Interaction Visualization among Molecules and Atoms by Synchrotron Radiation

- Electrostatic Potential and Electric Field Imaging in Materials by MaxEnt Analysis –

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High brilliance and extremely small divergence of synchrotron radiation(SR) beam of SPring-8 have made a great progress in improving the precision of x-ray structural materials science. With an accurate diffraction data, SR allows us to reveal not only an atomic arrangement but also precise charge density distribution relating to bonding nature of atoms and molecules. So far, our developed analytical method which is the combination of the MaxEnt analysis and Rietveld refinement, so called MEM/Rietveld method, has been successfully applied to the structure analysis of novel nano materials, ferroelectric materials, manganites and superconductors by SR powder data[1,2]. The obtained MEM charge density enabled us structure refinement as well as observation of bonding nature, charge transfer and etc. The electrostatic potential mapping based on experimental charge density should be more informative to investigate the interaction between atoms and molecules.

Recently, we have succeeded in developing electrostatic potential and electric field imaging based on MEM charge density analysis[3]. The obtained electrostatic potential of the typical ferroelectric material, tetragonal $PbTiO_3$ has uncovered the feature of electronic polarization in Ti-O and Pb charge densities. In addition, the result shows very good agreement with that obtained from the *ab initio* calculation[4]. Very recently, we have also succeeded in visualization of charge order associated with orbital order in manganites[5]. Our new method shall be promising for visualization of interplay between atomic arrangement and function properties of novel materials.

In the talk, our recent challenge to time resolved structural analysis of DVD media materials using pulse characteristics[6] of SR will be also presented.

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