

The Electron Density Distribution of Ti and O octahedron in Perovskite type Oxide crystals analysed by Maximum Entropy Method

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BaTiO₃ is a very well known compound, showing a ferroelectric phase transition at 403 degree K. On the other hand SrTiO₃, which is of a similar perovskite structure, show a different structural phase transition at 105 degree K. Such a difference in structural phase transitions has been understood as due to the condensation of different unstable phonon modes, zone center Γ_{15} ferroelectric mode for BaTiO₃ and zone boundary R₂₅ mode for SrTiO₃. The lattice dynamic of these two compounds must be closely related to the nature of their chemical bondings. In order to understand those phase transitions systematically on the basis of atomic bonding, we have shown at the last Denver Conference 2000 that the analysis by MEM on the basis of powder diffraction data is very promising. We have, then, shown that it is possible to see the difference of bonding nature between the tetragonal phase of BaTiO₃ and cubic phase of SrTiO₃. We extended the study to investigate the structural change before and after the phase transitions for those two compounds by producing again charge density distribution based on the analysis of MEM.

Synchrotron radiation and an imaging plate (IP) detector were used to obtain good counting statistics as well as high angular resolution (peak width at half maximum intensity of 0.03 degrees of 2 theta) from a large Debye-Scherrer camera installed at BL02B2, Spring-8. The wavelength used in this study was 0.5 Angstrom to measure over an angular range up to 80 degrees of 2 theta. A MEM/Rietveld analysis was used to calculate the charge-density distribution in the structures of four phases, that is above and below the phase transitions for BaTiO₃ and also for SrTiO₃.

Analysis showed that any particular difference was not seen in bonding nature of Ti and O octahedron for the paraelectric structures above their phase transitions, BaTiO₃ and Also SrTiO₃. While a significant different deformations of electron density distribution in Ti and O octahedron were noticed in the structures below the phase transition. The origin of the difference will be discussed.