Resonant Soft X-ray Diffraction as a Probe for Complex Magnetic Structures. <u>Christian Schuessler-Langeheine</u>. *II.Physikalisches Institut, Universitaet zu Koeln, Zuelpicher Str. 77, 50937 Koeln, Germany.*
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For the study of complex magnetic order in 3d-transition metal systems resonant diffraction of soft x-rays (RSXD) exists as a technique that is complementary to neutron diffraction. RSXD is characterized by a large magnetic scattering cross section and a high spectroscopic sensitivity. This sensitivity allows to do experiments not only selectively for a certain element in the sample but also for a certain oxidation state of a given element. In addition to magnetic order also charge and orbital order can be probed directly using RSXD. A realistic microscopic theory as well as sum rules allow for a quantitative analysis of the resonance spectra. While the rather long photon wavelengths, which is of the order of 10 to 20 Angstroms for 3d resonances, limits the accessible momentum space, many complex materials exhibit magnetic order on fairly long length scales and can be readily studied using RSXD. Examples are stripe phases as they are found in cuprates and nickelates or the complex charge, orbital and spin order pattern found in doped manganites. Also artificial systems like multilayers typically have periodicities in the nm range and can well be studied using RSXD. Interestingly not only static magnetic order but also fluctuating order that would occur in a neutron experiment in the inelastic channel can be probed. With the use of coherent photons an RSXD experiment gains an additional sensitivity to disorder on nm length scales and to changes of this disorder as a function of time or an external field. Coherent RSXD can hence be used to study magnetic domain dynamics as well as phase separation effects in complex materials. The talk will discuss the experimental possibilities of RSXD and will present results from Sr-doped La_2NiO_4, La_2CuO_4, and La_2CoO_4 as well as from ultrathin Ho-metal films.

Keywords: soft X-rays; X-ray anomalous scattering; transition-metal oxides

The Nature of Magnetic Coupling in the Martensitic and Austenitic Structures in Magnetic Shape-Memory Alloys Studied by Neutron Polarization Analysis. <u>Mehmet Acet</u>[a], Seda Aksoy[a], Eberhard F. Wassermann[a], Lluise Mañosa[b], Antoni Planes[b], Pascale P. Deen[c]. *[a]Experimentalphysik (AG-Farle), Universität Duisburg-Essen,D-47048 Duisburg. [b]Facultat de Física, Departament dEstructura i Constituents de la Matèria, Universitat de Barcelona, E-08028 Barcelona. [c]Institut Laue-Langevin, 38042 Grenoble.*
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Ni-Mn-*X*-based Heusler-type alloys (*X*: group IIIA-VA elements) undergo martensitic transformations from a high symmetry cubic austenitic state to a modulated orthorhombic martensitic state of lower symmetry. The presence of such a transformation is responsible for the rich variety of phenomena observed in these materials; mainly being the magnetic shape-memory effect, magnetic superelasticity, the magnetocaloric effect, magnetic field induced structural transformations, exchange-bias, and austenite arrest. To understand the cause of these magnetostructural effects, we study the structure and nature of the magnetic coupling below and above the martensitic transition with XYZ neutron polarization analysis experiments. We show that around the transition temperature M_s, the magnetic interactions are in the form of short-range antiferromagnetic correlations for $T < M_s$, whereas they persist as mixed ferromagnetic and antiferromagnetic short-range correlations for $T > M_s$ as well as beyond the Curie temperature of the austenitic state. We discuss magneto-structural phenomena in the various crystallographic states of these alloys in relation to the observed magnetic coupling.

Keywords: magnetic shape memory; polarization analysis; heusler alloys

Orbital Contribution to the Magnetic Moment in Co_2SiO_4. <u>Andrew Sazonov</u>[a,b], Vladimir Hutanu[a,b], Martin Meven[b], Gernot Heger[a]. *[a]Institut fuer Kristallographie, Rheinisch-Westfaelische Technische Hochschule (RWTH) Aachen, D-52066 Aachen, Germany. [b]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universitaet Muenchen (TUM), D-85747 Garching, Germany.*
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Synthetic Co_2SiO_4 has an orthorhombic crystal structure (space group *Pnma*, No. 62) and shows magnetic ordering below ~ 50 K. Both single-crystal and powder neutron diffraction were applied to determine precise crystal and magnetic structure parameters. Detailed symmetry analysis of the magnetic structure show that it corresponds to the Shubnikov magnetic group *Pnma* which allow the antiferromagnetic configuration (G_x,C_y,A_z) for 4*a* site with inversion symmetry $\bar{1}$ (Co1 position) and $(0,C_y,0)$ for 4*c* site with mirror symmetry *m* (Co2 position). The magnetic moments from the neutron diffraction data were found to be 3.86 ± 0.05 μ_B and 3.37 ± 0.04 μ_B for Co1 and Co2, respectively. An important orbital contribution to the total magnetic moment of Co^{2+} in Co_2SiO_4 was predicted by means of magnetic susceptibility and non-polarized neutron diffraction measurements. This prediction was independently proved by means of direct X-ray magnetic circular dichroism and polarized neutron diffraction studies which indicate a spin to orbital magnetic moment ratio $\mu_L / \mu_S \approx 0.25$. The results are in agreement with theoretical expectation of the spin-only value 3 μ_B for the Co^{2+} ion in the high spin state ($S = 3/2$, $t_{2g}^5 e_g^2$). Thus, the excess magnetic moment above 3 μ_B is caused by the orbital part. Spin-orbit coupling with this partially unquenched orbital moment in Co^{2+} is mainly responsible for the magnetocrystalline anisotropy in the cobalt olivine.

