Perovskites Yanfu Lu, Yakun Yuan, Venkatraman Gopalan and Susan B. Sinnott; The Pennsylvania State University, United States

Octahedral tilts are the most ubiquitous distortions in perovskite-related structures that can dramatically influence ferroelectric, magnetic, and electronic properties; yet the paradigm of tilt epitaxy in thin films is barely explored. Non-destructively characterizing such epitaxy in three-dimensions for low symmetry complex tilt systems composed of light anions is a formidable challenge. Here we demonstrate that the interfacial tilt epitaxy can transform ultrathin calcium titanate, a non-polar earth-abundant mineral, into high-temperature polar oxides that last above 900 K. The comprehensive picture of octahedral tilts and polar distortions is revealed by reconstructing the three-dimensional electron density maps across film-substrate interfaces with atomic resolution using coherent Bragg rod analysis. The results are in excellent agreement with density functional theory. The study could serve as a broader template for non-destructive, three-dimensional atomic resolution probing of complex low symmetry functional interfaces.

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EL03.06.14
Advanced Techniques in Ultralow Voltage Piezoelectric Characterization of Ferroelectric Thin Films with Piezoresponse Force Microscopy Aviram Bhalla-Levine[1], Ryan Wu[1], Sujit Das[1], Roger Proksch[2] and Ramamoorthy Ramesh[1]; [1]University of California, Berkeley, United States; [2]Asylum Research, United States

There is currently significant interest in ultralow power microelectronics for memory and logic functions. Recent reports have identified multiferroic systems as possible candidates for such applications, with the ultimate goal of reducing the switching voltage to below one hundred millivolts (translating to approximately one attojoule per unit operation). Thus, measuring the ferroelectric and piezoelectric responses of ultrathin ferroelectric layers at such low voltage scales is essential. Piezoelectric measurements are, in principle, easier to execute and analyze since the primary response arises solely from the ferroelectric state (unlike polarization based measurements that are susceptible to leakage and nonlinear dielectric effects). To understand switching at voltages on the order of one hundred millivolts, we are carrying out a careful study of the piezoelectric switching of five, ten, fifteen, and twenty nanometer thick lead zirconate titanate films as a model system. We specifically focused on characterizing the piezoresponse of such nanoscale thin films using very low alternating current voltages (down to ten millivolt excitations). Our research indicates that statistically credible piezoelectric switching information can be obtained at these voltages. We will report the results of these scaling studies using piezoresponse force microscopy (PFM) as well as pulsed polarization measurements.

EL03.06.15
New Lead-Free Materials on the Base of Sodium-Potassium Niobate and Sodium-Bismuth Titanate Perovskites Ekaterina Politova; Karpov Institute of Physical Chemistry, Russian Federation

New Lead-Free Materials on the Base of Sodium-Potassium Niobate and Sodium-Bismuth Titanate Perovskites
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Lead-free materials are being intensively studied in order to replace widely used Pb-based ones. We study influence of cation substitutions and preparation conditions on structure parameters, microstructure, dielectric, relaxor ferroelectric, and piezoelectric properties of solid solutions in the systems based on $(Na_{0..5}Bi_{0.5})TiO_3$ (NBT) and $(K_{0.5}Na_{0.5})NbO_3$ (KNN) perovskites.
Ceramic samples in systems $(Na_{0.5}Bi_{0.5})TiO_3$ - $BaTiO_3$ (NBT-BT) and $(K_{0.5}Na_{0.5})NbO_3$ – $BaTiO_3$ (KNN-BT) with compositions close to Morphotropic Phase Boundaries (MPB) were prepared by the two-step solid-state reaction method at temperatures of 900 – 1500 K. To modify properties of the samples, in A- and B-sites of perovskite lattice Li^+, La^{3+}, Mn^{3+}, Ni^{3+}, Fe^{3+}, Nb^{5+} , Sb^{5+} and W^{6+} cations were added. To improve density of ceramics

