We studied the influence of Mn doping on dielectric properties of high density (>95%) PMN-10PT ceramics by means of broadband dielectric spectroscopy in 20 Hz – 40 GHz range using flat capacitor (low frequencies), coaxial lines and waveguides (microwave range). The Mn-addition significantly decreases the dielectric permittivity and losses with strong indication of suppression of domain wall movement and mobility of polar nanoregions. Various relaxational processes were resolved and will be discussed during the presentation.

(EAM-P005-2018) Dielectric Response of the Methylammonium Lead Halide Solar Cell Absorbers

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Hybrid organic–inorganic perovskites have recently attracted overwhelming attention due to their excellent photovoltaic performance yielding efficiencies well exceeding 20%. This has been related to properties such as long charge carrier lifetime, the exceptionally large diffusion length, large absorption coefficient, high carrier mobilities, large open-circuit voltages, and direct band gap. The organo-lead-trihalide perovskite compounds, $CH_3NH_3PbX_3$, are the forerunners in efficiency. We address the key role of the dynamical nature of MA dipoles by combining large frequency range and temperature-dependent dielectric measurements with ultrasonic. Dielectric measurements were performed between temperatures 100 and 300 K and frequencies 10^2 –10^{11} Hz utilising a HP 4284A precision LCR meter, Agilent 8714ET vector network analyzer with a sample-terminated coaxial line and rectangular waveguide system with an Elmika scalar network analyser R2400. All measurements were performed at a rate of 1 K min^{-1}. We show that a sufficiently high dielectric constant exists across the entire frequency range allowing for efficient screening of charged entities. This is the fundamental effect facilitating the diffusion of photogenerated carriers. Furthermore, measurements are complimented by Monte Carlo simulations to show the antipolar nature of the structural phase transitions.

(EAM-P006-2018) Enhanced Curie temperature and piezoelectric properties of Sn doped (x)($Ba_{0.82}Ca_{0.13}Sn_{0.05}$)$TiO_3$ – (1-x) Ba($Zr_{0.15}Ti_{0.85}$)O_3 perovskite system

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Piezoelectric ceramics are used as electromechanical transducers in many applications such as sonars, actuators, ultrasonic transducers. Due to the toxicity of lead (Pb) and its detrimental effects to the environment, it is preferable to replace lead (Pb) in commercial piezoelectric ceramics. (Ba,Ca) (Zr,Ti)O_3 or BCZT has been proposed as a possible alternative to Pb-based piezoceramics such as PZT. Despite the fact that (Ba,Ca) (Zr,Ti)O_3 system exhibit large piezoelectric properties, their potential applicability is limited by low curie temperatures (i.e., T_C ~60 °C). In order to overcome this limitation of BCZT ceramics, we have constructed a new system of (x)(Ba Ca Sn) TiO_3 - (1-x) Ba(Zr Ti)O_3 perovskite solid solution, which exhibit an improved curie temperature T_C of up to ~100 °C. The introduction of tin (Sn^{+2}) at the A-site, leads to formation of a broad morphotropic phase boundary (MPB) region with coexisting rhombohedral and tetragonal phases. The volume fractions of rhombohedral and tetragonal phases changes with x in the MPB region. In this work, we investigated the correlations between the different crystallographic phases present and the dielectric, piezoelectric and ferroelectric properties of the (x)(Ba Ca Sn)TiO_3 - (1-x) Ba(Zr Ti)O_3 perovskite solid solution system.

(EAM-P007-2018) Influence of KBT on the structure and ferroelectric properties of BCZT ceramics

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Barium titanate ceramics modified by calcium and zirconium dopants, denoted BCZT, exhibit promising piezoelectric properties with a piezoelectric charge coefficient, d_{33}, in the region of 600 pC/N being reported at room temperature. The need for high sintering temperatures for densification of BCZT is a serious concern, particularly when considering the compatibility with certain substrates for thick film deposition. It has been proposed that the incorporation of bismuth-based perovskite compounds, such as $BiFeO_3$ and $Bi(Mg_{0.5}Ti_{0.5})O_3$ into BCZT could both increase the temperature-stability of properties and improve the sintering behavior. The aim of the present study was to determine the effects of adding ($K_{0.5}Bi_{0.5}$) TiO_3 (KBT) into BCZT solid solutions having 2 different calcium titanate contents. The effects of increasing KBT content, in the range from 0 to 65 mol%, on phase transition behaviour, densification, microstructure, dielectric, ferroelectric and piezoelectric properties of these ceramics were systematically investigated. Subsequently, further investigations were conducted to eliminate second phase formation and enhance the ferroelectric properties through the incorporation of excess bismuth oxide and optimisation of the heat treatment procedures.

(EAM-P008-2018) Ab-Initio Prediction of Novel 2D Group-III Oxides by Evolutionary Algorithms

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Combining an efficient evolutionary algorithm for the search of the energy landscape of two-dimensional (2D) materials with accurate density-functional theory (DFT) calculations, we predict new, low-energy 2D materials in the family of group-III oxides, A_2O_3 with A=B, Al, Ga, and In. For B_2O_3, we discover a planar 2D structure with a surprisingly low formation energy of about 20 meV/atom relative to bulk B_2O_3. For Al_2O_3, we identify a structure consisting of 2 Al and 3 oxygen layers with a formation energy of about 190 meV/atom. These formation energies are comparable to those of experimentally synthesized 2D materials indicating that these materials could be grown by techniques such as MBE and CVD. We find that 2D B_2O_3 and Al_2O_3 are semiconducting and that 2D Al_2O_3 is stable in aqueous environments, indicating potential applications in electronic devices and as protective layers.

(EAM-P009-2018) Effects of Dysprosium Oxide on Sintering Behavior and Electrical Conductivity of Samarium Doped Ceria

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Solid electrolytes based on rare earth-doped cerium dioxide are of considerable interest for potential application in intermediate-temperature solid oxide fuel cells, IT-SOFC. Nevertheless, some constraints related to their sintering behavior along with improvement of the ionic conductivity are still object of investigation. In this work, dysprosium ion was chosen as a second additive/dopant, aiming to obtain a ceramic solid electrolyte with optimized ionic conductivity. Compounds of $Sm_{0.2-x}Dy_xCe_{0.8}O_{1.9}$ with 0 % x % 0.2 were prepared by solid-state reaction, and the influence of the additive content on densification and ionic conductivity was analyzed by density, X-ray diffraction and impedance spectroscopy measurements. All compositions were found to exhibit cubic fluorite-type structure. The sintered solid electrolytes achieved densities higher than 92% of the theoretical value after sintering at 1500°C/3 h, and higher ionic conductivity than the $Sm_{0.2}Ce_{0.8}O_{1.9}$ parent electrolyte.