(EMA-S6-P015-2016) Controlling Spin Ordering in Rare-Earth Perovskite Vanadates

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We investigate the role and influence of local structure distortions on the antiferromagnetic spin ordering temperatures for large A-site radii RVO_3 perovskites (R=Yb-La) using a combination of data analytics (DA) and density functional theory (DFT). First, mode crystallography is used to parameterize the structural phase space. Next, we identify the important local structural features that correlate strongly with the Néel temperatures using Pearson correlation coefficients and principal component analysis. From this data, we then formulate a regression model using gradient boosted decision trees (GBDT) that returns the relative importance of each feature in predicting the Néel temperature. Our analysis indicates that the amplitude of the subtle Jahn-Teller active mode, which leads to variations in the V-O bond lengths and angles, could be used as an effective structural control parameter to modify the spin ordering temperature. We then validate these data-driven structure-property relationship in artificial vanadate structures using Néel temperatures based on both our GBDT model and a model Hamiltonian using DFT energies. This combined DA-DFT approach allows us to gauge the accuracy of existing models for the critical ordering temperatures in vanadates and opens possible strategies to deterministically design materials with targeted magnetic ordering temperatures.

(EMA-S6-P016-2016) Displacement Radiation Effects in Ferroelectric $BaTiO_3$: A Molecular Dynamics Study

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Displacement radiation effect can create a large number of defects in materials that may have a significant impact on the performance of materials and devices. For ferroelectrics, these defects will not only lead to polarization loss but also result in other serious problems such as ferroelectric fatigue and imprint failure. To obtain an atomistic understanding of the radiation effects in ferroelectric materials, the displacement radiation cascades in $BaTiO_3$ were simulated using molecular dynamics simulations with a modifed shell model. Primary knock-on atoms with different energies were introduced to the system and the resulting defects distribution and associated polarization loss were analyzed. Compressive strain was then introduced and it was found that the number of defects created decreases with increasing strain. Furthermore, polarization reversal was simulated to investigate the effect of radiation on the coercive field. Finally, the impact of the displacement radiation on the domain structure was studied.

(EMA-S6-P017-2016) Effects of doping on the magnetic ordering in $EuTiO_3$

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Eu-based perovskites have attracted considerable attention due to the strong spin-lattice coupling, that can potentially lead to robust multiferroicity. One particular member is $EuTiO_3$ (ETO), which is a complex oxide that displays a large magneto-electric effect, and undergoes a series of structural and magnetic phase transitions when subjected to pressure or epitaxial strain. ETO adopts a cubic structure and is paramagnetic at high temperatures, while at very low temperatures it transforms to an antiferrodistortive tetragonal structure with a G-type antiferromagnetic (AFM) ordering. Several approaches have been presented to tune the magnetic ordering from the G-type antiferromagnetism to the F-type ferromagnetism, often relying on external pressure or epitaxial strain. Doping at the europium sites or creating oxygen vacancies have also been proposed to lead to ferromagnetism. However, the fundamental mechanism by which excess from impurities or defects lead to ferromagnetic ordering is unclear. In this study, we explore the effects of doping on the magnetic ordering in $EuTiO_3$ through first-principles calculations. We show how itinerant carriers in the Ti-d-derived conduction-band states interact with the lower-lying europium f states, inducing an alignment of the large moments on the europium ions. The effects of doping on different types of magnetic ordering are considered, and possible ways of doping are discussed.

(EMA-S7-P018-2016) Development of radio transparent ceramic materials

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In recent times, scientists attention is paid to the synthesis of glass-ceramic and ceramic radio transparent materials based on celsian and slavsonite, which are characterized by ε ≤ 6-8, tgδ ≤ 1-50 • 10-4, have high melting temperature (1650 and 1760 ° C) low coefficient of thermal expansion ≤ 3,8 • 10-6 K-1 and high mechanical strength (E = 110 ÷ 115 GPa). With the purpose to expand the composition of radio transparent ceramic materials with low dielectric and high mechanical properties, the experiment was conducted with using of the simplex-lattice planning (Sheffs plans)). The area of technological compositions in ternary system SrO-Al2O3-SiO2 with the content of the components SrO - 25-45 wt. %, SiO2 - 30-50 wt. %, Al2O3 - 25-35 wt. % was selected for studying. Preparation of the samples was performed by the following technology. Raw ingredients was milled in a porcelain mill to the residue 4 - 6% on sieve 10,000 Holes. / Cm2. Pressing of the samples was performed on a hydraulic press P-125 at the specific pressure of 20 MPa. Pressed samples were dried in the oven at 110 ° C for 1 hour. Firing of samples was conducted in a laboratory oven at a temperature range of 1250-1450 ° C. On the basis of the research, new compositions of radio transparent ceramic materials, which are characterized by reduced values of dielectric permittivity (ε) - 5-9 and dielectric loss tangent (tg δ) - 60-110 • 10-4 were set.

(EMA-S7-P019-2016) Densification and Nanostructural Features of Al_2O_3 Ceramics Prepared with Nanoscale Powders by Microwave-assisted Sintering

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Al_2O_3 can be used for various engineering applications owing to its unique and useful physical features. Since the nanotechnology was introduced a few decades ago, much efforts has been made to fabricate nano-grained Al_2O_3 ceramics for various applications. In this study, densification and nanostructural features of Al_2O_3 ceramics prepared with nanoscale powders by microwave-assisted sintering (MWS) were investigated. To investigate the effects of initial powder size on the densification, Al_2O_3 powders with an average size of a few hundred nm were prepared and sintered by MWS and conventional sintering (CS). A MWS furnace equipped with a microwave generator (frequence: 2.45 GHz, power: 4 kW) was used. The structural features of the initial nanoscale powders and ceramics were examined by X-ray diffraction and transmission electron microscopy. The activation energy of the sintering processes was estimated to appreciate the kinetic behaviors of densification. The MWS of nanoscale powders yielded a relative density (RD) of over 90% when sintered at temperatures down to ~1200°C, whereas the same RD was achieved over ~1500°C by CS. In addition, nano-grained Al_2O_3 ceramics with RD of >90% can be obtained by MWS method. It was found that the response of nanoscale powders to microwave turns out to be more significant as the initial powder size decreases.

(EMA-S8-P020-2016) $BaTiO_3$ doped ceramics fractal sources dielectric properties

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The rare earth doped $BaTiO_3$-ceramics is investigated regarding their microstructural and dielectric characteristics influenced by the triple fractality “source”. Doped BaTiO3 were prepared using conventional solid state reaction and sintering at 1320 °C. Additive materials ensure the upper grain limit size to be 2-10 mm. Dielectric measurements were carried out as a function of temperature up to 180°C. The low doped samples (0.01wt%) sintered at 1320°C, display the high value of dielectric permittivity (e_r = 2300), at room