overstoichiometric KCl and LiF additives were used.
The samples were characterized using the X-ray Diffraction, Scanning Electron Microscopy, Second Harmonic Generation (SHG), Dielectric Spectroscopy (DS), and Atomic Force Microscopy in Piezorespone Force mode (PFM) methods.
The unit cell volume changes were observed in modified KNN- and NBT-based ceramics depending on ionic radii of substituting cations. Ferroelectric phase transitions at ~ 400-500 and 600 – 700 K were confirmed using the DS and SHG methods. Phase transitions near ~ 400 K in NBT-based compositions revealed typical relaxor behavior due to the presence of polar nanoregions in a nonpolar matrix. At high temperatures > 700 K effects of dielectric relaxation were observed in ceramics studied caused by formation of oxygen vacancies in compositions with aliovalent substitutions. At the room temperature, non monotonous changes of the dielectric parameters and increase in the spontaneous polarization value was proved for modified ceramics. Using the PFM method ferroelectric polarization switching at nanoscale was observed, and in some KNN-based ceramics high values of effective d_{33} piezoelectric coefficient up to 300 pm/V were observed. The results obtained confirmed prospects of new lead-free materials development on the base of modified KNN- and NBT-based compositions.

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EL03.06.16
Giant Polarization in Super-Tetragonal Ferroelectric Thin Films through a New Concept of Interphase Strain Linxing Zhang; University of Science and Technology Beijing, China

Generally, the chemical or physical properties strongly depend on the change of lattice. The control of lattice strain, therefore, much affects the chemical or physical properties of functional materials, which has been widely used in superconductivity, giant magnetoresistance, multiferroics, catalysis and etc. Ferroelectrics are an important functional material, which has been widely used in the field of ferroelectric memories, tunable microwave devices, large-capacity capacitors, piezoelectric sensor devices, etc. The intriguing properties of ferroelectric materials utilize the basic functional primitive parameter of polarization. This team has realized this method, interphase strain, by creating a single-lattice-parameter epitaxial composite film on $SrTiO_3$ substrate from two tetragonal materials but with different lattice parameters, $PbTiO_3$ ferroelectrics and PbO non-ferroelectrics. The results show that the method improves the lattice distortion of $PbTiO_3$ to c/a = 1.238, compared to 1.065 in bulk. The remanent polarization is as high as 236.3 $\mu C/cm^2$, which is near twice the highest value of the known ferroelectrics. This composite ferroelectric thin film is very stable, and the super-tetragonal ferroelectric phase is stable up to 725 °C, compared to the bulk transition temperature of 490 °C.
The proposed "interphase strain" is a new concept for strain engineering to regulate lattice strain of ferroelectrics, and successfully achieved giant polarization in the super tetragonal $PbTiO_3$/PbO based ferroelectric thin films. The idea of "interphase strain" is as follows: if two kinds of materials with similar crystal structures, but different lattice parameters, are growing into a single-lattice-parameter epitaxial film, the material of the small lattice is inevitably subjected to the tensile stress from the large lattice material, thereby introducing a large lattice strain. The regulation of lattice strain can cause significant changes in the physical and chemical properties of the material. This new approach of interphase strain for strain engineering can be utilized to enhance the physical and chemical properties of other functional materials, such as superconductivity, giant magnetoresistance, multiferroic, and catalysis.

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In-Plane Ferroelectricity in Epitaxial Dion-Jacobson $CsBiNb_2O_7$ Jie Jiang[1,2], Lifu Zhang[1] and Jian Shi[1]; [1]Rensselaer Polytechnic Institute, United States; [2]Kunming University of Science and Technology, China

Conventional ferroelectric perovskite materials carry a debatable critical thickness below which the depolarization field is large enough to destabilize ferroelectricity. 2D ferroelectric materials are discovered to hold robust in-plane polarization down to a single unit cell, contending the continuous miniaturization of ferroelectric devices. However, due to the nonuniformity of the electrostatic field from quasi-2D metal electrodes, the in-plane intrinsic dipoles would experience a mismatched screening (screening frustration) making the in-plane polarization switching