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A technique of X-ray magnetic diffraction (XMD) of ferromagnets was applied to an orbital ordering compound of YTiO₃. XMD, that is nonresonant X-ray magnetic Bragg scattering, is a unique experimental technique which enables one to measure spin- and orbital-magnetic form factor separately. The aim of this study is to observe directly the ordered orbital (wavefunction) in real space through the spin magnetic form factor measured by the XMD.

In YTiO₃ which is one of perovskite oxides, a Ti atom exists as a Ti³⁺ ion, and has one 3d electron in t_{2g} state which shows orbital ordering. Below 30K this compound is ferromagnetic, and spin ordering occurs together with orbital ordering.

The XMD measurement was performed at KEK-PF-BL3C3, and the spin-magnetic form factor was measured for more than 22 reciprocal lattice points. By the Fourier transformation of it the spin density distribution was obtained in real space. As each Ti atom has one 3d electron with spin aligned in one direction, spin density distribution corresponds to 3d electron distribution which is correlated with 3d electron wavefunction. The experimental spin density was compared with calculated electron density base on t_{2g} wavefunction. MEM analysis of spin density is planned and the result will be shown.

Keywords: magnetic X-ray scattering, spin density, titanium oxide compounds

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Charge Density Study of Cu₃(en)₂(CN)₄H₂O

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In our recent work we have studied distribution of the electron density in the model compounds for blue proteins. Two model compounds [1] representing the reduced and the oxidized form of the protein contains copper in state +1 and +2. The mixed-valence complex Cu₃(en)₂(CN)₄H₂O [2] contains copper atoms in both oxidation states, and so it should be possible to study electronic structure and particularly copper in both oxidation states not biased by different systematic errors. This provide us interesting comparison with our previous results.

Data were collected at the beamline F1 at HASYLAB/DESY in Hamburg (T = 100 K, λ = 0.5604 Å). For corrections, integration and data reduction programs SAPRO, SAINT, and SORTAV were used. Multipole refinement was performed with XD software package.

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