Multiple powder diffraction profiles for charge density study using synchrotron radiation X-ray.

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The electron density distribution in materials determines their properties and functions. We have developed both experimental analytical techniques for an accurate charge density study from powder diffraction data. Since the range of target materials of the powder diffraction is extensively broader than that of the single crystal diffraction. In addition, the powder diffraction technique easily provides us diffraction data under external fields such as temperature, pressure, electric fields.

We have developed a method based on multi-powder diffraction data[1)] for an improvement of the accuracy. Powder data with high reciprocal-space resolution, d~0.3 Å, are available by using the method. The method have been successfully applied charge density studies of silicon, diamond, and $CoSb_3$[2)] by a Maximum Entropy Method (MEM) and a multipole refinement[3,4)]. The recent application of the method is a charge density study of α-rhombohedral boron[5)]. We have successfully revealed a detailed bonding nature and also investigated the resolution dependence of the charge density study.

We have also developed a method for the determination of an element-selective structure from multi-wavelength anomalous powder diffraction (MAPD) via the combination of Rietveld and MEM charge density analysis [6, 7)]. We have successfully revealed charge density distributions of yttrium atom inside carbon cage in $Y@C_{82}$ from three distinct wavelength powder profiles[6)]. We have also visualized the charge density of gold atom in the Au(tmdt)2 using two distinct wavelength data [7)].

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