 - 14:20 - 15:00

Invited talk - APPLICATIONS

Fr-S-O-01

(INVITED) High-density ferroelectric random access memory using wall-current readout of binary information

Anquan Jiang [1], Jun Jiang [1], Zilong Bai [1], Cheol Hwang [2], James Scott [3]

[1] *Fudan University, Shanghai, China*
[2] *Seoul National University, Seoul, Korea, Republic of (South)*
[3] *St. Andrews University, St. Andrews, United Kingdom*

Ferroelectric polarization can be reversed by mechanical force, thermal heating, electron/light illumination, gas pressure or electrical fields, enabling applications in spatial visualization, electrochemical sensors, and terabit non-volatile ferroelectric memories with ns-to-ps programming times, near-unlimited cycle endurance and low energy consumption. One significant challenge for these

applications is the current capacitor-based technology that destructively reads out domain information through charge integration, requiring memory cells with >250 nm lateral sizes, although mechanical probe-based technology has demonstrated huge ferroelectric storage capacity of several Tb/in^2. Here we show a nanoscale non-destructive ferroelectric polarization readout method via electrical opening of charged-domain-wall conduction paths near the film surface layer under a horizontal read field. Our method is not only applicable for epitaxial $BiFeO_3$ thin films on (001) $SrTiO_3$ substrates with a diagonal polar axis but also successful for other nonorthogonal ferroelectrics. They have mesa-geometry three-terminal structures and functions via instantaneous domain-wall conduction upon voltage application. The operation principle of newly explored devices combines the merits of non-volatile ferroelectric memory and current-sensing resistance switching memory in ultrahigh storage density.

Keywords: ferroelectric thin film; domain wall current; nonvolatile memory

---

Fr-S-O-02

(INVITED) Optimization of BST phase shifter circuits for beam-steering applications

Devin Spatz, Guru Subramanyam, Weisong Wang, Eunsung Shin
University of Dayton, Dayton, United States

Voltage controlled analog phase shifters are optimized and implemented as part of a phased array antenna. The phase shifters designed are based on a parallel-plate varactor design with Barium Strontium Titanite (BST) thin- film used as the electrically tunable dielectric. Through the simulation of varactor device variations including parallel-plate area and dielectric thickness, potential phase shifter designs are studied. Optimization parameters for phase shifter selection include insertion loss, device size, and figure of merit in degrees of phase shift per dB loss. A 6 by 6 micron varactor based phase shifter with a dielectric thickness of 200 nm is determined to be optimal. MMIC and hybridized circuits are designed to test phase shifter performance in a phased array beam-steering circuit.

Keywords: Voltage tunable dielectrics, Ferroelectric phase shifters, electronic beam steering

Friday, September 8th, 2017 - Room1 - 15:00 - 16:15

Oral presentation - PROBE (NANOSCALE)

Fr-S-O-01

Imaging of non-collinear antiferromagnetic order and ferroelectric order in $BiFeO_3$

Stephane Fusil [1], Isabell Gross [2, 3], Waseem Akhtar [2], Luis Martinez [2], Saddem Chouaieb [2], Cecile Carretero [1], Patrick Appel [4], Patrick Maletinsky [4], Jean-Yves Chauleau [6], Nicolas Jaouen [7], Michel Viret [6], Joo-von Kim [5], Manuel Bibes [1], Agnes Bathelemy [1], Vincent Garcia [1], Vincent Jacques [2]

1 Unité Mixte de Physique, CNRS, Thales, Univ. Paris Sud, Université Paris-Saclay, Palaiseau, France
2 Laboratoire Charles Coulomb, Université de Montpellier and CNRS, Montpelier, France
3 Laboratoire Aimé Cotton, CNRS, Université Paris-Sud, ENS Cachan, Université Paris-Saclay, Orsay, France
4 Department of Physics, University of Basel, Basel, Switzerland
5 Centre for Nanoscience and Nanotechnology (C2N), Orsay, France
6 SPEC, CEA, CNRS, Université Paris-Saclay, Saclay, France
7 Synchrotron SOLEIL, Gif sur Yvette, France

Most magnetic multiferroics are actually antiferromagnets, including the archetypical BiFeO3. The easy plane of antiferromagnetic domains is correlated to the polar direction and switching the ferroelectric polarization affects the AF sublattice vector. In addition, BiFeO3 exhibits an incommensurate magnetic structure with a long range cycloid ordering of spins. Resorting to a non-invasive scanning magnetometer based on a single nitrogen-vacancy (NV) defect in diamond, we demonstrate the first real-space visualization of non-collinear antiferromagnetic order in a multiferroic thin film. Thanks to piezoresponse force microscopy, we highlight the correlation with the ferroelectric landscape and take advantage of the magnetoelectric coupling to manipulate the cycloid propagation direction with an electric field. Besides illustrating the unique potential of NV magnetometry for imaging complex antiferromagnetic order at the nanoscale, these results demonstrate how BiFeO3 can be used as a versatile platform for the design of reconfigurable nanoscale spin textures.

