Acta Cryst. (2002). A58 (Supplement), C38 MAGNETIZATION DENSITIES IN FERROMAGNETS

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Investigations of electron spin density by magnetic compton scattering with high energy synchrotron radiation, and magnetization density, i.e. Spin plus orbital components, by diffraction at conventional x-ray energies will be presented for a number of rare earth and transition metal ferromagnetic compounds and alloys. The methods for retrieving the weak magnetic signal from the charge scattering will be discussed and the success of the methods separately, and when combined, will be illustrated by reviewing recent results obtained by the warwick group at esrf and collaborators elsewhere.

Keywords: FERROMAGNETISM COMPTON SCATTERING

Acta Cryst. (2002). A58 (Supplement), C38 RESONANT X-RAY SCATTERING IN STRONGLY CORRELATED ELECTRON SYSTEMS

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The interplay between charge, orbital and spin degrees of freedom is the key ingredient underlying the physics of transition-metal oxides. An ideal tool for studying the consequences of such correlation is provided by Resonant X-ray Scattering (RXS), as was demonstrated by several experiments carried out during the past few years on manganites and other transition metal oxides.

RXS has its origin from processes in which photons are virtually absorbed by exciting core electrons to empty states, and subsequently reemitted when the excited electrons and core holes recombine. These processes give rise to anomalous tensor components in the atomic scattering factor, and the appearance of Bragg peaks at position forbidden by crystallographic space group if long-range order of magnetic moments, electronic orbital occupancy, or aspherical electron clouds is present. We present a brief overview of some recent experiments performed at ID20 beamline at ESRF.

Keywords: ORBITAL ORDERING, RESONANT X-RAY SCATTERING

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ELECTRON TRANSFER IN KONDO CRYSTAL CeB₆ AND RELATED COMPLEXES BY MULTI-TEMPERATURE EDD MEASUREMENT <u>K. Tanaka¹</u>Y. Onuki²

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Electron density distributions (EDD) in rare-earth complexes have been supposed to be impossible to measure by X-ray diffraction. However EDD in CeB₆ is highly interesting since 4f-electrons spontaneously flow from Ce to B₆ with a decrease in temperature by Kondo effect. However measurements at 100, 165, 230 and 298 K avoiding multiple diffraction and a refinement assuming a spin-orbit interaction for Ce 4f-electrons revealed essential nature of the changing system.

The multi-temperature EDD measurement revealed electron donation from Ce to B_6 and its process illuminating a role of entropy. The more 4f and 2p electrons in a B_6 octahedron are transferred at the lower temperature to B-B bonds connecting B_6 octahedra. The electron transfer changes potential of Ce atoms enhancing anharmonic vibration (AHV) of Ce toward the bond at low temperature. It explains prominent and diminished 4f-electron peaks in the deformation densities at 165 and 100 K, respectively. The enhanced AHV caused by the 4f-electron transfer corresponds to an increase in entropy. Since the electron transfer itself increase entropy, it cannot be stopped. EDD in La B_6 and Sm B_6 with zero and five 4f electrons, respectively, are also investigated to support the above discussion.

Keywords: 4F-ELECTRON DENSITY KONDO EFFECT MULTI-TEMPERATURE EDD MEASUREMENT

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ELASTICITY AND STRENGTH OF SIX-COORDINATED SILICATES AT PRESSURES OF THE EARTH'S LOWER MANTLE: STISHOVITE, CALCIUM SILICATE PEROVSKITE, AND PHASE D

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Single-crystal elastic properties and the yield strength are fundamental properties of materials that are not well understood at high pressures. We obtain new constraints on elasticity and strength using radial x-ray diffraction techniques in the diamond anvil cell. In this method, the lattice strain is measured as a function of orientation with respect to the loading axis of a sample under non-hydrostatic compression. The measured lattice strains contain information about single-crystal elasticity, yield strength, strength anisotropy, stress continuity, texturing, and even the equation of state. We have carried out radial diffraction studies at ambient temperature and pressures up to 60 GPa on three silicates relevant to the Earth's deep interior: stishovite (SiO₂), Calcium silicate perovskite (CaSiO₃), and the dense hydrous silicate, phase D (MgSi₂H₂O₆). This diverse set of six-coordinated silicates is representative of the range of structures likely to be encountered in the Earth's lower mantle. Our results show that the ratio of differential stress to shear modulus for these three materials increases weakly with pressure and ranges between 0.012-0.039. This ratio is lower than found for four-coordinated silicates such as olivine and ringwoodite. The yield strength of stishovite is markedly reduced as the stishovite-CaCl₂ phase boundary is approached, and our inversion for elastic stiffnesses provides experimental support the predicted instability in C₁₁-C₁₂. The yield strength of Ca-perovskite is 10 GPa at a pressure of 61 GPa whereas phase D supports a differential stress of 3.1 GPa at a pressure of 28 GPa

Keywords: HIGH PRESSURE, SILICATES, LOWER MANTLE