Abstract

English title: Verification of the crystal lattice and magnetic symmetry of selected materials

Diffraction studies of the crystal structure of selected M_2O_3 oxides (with trigonal corundum-type structure), MO_2 oxides (with tetragonal rutile-type structure) and chromium metal (with cubic bcc-type structure) were performed. The motivation for such studies was based on the disagreement between the symmetry of the observed magnetic phenomena and the symmetry assigned to the crystal structure. In α-Fe_2O_3 the antiferromagnetic ordering of Fe^{3+} magnetic moments with weak ferromagnetic contributions is forbidden in trigonal symmetry. For β-MnO_2 the observed helical type modulated magnetic ordering of Mn^{4+} magnetic moments is also forbidden in tetragonal symmetry. The spin density wave ordering observed in chromium is not permitted in cubic symmetry.

Experimental studies of the aforementioned materials together with some other oxides, e.g. Cr_2O_3, V_2O_3, Al_2O_3, Ti_2O_3, β-PbO_2, were done by using X-ray diffraction, synchrotron radiation diffraction and thermal neutron scattering. Measurements were perofrmed at different temperatures, both below and above the Néel temperature. Synchrotron radiation diffraction studies were done by using beamlines at ALBA-CELLS in Barcelona, the European Synchrotron Radiation Facility in Grenoble and the Diamond Light Source in Chilton near Oxford. Neutron diffraction studies were performed at the reactor sources in Helmholtz-Zentrum Berlin and the Institut Laue Langevin in Grenoble as well as the spallation neutron source ISIS in Chilton near Oxford. The description of non-modulated and modulated magnetic structures was done by using the formalism of magnetic space groups and superspace groups, respectively. The expression superspace groups is related to a four dimensional description of a three dimensional lattice with the modulation phase assigned to the coordinate along the fourth dimension.

A set of precise diffraction experiments together with non-standard analysis procedures provided information about the lattice parameters of the materials under study. The analysis based on the magnetic space groups and magnetic superspace groups provided a unified description with one common symmetry group for both magnetic phenomena and the crystal structure. For corundum-

type M_2O_3 oxides and for chromium the optimal symmetry is monoclinic, while for rutile-type MnX_2 compounds the optimal symmetry is orthorhombic.