

X-RAY ABSORPTION AND EMISSION SPECTROSCOPY OF RARE-EARTH MATERIALS

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Hard X-ray absorption spectroscopy (XAS) is a widely used technique at synchrotron radiation sources for analyses of the electronic structure of materials. There are several methods for measuring the variation of the absorption coefficient as a function of photon energy. Figure 1a shows schematically the experimental setup for XAS in transmission mode and medium energy

resolution fluorescence mode (using an energy dispersive X-ray detector). In conventional XAS experiments the large core-hole lifetime broadening, which is around 4 eV for rare earths L₃ edges give rise to broad spectral features. A spectral narrowing below the natural core-hole lifetime width can be achieved by employing an X-ray emission spectrometer [1] (cf. Fig. 1b).

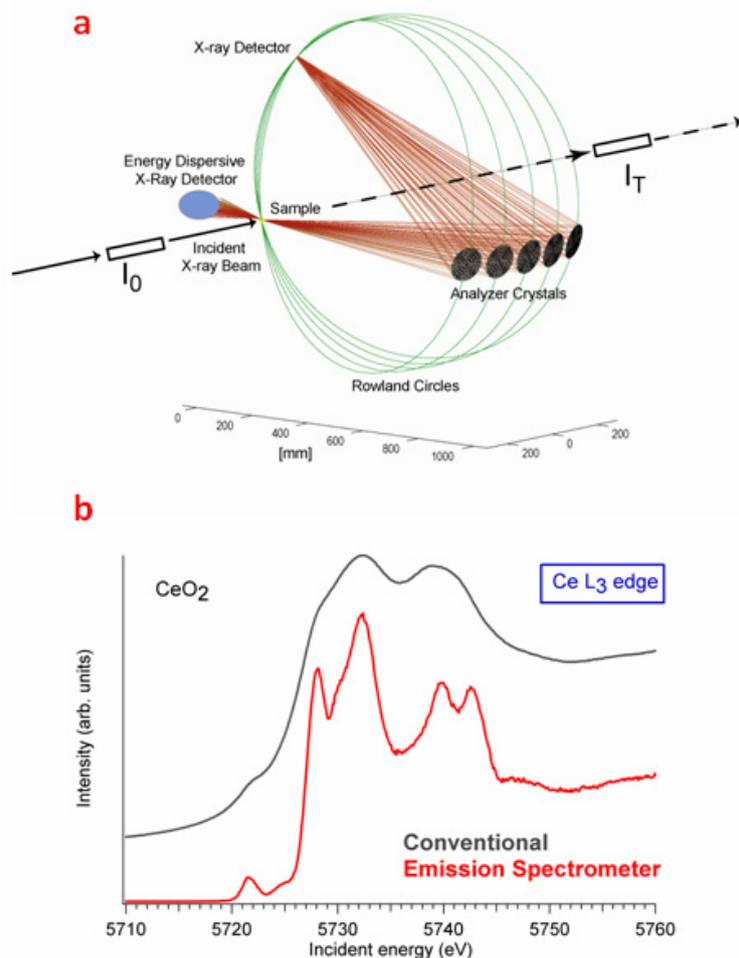


Figure 1. a) Schematic experimental setup for XAS in transmission (I_T), medium (energy dispersive X-ray detector) and high energy resolution fluorescence detection mode; b) standard (grey) and high energy resolution XAS (red) of CeO_2 at the Ce L₃ edge.

Figure 1a shows a schematic drawing of the X-ray emission spectrometer with five spherically bent crystal analyzers installed at beamline ID26 of the European Synchrotron Radiation Facilities (ESRF) in Grenoble. This contribution will provide an overview of the possible spectroscopic techniques, such as resonant inelastic X-ray scattering (RIXS) and high-energy-resolution fluorescence detected (HERFD) absorption spectroscopy [2] that become available using such an experimental setup.

We have studied the electronic structure of cerium, ytterbium and uranium systems in different oxidation states by means of HERFD and RIXS. In case of the latter we observed transitions between core levels as well as valence band excitations. The experimental spectral features were characterised using a variety of theoretical codes including the LDA+*U* approximation within DFT [3], atomic multiplet theory [4] and full multiple scattering FEFF [5]. We found that the experimental results for valence band RIXS in some cases can be modelled using a surprisingly simple theoretical model that uses the ground state electron density. We furthermore show how valence band RIXS can be used to

assess the effect of the core hole in inner-shell spectroscopy. We demonstrate that RIXS can provide important information for applied, environmental and fundamental science.

References

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