

Ab initio simulation of Surface Resonant X-ray Diffraction

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The variation with energy of the diffracted peak intensities around the absorption edges has been known for a very long time. The correspondent resonant elastic x-ray scattering (REXS) spectroscopy is today well established to study all kind of materials. *Ab initio* simulations are also realized for more than 10 years and have given many results for example regarding charge, orbital and spin-ordering in oxides. More recently, experiments performed on surfaces, for example in electrochemical environment,⁽¹⁾ or on thin films, have shown interesting dependence versus sample parameters such as film-thickness, or temperature, or beam polarization states. In this surface science context, simulations can bring new pieces of information to understand the data and extract quantitatively sample parameters and properties. For this purpose, we have developed the *ab initio* simulation of Surface Resonant X-ray Diffraction (SRXRD) inside the FDMNES project^(2,3).

After the necessary recalls (or calls...) on Surface X-ray Diffraction and the connection with reflectivity, the main ingredients for the calculation of SRXRD will be given. The relation between bulk and surface diffractions and between resonant scattering and x-ray absorption near edge structure (XANES) will be the track to understand the specificity and the sensitivity of SRXRD. At this stage, our approach is DFT, and we use both the multiple scattering theory and the Finite Difference Method to calculate the electronic structure probed by the photo-electron. We also go to understand why the building of a virtual diffraction set-up allowing the definition of operating modes, as in the “real” spectrometers is necessary, to confidently calculate first, the intensity emerging perpendicularly to the surface between the bulk diffraction peaks, the so-called crystal truncation rods allowed thanks to the surface, and second, the spectra at different points on these ones.

Examples of use concerning the study of a very-thin film of magnetite on silver and of halide-metal interaction at an electrochemical interface will be given.

(1) Y. Grunder, P. Thompson, A. Brownrigg, M. Darlington, and C. A. Lucas, *J. Phys. Chem. C*, **116**, 6283 (2012)

(2) www.neel.cnrs.fr/fdmnes

(3) Y. Joly *et al.* *J. Chem. Theory Comput.* (2017), DOI: 10.1021/acs.jctc.7b01032