Resonant Inelastic X-ray Scattering of transition metal oxides

Frank de Groot*[1]

[1]Debye Institute of Nanomaterials Science, Utrecht University, Netherlands

An overview is given of RIXS of transition metal oxides, including soft x-ray 2p3d RIXS and hard x-ray 1s2p and 1s3p RIXS spectra [1, 2]. Within a band model, 1s2p RIXS can be described as the convolution of the 1s x-ray absorption spectrum with the 1s2p x-ray emission spectrum, corrected for broadening effects. If the experimental 1s2p RIXS plane can be simulated as such, it does not contain any additional information. However the details of the convolution depend on both the Lorentzian and Gaussian broadenings and to determine those reliably the 2D RIXS plane is necessary to decrease the uncertainties of the fit. Our intention is to develop a 'RIXS plane tester' that generates the 2D plane from the 1s XAS and 1s2p XES spectra, which then can be compared with the experimental data. In the second part of the talk some recent examples of RIXS experiments will be shown. In 2p3d RIXS one scans through the 2p XAS edge and measures the optical excitation range. As an example, the RIXS spectra of CoO will be discussed. The experimental resolution of 100 meV allows the detailed observation of the electronic structure. Applying 2p3d RIXS to a mixed valence system under working conditions allows the detection of the optical spectrum of, for example, 1% Co^{2+} sites in a dominant Co^{3+} material. As example we analyse 2p3d RIXS of Co_3O_4 and compare it with a tetrahedral Co^{2+} system and an octahedral low-spin Co^{3+} system. In hard x-ray 1s2p RIXS we sow new RIXS-MCD data on CrO_2, which nicely shows the large MCD signal in the quadrupole peak and a much reduced MCD signal in the non-local peak. This analysis also shows that the pre-edge structure in normal 1s XAS spectrum of CrO_2 is related almost completely to the non-local peak.

References

[1] Core Level Spectroscopy of Solids, Frank de Groot and Akio Kotani (Taylor & Francis CRC press, 2008)

[2] Download the x-ray spectroscopy simulation software at http://www.anorg.chem.uu.nl/CTM4XAS/

*Corresponding author: f.m.f.degroot@uu.nl