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Using magnetic Compton scattering to study Invar and spin-polarised materials

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Invar and spin-polarised materials are two systems where magnetism plays the central role in determining their technologically useful properties. Magnetic Compton scattering is able to provide unique information concerning the magnetic ground state. The technique's sensitivity to the momentum density distribution enables the effects of the underlying electronic band structure to be studied. The fact that only the spin moment is measured enables the spin and orbital moments to be determined, and "spin-magnetometry" measurements can be made. A number of Invar systems have been studied using magnetic Compton scattering. In Fe_3Pt the momentum space spin density showed no temperature dependence. This is in disagreement with what would be expected for the Weiss two-state model proposed as a possible mechanism behind the Invar effect. $DyCo_2$ is another interesting Invar material, as it contains both *3d* and *4f* magnetism and their behaviour will be discussed in the talk. In the classic Invar system, Fe-Ni, the temperature dependence shows no apparent changes in the spin density distribution, but the technique's sensitivity to the spin moment reveals that the spin and orbital moments exhibit different behaviour in the Invar region. Details of the electronic structure, such as Fermi surface related features, are manifested in the shapes of the magnetic Compton profiles. This sensitivity had been exploited in the study of the highly spin-polarised $Co_{1-x}Fe_xS_2$ system, enabling us to investigate the underlying electronic structure and signatures of the band structure related to the changing spin polarisation that occurs on doping with Fe. This information can be used, in conjunction with calculations, to determine the spin polarisation at the Fermi level.

Keywords: spin density, magnetic materials, Compton scattering

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Magnetic Compton scattering under high pressure

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Magnetic Compton scattering using synchrotron radiation is an established technique for probing a spin-uncompensated momentum density distribution in materials with spontaneous magnetizations. A projection of the spin-uncompensated momentum density distribution on the x-ray scattering vector can be measured as a magnetic Compton profile (MCP) using circularly polarized x-rays due to the spin dependent terms in the scattering cross-section. For studies of an electronic structure in a material with spontaneous magnetization, a measurement of the spin-uncompensated momentum density distribution is very useful because it reflects the spin polarization in a momentum space of all occupied bands. The MCP is extracted from the difference between two energy spectra with alternative directions of magnetizations in the sample under the same experimental conditions. Then magnetic Compton scattering may be one of useful techniques to study an electronic structure in the material under high pressure because non magnetic materials do not contribute MCP. We have tried to measure MCPs of single crystalline Fe_2P under high pressures using a diamond-anvil-cell on beamline BL08W at SPring-8, Japan. Fe_2P is a ferromagnetic compound at ambient pressure and a new antiferromagnetic state appears in Fe_2P under pressure. In this antiferromagnetic phase, metamagnetic transition is observed at about 2 kOe. MCPs along the c-axis of Fe_2P were measured at ambient pressure and 2.5GPa with 25 kOe. The extracted MCP in the region of $pz < 1.0$ a.u. at 2.5GPa is little different from that at ambient pressure. Then this difference in MCPs is most likely caused by the change of contribution from spin-uncompensated itinerant electrons.

Keywords: compton profiles, pressure, magnetic material

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Spin and magnetization density in the kagome staircase system $Co_3V_2O_8$

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$Co_3V_2O_8$ represents the transition metal orthooxovanadates labelled as kagome staircase structures. These structures are characterized by edge-sharing CoO_6 octahedra ($3d^7$ Co) isolated by nonmagnetic VO_4 tetrahedra ($3d^0$ V). The crystallographic structure (orthorhombic space group Cmca [1]) is interesting with respect to the magnetic properties as the magnetic ions form buckled planes of corner-sharing isosceles triangles representing an anisotropic variation of the ideal kagome net. Within these buckled planes, the kagome staircases, cross-tie ions on crystallographic 4a sites link the linear chains of spine ions on 8e sites. The magnetic coupling is mainly effectuated via 90- Co-O-Co superexchange pathways [2], which motivates the investigation of the spin and magnetization density concerning two main points: Can the oxygen ions, which participate in the superexchange, clearly be identified? Does vanadium really act as an isolator or does it have an electronic configuration different than $3d^0$? In order to answer these questions a combination of Magnetic Compton Scattering, Polarized Neutron Diffraction and ab initio calculations has been employed, from which each of the applied methods reveals interesting features of the density distributions.

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