

## Poster Presentation

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### *Substitution Effects of Gd and Mg on Cubic Structure of Barium Titanate*

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Barium titanate BaTiO<sub>3</sub> is a ferroelectric oxide with low dielectric loss and high permittivity, which makes it a good insulator for industrial uses. However, the pure barium titanate is not always used for electronic devices. Gd- and Mg-doping in barium titanate is effective for the dielectrics in multilayer ceramic capacitors MLCCs, for example, to attain the uniform temperature-variation of dielectric constants in the wide temperature-range where MLCCs are practically used, while the Curie temperature is significantly decreased [1]. In this study, the structural characteristics of Gd- and Mg-substituted barium titanate (Ba,Gd)(Ti,Mg)O<sub>3</sub> (BGTM) in the cubic phase were investigated to clarify the effects of Gd- and Mg-substitution on the crystal structure and the chemical bonding. Synchrotron radiation x-ray powder diffraction measurements were carried out using the BGTM samples with the Mg content of  $x = 0 \sim 0.1$ . Lattice parameters, substitution sites of the Gd and Mg ions, thermal parameters, and electron charge density distributions in the crystals were analyzed by using the maximum entropy method (MEM)/Rietveld method. The Curie temperature decreased with increasing  $x$ . The phase transition did not take place in BGTM with  $x > 0.05$ . The Gd ion was confirmed to be substituted for the Ba ion with larger thermal vibration amplitude than that of the Ba ion. The amplitude was almost independent of the Gd content. It was revealed that the Gd ion occupied the off-centered positions slightly from the Ba-site along the  $\langle 100 \rangle$  directions at lower temperatures. Difference in thermal behaviors of the Gd and Ba ions can be attributed to the size difference between the smaller Gd ion and the larger Ba ion. The Mg ion was observed on the Ti-site. The substitution of the Mg ion for the Ti ion suppresses the ferroactivity of the Ti ion, which causes the lowering of the Curie temperature.

[1] Inoue, N., et al. *Jpn. J. Appl. Phys.*, vol. 48, pp. 09KF03/1-4, (2009).

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