Keywords: scanning probe microscopy, antiferromagnets, multiferroics

---

Fr-S-O-02

Probing local and global ferroelectric phase transition in single phase multiferroic thin films

Dhiren Pradhan [1, 2], Shalini Kumari [2, 3], Rama Vasudevan [4], Evgheni Strelcov [4], Sergei Kalinin [4], Ronald Cohen [1], Ram Katiyar [2]

[1] Geophysical Laboratory, Carnegie Institution for Science, Washington, United States
[2] Department of Physics and Institute of Functional Nanomaterials, University of Puerto Rico,, San Juan, United States
[3] Department of Physics and Astronomy, West Virginia University, Morgantown, United States
[4] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory,, Oak Ridge, United States

Piezoresponse Force Microscopy (PFM) has emerged as a powerful tool for experimental investigations of ferroelectric materials. In the imaging mode, PFM allows visualization of static domain structures with nanometer spatial resolution. Application of a sufficiently large voltage through a conductive scanning probe microscopy (SPM) tip can induce local polarization switching and can be extended for creation of tailored domain structures and ferroelectric data storage. Finally, acquisition of the piezoresponse signals during polarization reversal allows measurement of local hysteresis loops, which can be used for characterization of the switching process in the nanoscale area in the vicinity of the tip. The broad application of PFM for probing domain structures and polarization reversal in ferroelectrics demands deep understanding of the basic mechanisms involved. PFN ($Pb(Fe_{0.5}Nb_{0.5})O_3$) thin films were grown by optimized pulsed laser deposition (PLD) . The highly c-axis oriented growth containing only

(00*l*) diffraction peaks of PFN films along with in plane epitaxial relationship were confirmed by high resolution X-ray diffraction measurements. PFN thin films possess well saturated ferroelectric hystersis and weak ferromagnetism at room temperature. The existence of ferroelctricity at nanoscale is confirmed by band excitation PFM. The ferroelectric phase transition is also probed by the temperature dependence of piezoresponse studies. In addition to the temperature dependence of piezoresponse studies the phase transition is also confirmed by temperature dependent dielectric spectra. Detailed studies on effect of temperature on coercive field, imprint, switchable polarization, nucleation bias of PFN will be discussed in the meeting.

Keywords: Piezoresponse Force Microscopy (PFM), Phase Transition

---

Fr-S-O-03

Probing the domain structures and the extrinsic contributions in piezoelectric materials

Nan Zhang

Xi'an Jiaotong University, Xi'an, China

The morphotropic phase boundary (MPB) is very important in the study of piezoelectric materials both from the fundamental understanding as well as developing new materials. Here we present a combined PFM and synchrotron X-ray diffraction study on the domain structures and behaviours under electric-field on lead zirconate titanate single crystals. An increasing in both polarization rotation (intrinsic contribution) and domain switching (extrinsic contribution) are found when the monoclinic phase presents. Moreover, our in-situ high-resolution X-ray diffraction experiment make it possible to estimate the proportion of macroscopic deformation caused by domain switching. We are able to separate the multiple components of the Bragg peaks, from which, the individual shifts and the exchange of intensity between them. In this way, we show how the average macroscopic deformation accumulates through the inclusion of different domains into the probed material volume, and finally estimate the ratio between intrinsic and extrinsic contributions at different compositions in the phase diagram.

