no protein structure has been refined using the invariom model. The proteins under examination are lysozyme, insulin and myoglobin -- macromolecules with molecular weights of 6 to 17kDa. They all have important biological functions, so it is desirable to improve their refinement and to obtain a high quality electron density distribution. The latter allows to derive e.g. Bader's bond and atomic descriptors, electrostatic potentials and lattice energies. To achieve the necessary atomic resolution for the invariom refinement high intense synchrotron beamlines (Swiss Light Source, Diamond Light Source) were utilized.

Keywords: macromolecules, invariome, electron charge density

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Internal magnetic structure of a Mn_3 cluster determined by polarised neutron diffraction

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The self-assembly between metal centres and selected ligands into predetermined molecular architectures is especially relevant in the field of magnetic materials, since remarkable metal-metal interactions may be achieved.[1] The compound studied here exhibits fascinating features from the supramolecular and magnetism point of view.[2] It results from the fusion of two double-stranded helicates by 'click self-assembly' to form an unprecedented trinuclear helical structure(See figure). The magnetic response of the compound reveals that this is a rare lineal trinuclear MnII compound showing weak ferromagnetic interactions. Here we present the results of a polarized neutron experiment aiming to determine the spin density in the Mn atoms and to elucidate the magnetic interaction model. The understanding of the delicate interactions intra- and inter-clusters is crucial to permit in future the design of new magnetic interesting compounds.

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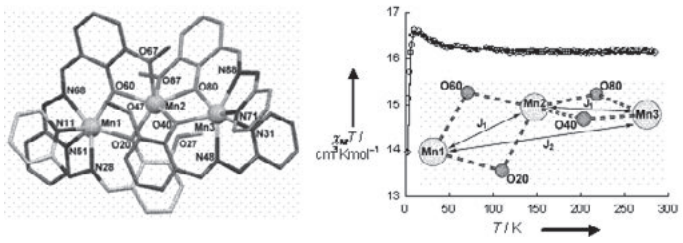

Keywords: molecular magnetism, spin density, self-assembly

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Magnetic frustration in $Gd_{7-x}Y_xPd_3$ single crystals

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Materials based on gadolinium are prospective for applications in magnetic refrigeration cycles. Magnetocaloric properties of polycrystalline Gd_7Pd_3 were investigated by Canepa et al. [1]. Wide investigations of the Gd_7T_3 (T = Rh, Pd) single crystals were performed [2, 3]. They crystallize in Th_7Fe_3 type hexagonal structure with c/a=0.63. Gd_7Rh_3 orders antiferromagnetically at 140 K while Gd_7Pd_3 becomes ferromagnetic at about 334 K. The aim of this work is to examine the influence of substitution of nonmagnetic yttrium into gadolinium sublattice. Single crystals of $Gd_{7-x}Y_xPd_3$ were grown by the Czochralski method from a levitated melt. The X-ray Berg-Barrett topography confirmed a good quality of the obtained crystals. The observed XPS, magnetic and electrical resistivity behaviour points to the coexistence of localized magnetism from the magnetic Gd^{3+} ions and itinerant ferromagnetism from 4d- and 5d-electron bands. The magnetic behaviour of the $Gd_{7-x}Y_xPd_3$ solid solutions in terms of three competition mechanisms: RKKY-interaction, magnetic frustration and spin-fluctuation is discussed. The change in TC across the $Gd_{7-x}Y_xPd_3$ series is consistent with change in the RKKY-interaction strength, while the spin-reorientation are probably governed by the vanishing of the magnetic frustration.

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Keywords: Czochralski method, ferromagnetics, magnetization

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Spin form factors of the samarium ions in $SmAl_2$

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We have tried spin-form factor measurements on $SmAl_2$ using the synchrotron radiation and established the method of analyzing the data using the operator-equivalent technique before [1]. It was, however, difficult to interpret the experiment and we have subsequently improved the experimental procedure and instrumentation. After that, a quantitative agreement with the theoretical estimates has been observed for, for example, $PrAl_2$ and $DyAl_2$ [3]. In this presentation, the newly measured results on $SmAl_2$ will be shown and discussed.

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Keywords: synchrotron radiation, magnetism, diffraction

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Study of spin and orbital magnetic form factors of $CeRh_3B_2$ by X-ray magnetic diffraction

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We have performed X-ray magnetic diffraction (XMD) on a single crystal of an intermetalic compound $CeRh_3B_2$ 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 $CeRh_3B_2$ 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 (Tc = 115K) among the known Ce compounds with nonmagnetic constituents. It is important to investigate the magnetic electrons of $CeRh_3B_2$ 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 $YTiO_3$ observed by X-ray magnetic diffraction experiment

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A compound of $YTiO_3$ is one of the orbital ordering systems. This compound has $GdFeO_3$-type perovskite structure and is ferromagnetic below 30K. The origin of magnetism of this compound is 3d electrons in t2g 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 $YTiO_3$. 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 $YTiO_3$. Obtained 3D spin-density distribution represents very well the electron orbital distribution of 3d-t2g state. In conclusion, we succeeded in direct observation of the ordered orbital of 3d electrons of $YTiO_3$ in the real space.

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

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The interplay between Ru and Mn moment in $CaRu_{1-x}Mn_xO_3$ 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), Jmag(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. $SrRuO_3$ and $CaRuO_3$ are attracting an attention in connection with the strongly correlated electron system. In particular, $CaRuO_3$ is paramagnetic though it has Curie constant corresponding to S=1 and relatively large negative Weiss temperature. The $CaRu_{1-x}MnxO_3$ system shows ferromagnetism with relatively large magnetic moment and higher TC than that of the ferromagnetic $SrRuO_3$ 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 $CaRu_{1-x}MnxO_3$ ($0.2 < x < 0.9$) 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