

## Experimental Study of Solid Solutions of ferroelectric Bismuth Sodium Titanate

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We fabricated several kinds of perovskite-type solid solutions of ferroelectric Bismuth Sodium Titanate for the lead-free application to vibration energy harvesters. The samples were prepared by powder sintering. Their crystal structures were investigated by X-ray diffraction. The results show that the samples are well solid-solutionized. We expect that the systems will be fundamental to the devices of our interest. The results including measurements of dielectricity will be presented systematically.

## Synthesis of Nanocube Crystals of Barium Titanate

- toward The Integration through Stirring

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We fabricated nanocube crystals of barium titanate by hydrothermal synthesis and also solvothermal, according to the methods of prior studies (H. Itasaka, K. Mimura, and K. Kato, *Nanomaterials* 8, 739 (2018), and references contained in this paper). Each particle is the single crystal and has the well-known conventional crystal structure, which was confirmed by TEM and X-ray diffraction. Currently, we are trying to build the oriented dense assemblage by stirring the particles in a small container. The result will be presented.

## Study of Molecular Orbital Calculation on Electric Conduction and Insulation of Bismuth Ferrite and Its Solid Solutions

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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.