Keywords: piezoelectricity; domain switching; PZT; synchrotron; PFM

Fr-S-O-04

Chemical phenomena of local polarization reversal in ferroelectric thin films

Anton V. Ievlev, Chance Brown, Petro Maksymovych, Sergei V. Kalinin, Olga Ovchinnikova

Center for Nanophase Material Sciences, Oak Ridge National Laboratory, Oak Ridge, United States

Functionality of ferroelectric materials is defined by the number of physical and chemical phenomena on the nanoscale, which requires using of nanoscale investigative techniques. Atomic Force Microscopy (AFM) is one of such techniques, which is widely used for characterization of the ferroelectric physical properties. But at the same time, chemical contribution in the ferroelectric phenomena in the most cases

are ignored. However, these studies can be carried out by combination of AFM with Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), allowing nanoscale local investigations of the chemical properties. Here, we utilize combine AFM/ToF-SIMS approach for correlated investigations of the functional and chemical phenomena in $PbZr_{0.2}Ti_{0.8}O_3$ thin film. In the studies, we used AFM to induce local ferroelectric switching by the electric field of the biased tip and study associated local changes in the chemistry of the film by ToF-SIMS. Investigations showed 3 - 5% change in the spatial concentrations of the base chemical elements close to the sample surface. Those changes were localized within 3.5 nm surface layer are caused by the screening process minimizing depolarization electric fields produced by the boundary charges. Observed phenomenon was also found to be reversible by application of the electric field of opposite polarity, which confirms its ferroelectric origin. Results of the study shed light on the chemical phenomena associated with ferroelectric properties and are important for their fundamentals investigations and practical applications.

This work was conducted at the Center for Nanophase Materials Sciences, which is a Department of Energy (DOE) Office of Science User Facility.

Keywords: Atomic force microscopy, Time-of-Flight Secondary Ion Mass Spectrometry, Local polarization reversal, Chemical phenomena, Domains

Friday, September 8th, 2017 - Room2 - 15:00 - 16:15

Oral presentation - THz/IR/RAMAN II

Fr-S-O-01

Ferroics and multiferroics for terahertz device design

Moumita Dutta [1], Soutik Betal [1], Amar Bhalla [1], Xomalin Peralta [1], Ruyan Guo [1], Kamaraju Natarajan [2], Michael. R.C Williams [2], Rohit. P Prasankumar [2]

[1] *The University of Texas at San Antonio, San Antonio, United States*
[2] *Center for Integrated Nanotechnologies: Los Alamos National Laboratory, Albuquerque, United States*

With the advancements in femto-second laser technology and the coherent generation and detection of Terahertz(THz) radiation (ranging from 0.1 THz to 30 THz), this spectral region is finding applications in various disciplines like imaging, communications, explosive-detection, spectroscopy of molecular vibrations etc. However, in order to realize full-fledged THz applications, efforts need to be directed towards the design and implementation of efficient THz modulators and switches. In this work the interaction of THz waves with different ferroic and multiferroic materials has been performed employing time-domain spectroscopic detection technique to reveal the role of their ferroic behaviours in the propagation control of THz waves. Temporal traces thus recorded using optical interferometry has been converted to its frequency domain responses. External field-dependent index of refraction and absorption coefficient dispersion function and their influence on the THz propagation has been retrieved

for the design of dynamically controlled THz modulators. These modulators are envisioned to be the opto-electronic units for the future optical-communication/computing.

Keywords: Terahertz, Spectroscopy, Multiferroic, Modulators

Fr-S-O-02

Second-harmonic phonon spectroscopy of the model oxide α-quartz

Christopher J. Winta, Martin Wolf, Alexander Paarmann

Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Nonlinear optical spectroscopy in solid state media is intriguing as it opens up additional experimental degrees of freedom which can help to disentangle congested linear spectra, while providing improved sensitivity. Most notably, this can be exploited to isolate different symmetry contributions to the measured signal and in consequence gain information about the crystal structure of the sample at hand. In particular, second-harmonic generation (SHG) as an even-order nonlinear process is (in leading electric-dipole order) only allowed in non-centrosymmetric media which makes it a very suitable tool for the investigation of ferroelectrics due to their naturally broken inversion symmetry [1]. However, these approaches have so far been restricted to the visible and near-infrared. Here, we demonstrate second-harmonic phonon spectroscopy [2] in the far-IR as a novel approach to study polar dielectrics with broken inversion symmetry and exemplify the technique for α-quartz. We observe a strong enhancement of the SHG yield at transversal optical phonon frequencies whereby the azimuthal behavior allows distinguishing the different symmetries of the respective modes. Temperature-dependent measurements demonstrate the sensitivity of our technique to symmetry changes upon the α-β phase transition selectively for the different phonon modes. Given the sensitivity to structure via phonon resonances and crystal symmetry via the nonlinear susceptibility tensor, our novel technique presents itself as a promising tool to study ferroic materials such as multiferroics and ferroelectrics.

References

[1] Denev et al., J. Am. Ceram. Soc. 94, 2699 (2011).

