Valence Electron Distributions of Ferroactive ions in Perovskite Oxides and Polar Lattice Distortions

Yoshihiro Kuroiwa

Department of Physical Science, Hiroshima University, Japan

e-mail: kuroiwa@sci.hiroshima-u.ac.jp

The polar lattice distortion and the lattice stability of perovskite-type oxides with the chemical formula ABO_3 are strongly influenced by substituting other ions for the *A*- and/or *B*-site ions. For example, primal 2nd-order (pseudo) Jahn-Teller distortions are caused in $BaTiO_3$ by the octahedrally coordinated high-valent d^0-ness Ti ion at the *B*-site, whereas a structure with a large tetragonal distortion is stabilized up to higher temperature in $PbTiO_3$ by cooperation of the Ti ion at the *B*-site and the Pb ion with lone pair electrons at the *A*-site. Most of valence electrons in perovskite-type oxides are distributed in shells of oxygen ions in general, while a small part of valence electrons of such ferroactive ions remains at the *A*- and/or *B*-sites to form covalent bonding with oxygen ions. The chemical bonding between the ferroactive ions and the oxygen ions is a clue for understanding phase transitions in perovskite-type oxides.

Our group has been devoted to visualizing the electron density distributions of perovskite-type oxides by analyzing the synchrotron-radiation x-ray powder diffraction (SXRD) data measured at SPring-8 using the maximum entropy method (MEM)/Rietveld method [1, 2]. In this study, the distributions of valence electrons in the outer shells of atoms are derived accurately from the SXRD data of various perovskite-type oxides to prove the characteristic chemical bonds which govern the ferroelectric phase transition. The obtained results provide direct experimental evidence that the hybridization of orbitals forming the *B*-O bonds weakens the short-range repulsion force, and causes the polar lattice distortion on the BO_6 octahedron.

References

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