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Keywords: synchrotron radiation, magnetism, diffraction

## P14.08.23

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### Study of spin and orbital magnetic form factors of $\text{CeRh}_3\text{B}_2$ by X-ray magnetic diffraction

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We have performed X-ray magnetic diffraction (XMD) on a single crystal of an intermetallic compound  $\text{CeRh}_3\text{B}_2$  at KEK-PF-BL3C in Japan. In this method the spin and orbital magnetic form factors of ferromagnets can be selectively measured by adjusting the angle between the directions of the sample magnetization and the incident X-rays on the sample. Spin and orbital magnetic form factors in reciprocal space are transformed to the density distribution of spin and orbital magnetic moments respectively in the real space by the Fourier inverse transform. The purpose of this study is to reveal the magnetic properties of  $\text{CeRh}_3\text{B}_2$  through the spin and orbital magnetic moment density in the real space obtained by the XMD experiment. This compound has attracted many scientists for its anomalous ferromagnetism. This material has the highest Curie temperature ( $T_c = 115\text{K}$ ) among the known Ce compounds with nonmagnetic constituents. It is important to investigate the magnetic electrons of  $\text{CeRh}_3\text{B}_2$  for understanding magnetism of this compound. We have obtained spin and orbital magnetic form factors for 26 reciprocal lattice points of  $hk0$  series by the XMD. The observed spin magnetic form factor obviously suggests anisotropic distribution in the real space, but the orbital magnetic form factor does not. We will obtain the density distribution of the spin and orbital magnetic moment in the real space by the Fourier inverse transform (or MEM analysis) of the observed spin and orbital magnetic form factors. Detail discussion will be given in the conference.

Keywords: X-ray magnetic scattering, spin density, rare-earth materials

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### 3D spin density and orbital ordering of $\text{YTiO}_3$ observed by X-ray magnetic diffraction experiment

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A compound of  $\text{YTiO}_3$  is one of the orbital ordering systems. This compound has  $\text{GdFeO}_3$ -type perovskite structure and is ferromagnetic below 30K. The origin of magnetism of this compound is 3d electrons in  $t_{2g}$  states of Ti atoms. In the previous experiment,

we applied the X-ray magnetic diffraction (XMD) experiment to this compound, and we obtained the spin magnetic form factor for reciprocal lattice points of  $h0l$  series. In this study, we apply the upgraded XMD experimental system in order to obtain the spin magnetic form factor for  $hk0$  and  $0kl$  series. We aim to observe three-dimensional spin-density distribution and orbital ordering of  $\text{YTiO}_3$ . The experiment was performed on the beamline BL3C of KEK-PF. White beam X-rays of elliptically polarized synchrotron radiation was irradiated on the sample crystal. The diffracted X-ray intensity was measured with pure Ge SSD. Sample temperature was 15K. Sample crystal was magnetized with an electromagnet. Applied magnetic field was 2.15T that was enough to saturate the magnetization of this compound along the hard magnetization axis (b axis). By adjusting the angle between the directions of the incident X-rays and the magnetization of the sample we measured selectively spin magnetic form factor. We obtained the spin magnetic form factor for the 30 reciprocal lattice points of  $hk0$  and  $0kl$  series. We applied Maximum Entropy Method (MEM) to the present and previous data of total 76 reciprocal lattice points. We obtained three-dimensional spin-density distribution of  $\text{YTiO}_3$ . Obtained 3D spin-density distribution represents very well the electron orbital distribution of 3d- $t_{2g}$  state. In conclusion, we succeeded in direct observation of the ordered orbital of 3d electrons of  $\text{YTiO}_3$  in the real space.

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

## P14.08.25

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### The interplay between Ru and Mn moment in $\text{CaRu}_{1-x}\text{Mn}_x\text{O}_3$ by magnetic Compton scattering

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A magnetic Compton scattering (MCS) is a powerful tool to study magnetic structure of materials because magnetic Compton profile (MCP),  $J_{\text{mag}}(pz)$ , provides the electron momentum distribution of all electrons into a material and distinguishes between s, p, d, and f electrons by the difference of the electron momentum density, which directly related to wave function. Additionally, it can evaluate not only the total magnetic moment but the magnetic moment on composite ions separately.  $\text{SrRuO}_3$  and  $\text{CaRuO}_3$  are attracting an attention in connection with the strongly correlated electron system. In particular,  $\text{CaRuO}_3$  is paramagnetic though it has Curie constant corresponding to  $S=1$  and relatively large negative Weiss temperature. The  $\text{CaRu}_{1-x}\text{Mn}_x\text{O}_3$  system shows ferromagnetism with relatively large magnetic moment and higher TC than that of the ferromagnetic  $\text{SrRuO}_3$  by very small substitution of the transition metal ions to the Ru site, however, the existence of magnetic moment on Ru and magnetic ground states have not been confirmed. The study on magnetic ground states of  $\text{CaRu}_{1-x}\text{Mn}_x\text{O}_3$  ( $0.2 < x < 0.9$ ) was carried out by MCS using the high-flux x-ray beam of synchrotron radiation at SPring-8. This study reveals that the Mn doping creates inhomogeneous magnetic ground states at whole range of this system. All Ru and Mn ions ferromagnetically ordered and antiferromagnetic coupling between Mn and Ru spin moments makes a ferrimagnetic

structure at  $x = 0.5$ . Low Mn doping sample ( $x < 0.5$ ) comprises paramagnetic and ferrimagnetic states and high Mn contained samples ( $x > 0.5$ ) become a ferrimagnetic and antiferromagnetic states. The ferrimagnetism is caused by the moment of  $\text{Ru}^{4.5+}$  and  $\text{Mn}^{3.5+}$  ions in frame of the mixed valence model.

