

XAFS STUDIES ON (Ba,Sr)TiO₃ THIN FILMS

Strontium titanate (SrTiO₃) and a related compound, barium strontium titanate ((Ba,Sr)TiO₃) are attractive candidates for the dielectric capacitors of large-scale integrated circuits devices because of their high dielectric constants [1]. The precise dielectric properties of SrTiO₃ and (Ba,Sr)TiO₃ depend, however, upon their deposition method and atomic composition. The composition dependence of the dielectric properties of SrTiO₃ thin films has been reported previously [2]. Stoichiometric (Ba,Sr)TiO₃ ((Ba+Sr)/Ti=1) thin films possess superior dielectric properties compared to SrTiO₃. Furthermore, the dielectric properties are inferior when the (Ba+Sr)/Ti ratio is moved away from unity. Characterization by X-ray diffraction revealed no clear relation between dielectric properties and crystal structure. Therefore, to clarify the relationship between dielectric properties and structure, we studied local structure in (Ba,Sr)TiO₃ thin films.

Three kinds of (Ba,Sr)TiO₃ thin films were prepared: stoichiometric ((Ba+Sr)/Ti = 1), Ti-rich ((Ba+Sr)/Ti < 1) and (Ba+Sr)-rich ((Ba+Sr)/Ti > 1). 35 nm-thick (Ba,Sr)TiO₃ thin films were deposited on metal-coated Si substrates using an

electron cyclotron resonance plasma chemical vapor deposition method at low temperature [3]. After deposition, a rapid thermal annealing was performed in order to crystallize the film.

Ba L₃-edge XAFS was studied in order to obtain the local structure around Ba atoms. However, it was difficult to analyze the Ba L₃-edge XAFS spectra of (Ba,Sr)TiO₃ due to interference with Ti K-edge XAFS. Therefore, we planned to measure the Ba K-edge XAFS at SPring-8, because high-energy X-rays of sufficient flux are available for use. XAFS measurements were carried out using a Si(311) double crystal monochromator at beamline **BL01B1**. Fluorescence measurements of total reflection were carried out on the Ba K-edge at room temperature using a Ge-SSD detector in order to obtain the XAFS signal of the surface layer selectively.

A typical absorption spectrum near the BaK-edge of the (Ba,Sr)TiO₃ thin film is shown in Fig.1. Figure 2 shows the Fourier transforms of EXAFS oscillation around Ba atoms. The peak positions and heights appear to be different from one other, indicating that differences in the local structure around Ba atoms correspond to variations in dielectric properties. Thus, the aggravation of the dielectric properties in (Ba,Sr)TiO₃ thin films may be due to the imperfections in local structure and/or the impurity phases.

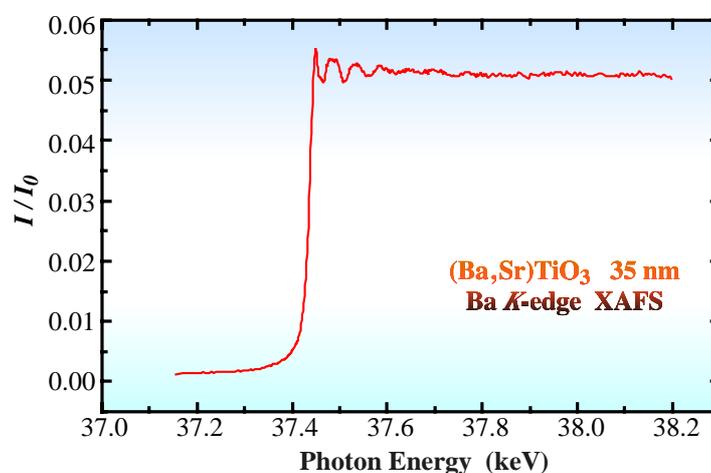


Fig. 1. Total reflection fluorescence XAFS spectrum near Ba K-edge of (Ba,Sr)TiO₃ thin film.

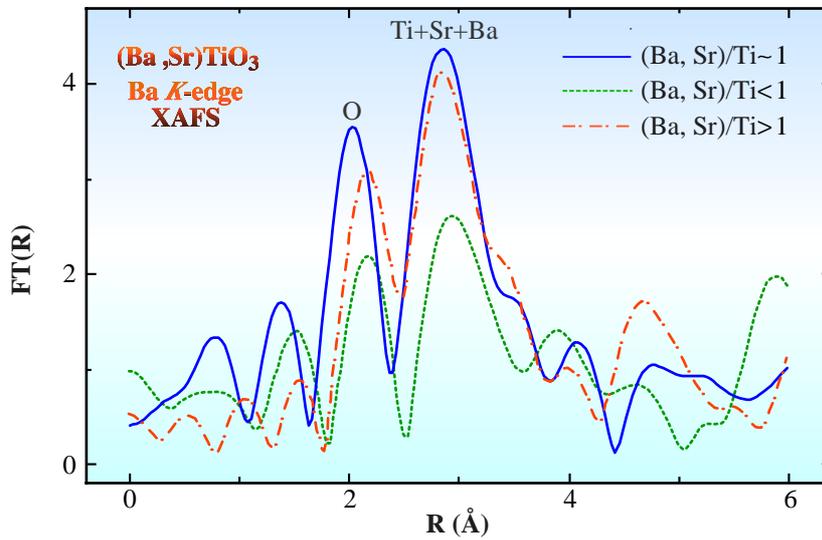


Fig. 2. Fourier transforms of EXAFS oscillation around Ba atoms of the (Ba,Sr)TiO₃ thin films.

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References

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