MS25-P2 Magnetic order and crystal structure of FeOCl described in superspace

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The metal(III) oxyhalide FeOCl crystalizes at room temperature in orthorhombic space group symmetry Pmmn. The structure is built by slabs consisting of Fe2O2 bilayers enclosed by layers of Cl atoms; the interaction between the slabs is of van der Waals type [1,2]. An antiferromagnetic phase transition was first observed by means of Mössbauer spectroscopy [3] and then confirmed by other techniques [4–6] while the reported values for TN are in the range of 80 – 92 K. Two different models for the magnetic superstructure are proposed, an incommensurate cycloïdal one [4] and a commensurate spiral one [6]. Both models are based on orthorhombic symmetry.

We have performed low-temperature neutron powder diffraction experiments at instrument SPODI (FRM2, Garching, Germany) and low-temperature single crystal X-ray diffraction at beamline D3 (Hasylab/DESY, Hamburg, Germany) to explore and describe the magnetic and nuclear superstructures.

The analysis of our experiments shows that the magnetic phase transition occurs at TN = 82.0(2) K and is of second order, that the magnetic and structural modulation wave vector varies in an intermediate temperature range with temperature and that this transition is accompanied by the development of a monoclinic lattice distortion at low temperatures [5], indicating a strong magnetoelastic coupling. Those findings have been also reported for the other MOCl compounds VOCl and CrOCl [7,8]. In our contribution we will propose models for the magnetic and nuclear structures applying magnetic superspacegroup symmetry [9,10]

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MS25-P3 Occupation disorder in $Mn_2Co_{1-x}Rh_xSn$ compounds

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The structure of Mn_2CoSn is the Heusler cubic lattice A_2BC. Since Mn is more electropositive than Co, the basic structure of this compound is inverted, i.e. the Mn ions occur in both fcc lattices mutually shifted by one fourth of the body diagonal. We have investigated a series of $Mn_2Co_{1-x}Rh_xSn$ polycrystalline samples by powder diffraction using CoK_α and CuK_α lines, and by EXAFS. From powder diffraction it follows that the structure undergoes a tetragonal distortion at approx. x=0.3. Several types of the occupation disorder in Heusler alloys exist in the literature; however some types can be excluded a-priori due to the absence of specific peaks in the powder diffraction patterns. We have determined the disorder type by fitting of the integrated diffraction intensities and of the EXAFS data to particular disorder models. The comparison of the measured and simulated EXAFS spectra demonstrated that the occupational disorder is a necessary feature, which must be considered in the analysis of EXAFS data, otherwise the fitting results are not physically feasible.

Keywords: Heusler alloys, occupation disorder, x-ray diffraction, EXAFS