Crystal structure of functional materials by synchrotron radiation X-ray diffraction

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Needless to say, structure analysis is one of important techniques to discuss functionality of materials. Synchrotron radiation (SR) X-rays have been popular for us and it enables us to get high quality diffraction data easily and quickly. Not only average crystal structure which provides periodic nature (i.e. crystal structure in normal sense) of materials but also local structure, structure correlation, nanostructure, and inhomogeneous structure can be discussed by SR measurements. Nowadays the accurate determination of the average crystal structure is available under multiple external conditions such as temperature, electric field, light, gas, and so on. The time-course measurement technique has also been developing. In this talk, our recent SR X-ray diffraction studies of several oxide materials are presented together with basic knowledge of X-ray diffraction. All the SR X-ray diffraction measurements presented here were done at the beamlines BL02B2 (powder diffraction) [1,2] and BL02B1 (single crystal diffraction) [3] of the third generation synchrotron facility SPrgin-8 in Japan.

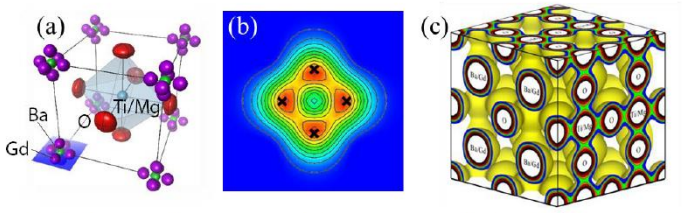

Figure 1. Example of crystal structure analysis of Gd- and Mg-substituted Barium Titanate in cubic phase by SR powder diffraction [4,5]. (a) Position and thermal amplitude of constituent ions. (b) Two dimensional map of probability density distribution of Gd ion on (001) plane derived by anharmonic atomic displacement parameter analysis. (c) Three dimensional electron charge density distribution map .

Figure 1 shows an example of determination of the atomic thermal vibration and electron density distribution of Barium Titanate based solid solutions in the cubic phase by the powder diffraction method [4,5]. The analysis of anharmonic atomic displacement parameters [6] clarified the 6-site off- centering of the partially substituted Gd ions. The electron charge density revealed covalent nature between the Ti/Mg and O ions. Figure 2 shows a time-course single crystal diffraction study of a tetragonal Barium Titanate under the application of voltage *V*. Tetragonality *c/a* oscillated during piezoelectric vibration induced by abrupt change of *V*. Other examples will also be introduced.

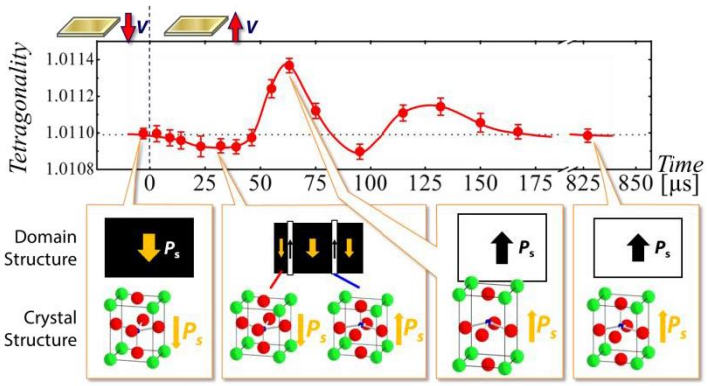

Figure 2. Example of time-course structure measurement of tetragonal Barium Titanate single crystal plate by pump-probe SR single crystal diffraction. Tetragonality *c/a* change during piezoelectric vibration induced by application of voltage were detected for millionths of a second [7].

References

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