

Molecular Orbital Calculation for Evaluation of Electric Conduction and Insulation of Bismuth Ferrite and Its Solid Solutions / N. Takesue, K. Asakura, K. Kiba (Fukuoka Univ.), J. Saito (JAEA) / Bismuth ferrite is a perovskite-type ferroelectric, and is promising for the lead-free application to vibration energy harvesters because of its exclusively large electric spontaneous polarization. However, the pure substance is somehow electrically conductive, which tends to prohibit reversing the polarization; therefore, it is difficult to obtain the highly oriented polycrystals through the conventional simple treatment. A possible method for the insulation is considered to solid-solutionize bismuth ferrite with the other resemblances. So we performed molecular orbital calculation to investigate density of states of the solid solutions systematically modeled, as well as the overlap populations. Effects of the solutionization on the conductivity or insulation will be presented.

Experimental study of perovskite BNT-base ferroelectric solid solutions / K. Asakura, K. Kiba (Fukuoka Univ.), J. Saito (JAEA), N. Takesue (Fukuoka Univ.) / We fabricated perovskite ABO_3 ferroelectric solid-solution systems of a bismuth-sodium titanate base; the fabrications were done by flux powder sintering. Crystal structures of the samples were investigated by X-ray diffraction; (111) and (200) Bragg reflections of the typical primitive cell were monitored carefully. The results of, e.g. $(Bi_{1/2}Na_{1/2})TiO_3$ - $BaTiO_3$, show a possible morphotropic feature over phase states of both tetragonal and rhombohedral structures. We expect that this system will be the fundamental system for excellent piezoelectric properties. The results including dielectric constant d_{33} measurements will be presented systematically, also for other systems.

Synthesis of Nanocube crystals of Barium Titanate - toward The integration through Stirring / K. Kiba, K. Asakura (Fukuoka Univ.), J. Saito (JAEA), N. Takesue (Fukuoka Univ.) / We fabricated nanocube crystals of barium titanate by hydrothermal synthesis and also solvothermal, according to the methods of prior studies. Each particle is the single crystal and has the well-known conventional crystal structure, which was confirmed by TEM and X-ray diffraction. We have tried building the oriented dense assemblage by stirring the particles in a small container. We expect that this kind of assemblage has a gigantic electric polarization which can be utilized for the lead-free application to vibration energy harvesters.

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