[2] Paarmann et al., Phys. Rev. B 94, 134312 (2016).

Keywords: Nonlinear spectroscopy, second-harmonic generation, far-infrared, phonons, phase transition

---

Fr-S-O-03

(INVITED) On the origin of ferroelectricity in $Hf_{0.5}Zr_{0.5}O_2$ thin films

Yingfen Wei [1], Pavan Nukala [2], Mart Salverda [1], Jamo Momand [1], Graeme R. Blake [1], Bart J. Kooi [1], Brahim Dkhil [2], Beatriz Noheda [1]

[1] *Zernike Institute for Advanced Materials, University of Groningen, 9747 AG, Groningen, Netherlands*
[2] *Laboratoire Structures, Propriétés Modélisation des Solides (SPMS) Centrale Supélec CNRS UMR8580, Université Paris-Saclay, 92290, Châtenay-Malabry, France*

Recently, ferroelectric properties and metastable polar phases have been observed in thin layers of doped hafnia and in the solid solution of zirconia with hafnia with composition $Zr_{0.5}Hf_{0.5}O_2$ [1]. Great technological interest has been raised due to their silicon compatibility, chemical simplicity and low toxicity [2]. Although ferroelectricity has been shown to be robust [3], its origin remains elusive and only recently the exact space group of the polar phase has been reported in Gd-doped hafnia [4]. The complexity arises from the fact that only ultra-thin films are ferroelectric and single-phase films are difficult to synthesize. Here, single-phase orthorhombic $Zr_{0.5}Hf_{0.5}O_2$ ferroelectric films have been obtained by Pulsed Laser Deposition on perovskite substrates. The samples grow epitaxially despite the large differences in structure between film and substrate. These differences are accommodated by means of (111)-oriented films, which are organized in four domains (although the (001) orientation also appears in lesser amounts). The single-phase character allows obtaining meaningful TEM images that bring new insight on the origin of the ferroelectric phase.

References

[1] J. Müller et al., NanoLett. 12, 4318 (2012).

[2] M. H. Park et al., Adv.Mater. 27, 1811 (2015).

[3] T. Shimizu et al., Appl.Phys. Lett. 106, 112904 (2015).

[4] X. Sang et al., Appl.Phys. Lett. 106, 162905 (2015).

Keywords: ferroelectric, thin films, zirconia, hafnia, pulsed laser deposition.

Fr-S-O-04

Dielectric and ferroelectric properties of rare earth doped lead zirconate titanate ceramics

Mohan Bhattarai [1], Shojan Pavunny [1, 2], Ram Katiyar [1]

[1] *Department of Physics and Institute for Functional Nanomaterials, University of Puerto Rico, P.O. Box 70377, San Juan, 00936-8377, Puerto Rico, United States*
[2] *ASEE fellow at US Naval Research Laboratory, 4555 Overlook Ave SW, 20375, Washington DC, United States*

We have synthesized La^{3+} and Sc^{3+} doped lead zirconate titanate electroceramics with the stoichiometric formula $(1-x/2)[PbZr_{0.53}Ti_{0.47}]-x[Li_ySc_{1-y}]O_3$ (PLZTS), where x = 0.1 and y = 0.2, 0.4, 0.6 & 0.8, by a conventional solid-state reaction method & investigated its structural, microstructural, dielectric, electrical and ferroelectric properties. X-ray diffractometry was used to probe the phase purity and to

derive the crystallographic parameters. Furthermore, structural phase transition was investigated by analyzing Raman spectra recorded in the temperature window of 80-580 K. The size, shape, and the distribution of grains were examined through a scanning electron microscope (SEM) and the sample was subjected to energy dispersive spectroscopy (EDS) for elemental analysis.We have carried out dielectric and electrical measurements on Pt/PLZTS/Pt metal-ferroelectric-metal capacitors using impedance analyzer and electrometer, respectively, as a function of temperature (100-600 K) and frequency (10^2-10^6 Hz). High dielectric constants (ε') of ~280, ~500, ~1800 & 1000 for y = 0.2, 0.4, 0.6 & 0.8 respectively were observed at room temperature. We measured hysteresis loops which proved the existence of ferroelectricity in all prepared samples of different compositions. These results provide insights into functionality of PLZTS ferroelectric materials for its potential applications in the future electronic devices.

