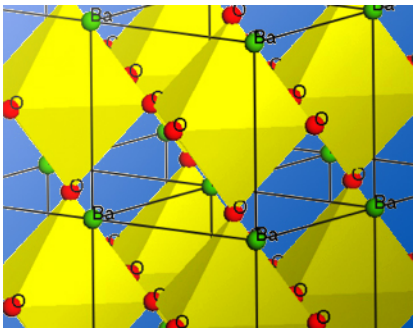
CASE STUDY

IMPROVED FERROELECTRIC MATERIALS - STRUCTURAL CHARACTERIZATION OF EUROPIUM-DOPED BATIO3 TERNARY OXIDE CERAMICS



Materials Studio Reflex prvides structural insights in novel systems as high temperature electronic super-conductors

Module used

- Materials Studio - Reflex

Industry Sectors

- Chemicals
- Ceramics

Organizations

- Graduate School of Science and Engineering, Yamagata University, Yonezawa, Japan
- Faculty of Engineering, Yamagata University, Yonezawa, Japan
- Department of Applied Physics, Harbin Institute of Technology, Harbin, China

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, $Ba_{1-x}Eu_xTiO_3$ ($0.1 \leq x \leq 0.4$) phases synthesized at high pressure and temperature as a function of Eu composition. The $Ba_{1-x}Eu_xTiO_3$ ($0.1 \leq x \leq 0.4$) phases showed an interesting orthorhombic-tetragonal-cubic structural transformation with the increase in Eu composition in $Ba_{1-x}Eu_xTiO_3$.

$BaTiO_3$ is an industrially important ferroelectric material. Its structure has a network of corner shared TiO_6 octahedra stabilized by the Ba^{2+} cations (Fig. 1). Various doping studies have been carried out in $BaTiO_3$ 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.

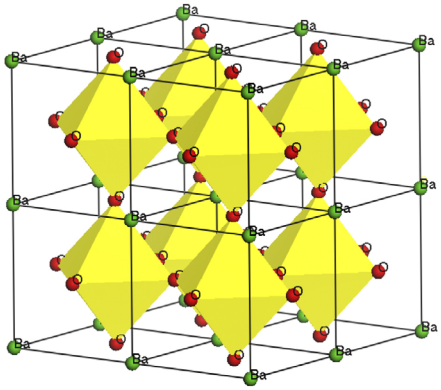


Fig. 1 *Crystal structure of $BaTiO_3$*

Reporting in the journal Crystal Research and Technology,[1] Lu and co-workers high-pressure synthesized the doped $Ba_{1-x}Eu_xTiO_3$ 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 $Ba_{1-x}Eu_xTiO_3$ was single-phase up to $x \leq 0.4$, the $x = 0.5$ composition is a mixture of tetragonal $BaTiO_3$ and Pyrochlore $Eu_2Ti_2O_7$ type impurity. The authors concluded that the single phase solid solution limit for $Ba_{1-x}Eu_xTiO_3$ type phases is $x = 0.4$.

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Eu composition 'x' in $Ba_{1-x}Eu_xTiO_3$	Crystal structure
0.1	Orthorhombic
0.2	Tetragonal
0.3	Cubic
0.4	Cubic
0.5	Mixtrue of Tetrogonal $BaTiO_3$ and $Eu_2Ti_2O_7$ Pyrochlore

Table 1 *Crystal structure of Ba1-xEuxTiO3 as a function of Eu composition*

REFERENCE

1. D.-Y.Lu, M. Sugano, W.-H.Su, and T. Koda, X-ray diffraction structural characterization of $Ba_{1-x}Eu_xTiO_3$ ternary oxides, Crys. Res. Technol., **2005**, 40, No.7, 703-708.