Keywords: Compton profiles, ruthenium oxide compounds, manganese oxide compounds

## P14.08.26

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### Development of magnetic Compton scattering using a 9T cryomagnet at the ESRF

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We report on the installation and use of high-field spin-polarised Compton scattering measurements at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France. To achieve this, an Oxford Instruments "Spectromag" cryomagnet was purchased. This can provide magnetic fields up to 9 Tesla, at temperatures down to 1.3K, whereas previously the sample environment was limited to a maximum field of 1T, with temperatures down to 2.2K. The commissioning of this new facility was successful, and it will vastly increase the range of problems that can be addressed using the technique at the ESRF. There are technical aspects of conducting these experiments associated with the use of the new magnet. A suitable methodology has been devised, and the first measurements have been made. Results for our recent research on the magnetocaloric material  $\text{Gd}_7\text{Pd}_3$  and the metamagnetic system  $\text{Sr}_3\text{Ru}_2\text{O}_7$  are presented in the poster.

Keywords: magnetic Compton scattering, cryomagnet, spin density

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### Magnetic Compton profile of $\text{ErCo}_2$ under high pressure

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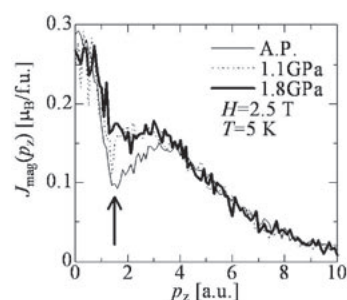
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Magnetic phase transition of Laves phase  $\text{ErCo}_2$  changes from first-order to second-order with increasing pressure [1], modification in the electronic state is of basic interest. We have recorded magnetic Compton profile (MCP) of  $\text{ErCo}_2$  under high pressure up to 1.8 GPa using a diamond-anvil-cell and determined the spin-polarized momentum distribution quantitatively. The figure illustrates pressure variation of the normalized MCP. The dip indicated by the arrow gradually shallows with increasing pressure. Fitted profiles

using the Hartree-Fock calculations reveal that the Co 3d spin moment decreases from 1.0 to 0.6 Bohr magnetons/atom and the Er 4f spin moment is reduced from 3.5 to 3.1 Bohr magnetons/atom. The suppression in the Co 3d moment is more significant in comparison with that of the Er 4f moment. This is consistent with the previous result of X-ray magnetic circular dichroism measurement [2]. Therefore, the instability of the Co 3d moment under pressure is closely associated with the magnetic phase transition.

[1] O. Syshchenko, et al., *J. Alloys and Compounds* 317-318 (2001) 438.

[2] N. Ishimatsu, et al., *Phys. Rev. B* 75 (2007) 180402(R).



Keywords: high-pressure physics, Compton scattering, magnetic phase transitions

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### Magnetic Compton scattering from ferromagnetic perovskite oxide $\text{YTiO}_3$

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$\text{YTiO}_3$  is one of the compounds which show orbital ordering phenomenon. The 3d electrons of  $\text{Ti}^{3+}$  ions in  $t_{2g}$  configuration exhibit orbital ordering. Crystal structure of  $\text{YTiO}_3$  is the perovskite (Pbnm). This compound is ferromagnetic below 28K, and is an insulator. The Magnetic Compton scattering (MCS) is one of the methods of observing the electronic structure. The physical quantity obtained from this experiment is Magnetic Compton Profile (MCP). The MCP is directly linked to the wave function of magnetic electrons in solids. The experiments were performed at the KEK-PF-AR-NE1A1. We measured the MCPs of  $\text{YTiO}_3$  along the a- and c-axis. These two MCPs showed clearly directional anisotropy. We calculated the MCPs by using an atomic model wave function of a linear combination of two 3d- $t_{2g}$  orbitals,  $u_{yz} + v_{dzx}$  ( $u^2 + v^2 = 1$ ) for the four Ti sites. Calculation of the MCPs was performed for various values of coefficient  $u$  (0.63-0.89). The calculated MCP for the c-axis depends much stronger on the parameter  $u$  than the one for the a-axis. Fitting analysis using the MCP for the c-axis was performed, and the best fit was obtained for  $u = 0.84$  and  $v = 0.54$ . MCP measurement for the b-axis has been made at the SPring-8 BL08W. The b-axis is the hard magnetization direction of this compound, and stronger magnetic field is needed for the MCP measurement of the b-axis than those of the a- and c-axis. The detailed analysis is being performed and the result will be given at the conference.

Keywords: magnetic Compton scattering, orbital ordering,  $\text{YTiO}_3$