Poster Presentation

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Magnetic electron density in Fe3O4 examined by RXMS at Fe K edge

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It is known that a difference-Fourier synthesis of the Fourier series provides a mean for the location of bonding electrons, by subtracting out the electron density of all atoms in the crystal structure. Here the Fourier technique in X-ray diffraction was applied to observe the magnetic electron density of magnetite Fe3O4. An asymmetrical ratio in the resonant X-ray magnetic scattering (RXMS) provides information on the magnetic moments, which can be estimated from an intensity difference between the right-handed and left-handed polarized X rays. The ratio is proportional to the real part of the product of the spin-contributed structure factor F(hkl) and the complex conjugation of charge-scattered F(hkl). Expanding the equations in difference–Fourier formalization, the spin density can be represented with the observed f"m of RXMS. Synchrotron RXMS experiments were performed at the PF-BL-6C beamline using an AFC-5u four-circle diffractometer. Through a diamond phase retarder the incident X rays were circularly polarized at the Fe K absorption edge, where a wavelength of λ = 1.7439 Å (E = 7.1094 keV) was selected within the pre-edge. A spherical crystal of 0.13 mm in diameter was mounted along the a3 axis with the glass fiber on rare-earth magnet and goniometer head. The intensity data of RXMS were collected for Bragg reflections up to 2θ = 131°. After crystal-structure refinements with scaling of the RXMS data, difference-Fourier syntheses were made in triclinic symmetry with a total of 165 reflections by using the software FRAXY. The syntheses are superior in examining the magnetic effect in the polarization difference and eliminating other effects such as charge scattering, experimental errors and the termination effect. The difference of magnetic electron density between left-handed and right-handed circular polarizations at E was estimated in the Fourier series of partially observed F(hkl). The magnetic electron density on Fourier maps will be discussed in the presentation.

Keywords: magnetic electron density, magnetite, resonant X-ray magnetic scattering