Magnetic Circular Dichroism effects in the Resonant Inelastic Xray Scattering at the K (pre) edge of 3d transition metal ions: an outlook

<u>A. Juhin,^{1,2} F. M. F. de Groot,¹ Ch. Brouder,² Ph. Sainctavit,² P. Glatzel³</u>

¹ Debye Institute for Nanomaterials Science, Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan 16, 3584 CA Utrecht, The Netherlands

² Institut de Minéralogie et de Physique des Milieux Condensés, UMR 7590, Universités Paris 6, 7 et IPGP. 140 rue de Lourmel 75015 Paris, France

³ European Synchrotron Radiation Facility, 6 rue Jules Horowitz, BP220, 38043 Grenoble Cedex 9, France

Transition metal elements play an essential role in physics (magnetic materials, superconductors), chemistry (catalysis) and geophysics (3d elements are major constituents of the Earth and planets). Properties such as magnetism, catalytic activity and optical absorption are governed by the 3d orbitals, which can be probed by X-ray spectroscopies at the K pre-edge ($1s \rightarrow 3d + 4p$ transitions), such as X-ray Natural Linear Dichroism, Resonant Inelastic X-ray Scattering and X-ray Magnetic Circular Dichroism. Compared with the L_{2,3} edges ($2p \rightarrow 3d$ transitions), the smaller interaction between the core-hole and the 3d orbitals enables to make a more direct connection to the ground state properties. However, XMCD effects are very small, due to the absence of spin-orbit coupling in 1s core-hole. This drawback has so far hampered the interpretation of XMCD at the K-edge.

Here, I will present results obtained on Cr-containing oxides with K pre-edge spectroscopies performed at ID26 beamline. The XNLD has been recorded on a single crystal of MgAl₂O₄:Cr^{3+,} and a theoretical approach combining monoelectronic and multielectronic methods has enabled us to fully interpret the dichroic signature of Cr³⁺. Crystal field excitations (*3d-3d* transitions) have been measured with RIXS on MgCr₂O₄, with an energy resolution of 0.6 eV.

Finally, our project to couple XMCD and RIXS spectroscopies at the K edge of 3d ions will be discussed. Preliminary calculations performed on CoO in the multiplet approach show that large XMCD effects are visible, both in the 1s3p RIXS (K β fluorescence) and also directly in the pre-edge structure when measured with a high-resolution fluorescence detector. These theoretical simulations suggest that RIXS-MCD could be used in the future to measure magnetic polarization of the 3d orbitals, with bulk sensitivity, high energy resolution, and the possibility to study samples in demanding environments such as high-pressure cells.