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Structural, Magnetic and Electric Properties of $GaFe_{1-x}Mn_xO_3$. <u>M.Bakr</u>[a], A. Senyshyn[a], H. Wang[a], G. Parzych[b], L.Dobrzynski[b,c], K.Szymański[c], H. Fuess[a].

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Gallium iron oxide ($GaFeO_3$) is a member of a multiferroic family which exhibits ferrimagnetic and piezoelectric properties below room temperature [1-2].This material has orthorhombic (double HCP Closed-Pack) crystal structure with space group $P c 2_1 n$ with four different cation sites labeled Ga1, Ga2 (mostly occupied by gallium) and Fe1, Fe2 (mostly occupied by iron) [3-5]. The different physical properties of $GaFeO_3$ are strongly dependent on the distribution of cations within the structure. The magnetic properties of $GaFeO_3$ strongly depend on the preparation method which affects the cations distributed over different sites. Polycrystalline $GaFe_{1-x}Mn_xO_3$ materials have been prepared by a traditional solid state reaction (SR) and sol-gel (SG) methods. Structural analyses showed that the maximum Mn content is 10% and 50% for samples prepared by SR and SG, respectively. All samples crystallise in the orthorhombic system with $P c 2_1 n$ space-group. The Curie temperature (T_C) for $GaFeO_3$ (SR) is about 190K and increases or reaches room temperature when the temperature of preparation is decreased from 1400°C to 700°C. The Curie temperature for SG reaction is slightly above room temperature. With increasing the Mn content the transition temperatures as well as the coercive field decrease. Dielectric investigations revealed a temperature independent anomaly at around 255 K with frequency dispersion of dielectric constant only for $GaFeO_3$ prepared at 700°C (SG) and Mn doped samples prepared by both methods. It follows from the neutron powder diffraction and Mössbauer spectroscopy revealed that $GaFeO_3$ exhibits a ferrimagnetic order with spins parallel to c-axis. Both, the cation and magnetic, orderings depend strongly on the preparation conditions.

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Keywords: multiferroics; magnetic; dielectric

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Neutron Diffraction Study of $DyVO_3$ and $HoVO_3$. <u>Manfred Reehuis</u>[a], Clemens Ulrich[b], Jun Fujioka[c], Shigoki Miyasaka[c], Yoshinori Tokura[c], Bernhard

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Vanadates with the formula RVO_3 (R = Y or rare-earth element) exhibit many exciting properties, which can be related to orbital or spin rearrangements [1], [2]. In order to provide a more complete basis for the theoretical description of the electronic properties of these compounds we have started to carry out a comprehensive investigation of the crystal and magnetic structures of YVO_3, $NdVO_3$ and $TbVO_3$ [3], [4]. In the room-temperature lattice structure the influence of the relative ionic sizes leads to tilts of the VO_6-octahedra. From La^{3+} to Lu^{3+} the distortions show a continuous increase due to the well-known lanthanide contraction. With decreasing temperature the vanadates show a structural phase transition at T_{S1}, where the orthorhombic structure (*Pbnm*) changes to a monoclinic structure with the space group $P2_1/b$ due to the onset of the cooperative *Jahn-Teller* effect and the onset of orbital ordering. In the monoclinic phase the magnetic moments of the V^{3+}-ions show antiferromagnetic ordering with the modes C_x, C_y and G_z, where the z-component is the weakest. A second structural phase transition (T_{S2}) could be observed for vanadates containing smaller R^{3+}-ions (R^{3+} = Y^{3+}, Ho^{3+} − Lu^{3+}) [1]. Below T_{S2} the crystal structure changes back to the orthorhombic structure and the vanadium moments are purely G-type ordered along z [3], [4]. In $DyVO_3$, where the R^{3+}-ion is slightly larger than Ho^{3+}, a critical phase competition between different spin-orbital-ordered states was observed only recently [5]. Our neutron diffraction experiments of $DyVO_3$ showed that the transition to the pure G-type ordering sets in at T_{S2} = 63(1) K. For YVO_3, where Y^{3+} is only slightly smaller than Dy^{3+}, this transition sets in at considerably higher temperature T_{S2} = 77(1) K. As found earlier for YVO_3 the G-type ordering in $DyVO_3$ remains stable upon cooling from T_{S2} down to 6 K. But with increasing temperature the monoclinic C-type phase surprisingly appears in $DyVO_3$ between 13 and 23 K. For $HoVO_3$ this intermediate phase could not be observed. On the other hand the second phase transition of this vanadate sets in (cooling process) at the strongly reduced temperature T_{S2} = 26(1). With increasing temperature it sets in at the higher value T_{S2} = 36(1) K, indicating the presence of strong hysteresis effects. Further it is important to note that both the magnetic moments of the Dy^{3+}- and Ho^{3+}-ions show a long-range ferrimagnetic order up to the unusually high temperatures 23(1) K and 36(1) K, respectively. Our study clearly showed that strong exchange interactions between the magnetically ordered V-moments and the magnetic Dy^{3+}- and Ho^{3+}-ions lead to a reduction of the transition temperature T_{S2} as well as to an increasing of the magnetic ordering temperature of the R^{3+}-ions.

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