Valence electron density and electrostatic potential in ferroelectric materials evaluated by MEM analysis of X-ray diffraction

Hiroshi Tanaka

Department of Materials Science, Shimane University, Japan

e-mail: h.tanaka@riko.shimane-u.ac.jp

The maximum entropy method (MEM) analysis of X-ray diffraction data is a powerful tool, which enables us to reproduce *total* electronic charge density in detail from a limited number of experimental data [1]. Kuroiwa and coworkers applied the method to $PbTiO_3$, and showed the first experimental evidence for covalency between Pb and O ions [2]. The *valence* charge density is, however, more informative in many cases from the viewpoint of materials design. Then we have proposed a smart method evaluating valence charge density, and shown an example for crystalline Si [3]. It is now improved, and applicable to any crystal structures consisting of most kind of atoms in the periodic table.

We also developed a method evaluating the electrostatic potential and electric field on the basis of MEM, and applied it to $PbTiO_3$. Visualized electrostatic potential and electric field on the isosurface of charge density distribution give a direct evidence for the dipolar polarization of the Pb ion. They show close agreement with results by *ab initio* calculations [4]. We extended the scheme in order to deal with materials showing large anisotropic thermal vibrations.

In this talk, we explain how to evaluate the valence charge density and electrostatic potential from the synchrotron radiation data by using MEM, and show some new results for $PbTiO_3$ and $BaTiO_3$. They are compared with those obtained by *ab initio* calculations, and reliabilities of the method will be discussed.

References

1. M. Takata, E. Nishibori, and M. Sakata, Z. Kristallogr. **216**, 71 (2001), and references there in.
2. Y. Kuroiwa, S. Aoyagi, A. Sawada, J. Harada, E. Nishibori, M. Takata, and M. Sakata, Phys. Rev. Lett. **87**, 217601(2001).
3. H. Tanaka, M. Takata, and M. Sakata, J. Phys. Soc. Jpn. **71**, 2595 (2002).
4. H. Tanaka, Y. Kuroiwa, and M. Takata, Phys. Rev. B74, 172105 (2006).