Keywords: X-Ray Diffraction, Raman Spectroscopy, Energy Dispersive Spectroscopy, Dielectric Measurement, Hysteresis Loop

Friday, September 8th, 2017 - Room3 - 15:00 - 16:15

Oral presentation - APPLICATIONS

Fr-S-O-01

ZnO/Si Lamb wave SAW devices

Lokesh Rana [1], Reema Gupta [1], Anjali Sharma [3], Monika Tomar [2], Vinay Gupta [1]

[1] *Department of Physics and Astrophysics, University of Delhi, Delhi 110007, INDIA, Delhi, India*
[2] *Physics Department, Miranda House, University of Delhi, Delhi, India*
[3] *Department of Physics, Atma Ram Santan Dharma College, University of Delhi, Delhi, India*

Surface acoustic wave devices have widespread applications in various fields including in communication and wireless sensing devices. However there are some shortcomings like lower sensitivity and the corrosion of IDT's limit their application as sensing devices. Lamb wave SAW devices have proved to be promising for sensing applications. Rayleigh wave SAW devices fabricated over a membrane with the thickness of membrane smaller than the acoustic wavelength leads to the generation of the lamb waves. The Rayleigh waves travel on both sides of the membrane causing the formation of the antisymmetric and symmetric modes of lamb waves. This design gives the feasibility of integrating the liquid media as required for biosensors from the back side protecting the IDTs. Moreover lamb wave SAW devices are fabricated on silicon membrane making them IC compatible. In the present work lamb wave SAW devices have been fabricated with four different acoustic wavelengths (20 μm, 40 μm, 60 μm and 80 μm). The devices have been fabricated using conventional photolithography technique on Silicon substrate. Piezoelectric ZnO thin film deposited using rf sputtering technique has been integrated with the Si substrate. The bulk etching of Silicon has been carried out from back side of each device using wet etching. The devices are packaged and frequency response is studied using a network analyzer. The antisymmetric and symmetric modes in these devices

have been identified and variation of acoustic velocity for both the mode is plotted as a function of the normalized thickness of the plate.

Keywords: SAW, Lamb Wave, ZnO

Fr-S-O-02

Effect of mechanical and electrical strain on bilayer polymer nonvolatile memory devices

Deepa Singh, Deepak ., Ashish Garg

Department of materials Science & Engineering, Indian Institute of Technology Kanpur, Kanpur, India

Ferroelectric polymers such as poly(vinylidenedifluoride–trifluoroethylene) P(VDF-TrFE) are great alternative to conventional ceramics based non-volatile memory (NVM) devices owing to their low temperature and easy processing, compatible with flexible electronics. Despite its excellent properties, large roughness and leakage are the main issues with P(VDF-TrFE). A thin layer of PMMA, an insulating polymer, is introduced to further improve the leakage current and roughness. To study the reliability of flexible ferroelectric capacitors (FeCaps), in this work P(VDF-TrFE)/PMMA bilayer devices were subjected to the individual as well as the combined effect of mechanical and electrical strain cycling. The effect of these strains on ferroelectric behavior was different depending on the way PMMA was incorporated (i.e. either on top of P(VDF-TrFE, or at the bottom of it). FeCaps with PMMA above P(VDF-TrFE) showed better electrical and mechanical endurance. The electrical and mechanical fatigue measurements exhibited that the flexible FeCaps are more likely to suffer from electrical fatigue than mechanical fatigue at moderate strains. The results suggest that increasing the bending strains to ~0.5% results in a slight increase in the coercivity of the samples whilst no severe decrement in polarization after testing up to 30000 bending cycles (with bending radius of 12 mm) accompanied by a formation of a few black spots and cracking on the top electrode. Moreover, electric field cycling, with or without the mechanical strain, results in a severe drop in the ferroelectric polarization of the devices, manifested in extensive degradation and delamination of the top electrode.

Keywords: P(VDF-TrFE), Non-volatile memory, mechanical endurance

---

Fr-S-O-03

Optimizing the performance of (Ba,Sr)TiO_3 tunable capacitors for high figures of merit

Christopher Freeze [1], Cedric Meyers [2], Susanne Stemmer [1]

[1] *Materials Department University of California, Santa Barbara, Santa Barbara, United States*
[2] *Department of Electrical and Computer Engineering University of California, Santa Barbara, Santa Barbara, United States*

