

Improved Ferroelectric Materials - Structural Characterization of Europium-doped BaTiO₃ Ternary Oxide Ceramics

Researchers at the Yamagata University, Japan, and Harbin Institute of Technology, China, have used Materials Studio's Reflex tools to characterize the crystal structure of Europium (Eu) doped Barium Titanate BaTiO₃ ceramics. The scientists studied the structural evolution of doped, Ba_{1-x}Eu_xTiO₃ (0.1 ≤ x ≤ 0.4) phases synthesized at high pressure and temperature as a function of Eu composition. The Ba_{1-x}Eu_xTiO₃ (0.1 ≤ x ≤ 0.4) phases showed an interesting orthorhombic-tetragonal-cubic structural transformation with the increase in Eu composition in Ba_{1-x}Eu_xTiO₃.

BaTiO₃ is an industrially important ferroelectric material. Its structure has a network of corner shared TiO₆ octahedra stabilized by the Ba²⁺ cations (Fig. 1). Various doping studies have been carried out in BaTiO₃ with an objective to improve its properties. For example, rare earth elements such as cerium (Ce) and lanthanum (La) have been partially doped in the Barium site to shift the dielectric maximum towards room temperature.

Reporting in the journal *Crystal Research and Technology*,¹ Lu and co-workers high-pressure synthesized the doped Ba_{1-x}Eu_xTiO₃ compositions and characterized the crystal structures of the products using X-ray diffraction. Analysis and refinement of the X-ray diffraction data was carried out using Materials Studio's Reflex tool.

The analysis of the X-ray diffraction data with the Reflex Pawley refinement tool indicated a series of phase transformations with a change in Eu composition. Table 1 shows the observed composition and structure. The Ba_{1-x}Eu_xTiO₃ was single-phase up to x ≤ 0.4, the x = 0.5 composition is a mixture of tetragonal BaTiO₃ and Pyrochlore Eu₂Ti₂O₇ type impurity. The authors concluded that the single phase solid solution limit for Ba_{1-x}Eu_xTiO₃ type phases is x = 0.4.

Eu composition 'x' in Ba _{1-x} Eu _x TiO ₃	Crystal structure
0.1	Orthorhombic
0.2	Tetragonal
0.3	Cubic
0.4	Cubic
0.5	Mixture of Tetragonal BaTiO ₃ and Eu ₂ Ti ₂ O ₇ Pyrochlore

Table 1 Crystal structure of Ba_{1-x}Eu_xTiO₃ as a function of Eu composition

Module used

Materials Studio – Reflex

Industry sectors

Chemicals/ Ceramics

Organizations

Graduate School of Science and Engineering, Yamagata University, Yonezawa, Japan

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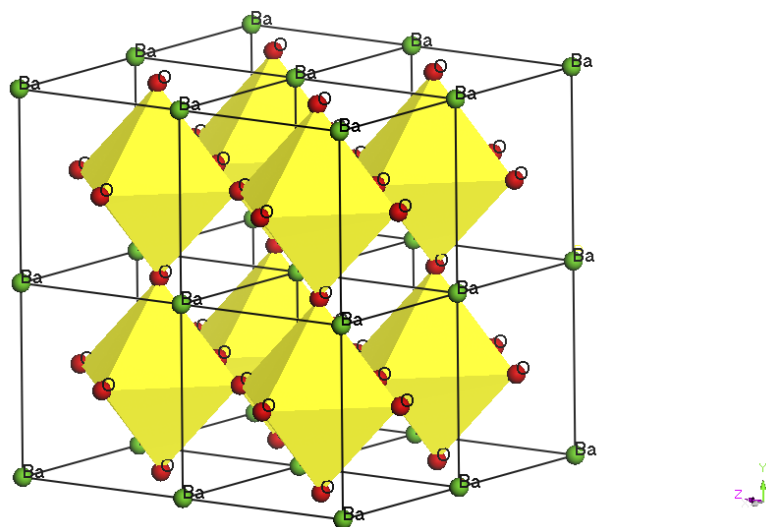


Fig. 1 Crystal structure of BaTiO₃

Reference

1. D.-Y.Lu, M. Sugano, W.-H.Su, and T. Koda, X-ray diffraction structural characterization of Ba_{1-x}Eu_xTiO₃ ternary oxides, *Crys. Res. Technol.*, **2005**, *40*, No.7, 703–708.