Ferroelectrics, particularly $Ba_xSr_{1-x}TiO_3$, have shown great promise for microwave-frequency devices such as electric field tunable dielectrics. A recurring challenge has been achieving simultaneous high

quality factor ($Q=1/\tan\delta>100$) while also enabling tunable capacitance by at least a factor of two. In this work, parallel plate capacitors are fabricated with $Ba_{0.3}Sr_{0.7}TiO_3$ thin films grown by hybrid molecular beam epitaxy on epitaxial Pt bottom electrodes. They exhibit device quality factors above 1000, which is higher than that grown by any other method. We investigate the influence of the top-electrode interface on device properties. Two different electrode deposition approaches are considered, which result in different interface quality – electron-beam evaporation at room temperature and sputter deposition after a high-temperature oxygen anneal. Using fits to the tunable capacitance, interfacial capacitances are extracted for samples with both contact deposition methods. The effective removal of the interfacial contaminant layer by using high-temperature sputtering deposition is demonstrated. While the removal of interfacial contaminants does not strongly affect quality factors, dielectric tunability is enhanced in devices with these cleaner interfaces. The combination of high tunability and high device quality factors results in record device figures of merit. We also report on the effects of different etch processes for the $Ba_{0.3}Sr_{0.7}TiO_3$ mesa – a high-aspect-ratio Ar ion mill and a dilute HF wet etch. While the effect on device quality factors is not significant for low biases, the damage induced by the ion mill allows leakage paths which become active at lower biases.

Keywords: tunable dielectric, loss, quality factor

Fr-S-O-04

Device physics of polymeric ferroelectric memory diodes

Thomas Lenz [1], Matteo Ghittorelli [2], Hamed Sharifi Dehsari [1], Fabrizio Torricelli [2], Kamal Asadi [1]

[1] *Max-Planck Institute for Polymer Research, Mainz, Germany*
[2] *University of Brescia, Department of Information Engineering, Brescia, Italy*

Ferroelectric polymers are well-suited candidates for low-cost, flexible non-volatile memory applications. The ferroelectric polarization is employed to store information in binary form. The basic memory element is a polymeric ferroelectric capacitor. The readout operation of the ferroelectric capacitors however is destructive, which complicates its integration in large arrays. The challenge of non-destructive read-out was overcome by blending semiconducting and ferroelectric polymers that yields phase-separated networks. Excellent bistable current rectification with high on/off current ratios has been demonstrated. The combination of ferroelectric bistability with (semi)conductivity and rectification allowed for demonstration of a 1 kbit solution-processable non-volatile reconfigurable memory arrays on foil with a simple cross-bar architecture that can be read out non-destructively. There is however still a limited understanding of the device physics, which is required for the technological implementation of high-density arrays. In this contribution, bistable ferroelectric diodes are fabricated by using both phase separation method, and the soft lithography method by solution micromolding. We have developed a morphology relevant device model and elucidate on the operation mechanism of the ferroelectric diode and show that the operation is based on the modulation of the injection barrier. Since the dependence of polarization on electric field is explicitly taken into account, the current-voltage characteristics of the diodes can be quantitatively described. The model provides design rules for the implementation of organic ferroelectric memory diodes, and predicts an ultimate theoretical memory density in the order of $Tbit/cm^2$ for a polymeric ferroelectric diode arrays.

Keywords: Ferroelectric diode, nonvolatile memory, device physics, memory array

---

Fr-S-O-05

Magnetoelectric nanorobots for remote controlled dynamically targeted live cell manipulation

Souik Betal, Moumita Dutta, Amar Bhalla, Ruyan Guo

Department of Electrical and Computer Engineering, University of Texas at San Antonio, San Antonio, United States

A remotely controlled dynamic process has been developed for manipulation of targeted biological cells using magnetoelectric nanocomposites which are core-shell nanoparticles comprised of single crystalline ferromagnetic cores (CoFe2O4) and ferroelectric crystalline thin film shells (BaTiO3). We demonstrated that these nanocomposites behaves as a unique family of inorganic magnetoelectric nanorobots (MENRs), which can be controlled remotely by ac or dc magnetic fields for dynamic cellular manipulation including cell targeting, permeation, and transport. MENRs performs these functions via localized electric periodic pulse generation, local electric-field sensing, or thrust generation and acts as the unique tool for remotely controlled dynamic cellular manipulation. We have designed a custom build systematic setup to accurately examine the MENRs-cellular interaction and performed experiments in microvascular structured microfluidic chamber (MSMC) with complex junctions and variable pressure gradient corresponding to vascular environment. The details of these MENRs and their performance will be presented in this paper.

Keywords: Magnetoelectric Nanorobots, multiferroics, core-shell magnetoelectric nanoparticles, targeted single cell electroportion, live cell manipulation

Author's Index