Simulating the energy-loss near edge structure for interferometric EELS in reciprocal space

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Numerical simulations are an integral part of analysing experimental electron energy loss spectrometry (EELS) data as well as for the fundamental understanding of it. Especially the energy-loss near edge structure (ELNES) – which can be exploited, for example, to determine the environment of particular atoms – requires extensive calculations. One commonly employed technique to simulate such ELNES is density functional theory (DFT).

Since the advent of field-emission guns (FEG) with their improved coherence properties, a new aspect has to be considered in EELS, however: interferometry. Due to the strong elastic scattering of the probe beam in the sample, it has to take into account multiple coherently diffracted beams as well. In addition, it is insufficient for EELS to only consider diffraction for the incident beam. After the inelastic interaction, the outgoing beam is again subject to elastic scattering. The final intensity measured at the detector is thus determined by the interference of dynamically diffracted beams both before and after the inelastic scattering event [1].

Thus far, most commonly available programs have only treated one of the two aspects of elastic and inelastic scattering. For some experiments, both aspects are important, however. For example, in energy-loss magnetic chiral dichroism (EMCD), interferometry is exploited to measure differences between the majority and minority spin populations in a magnetic material, leading to characteristic differences in the L₂ and L₃ EELS edges [2]. The accurate, complete simulation of these effects inherently requires both elastic and inelastic effects. Similarly, the energy-loss by channelled electrons (ELCE) method uses the different excitation of Bloch waves to locate atoms, but also to distinguish different configurations and different environmental effects at different positions in the unit cell [3].

In this work, we present a freely available simulation software package that enables scientists to calculate interferometric ELNES based on the state of the art DFT software WIEN2k [4]. In our program, both the incident and outgoing waves are treated in a Bloch wave formalism to incorporate elastic scattering effects. The inelastic interaction is modelled using the mixed dynamic form factor (MDFF) [3]. Several models for the MDFF are available, ranging from a simple dipole model for fast calculations to an accurate model based on DFT data. In addition to calculating spectra, the program is also capable of producing thickness and tilt maps, to show the origin of certain contributions to the signal in the sample [1], and even to produce a whole data (hyper) cube.

The simulations shown in figs. 1 and 2 were performed using a primary beam energy of 200 keV and a sample tilted into a systematic-row condition. Fig. 1 shows that for the artificial case of no elastic scattering in a Si single crystal, the output of our software package is indeed in perfect agreement with that of Telnes.3 (which is part of WIEN2k). Fig. 2 shows a more realistic calculation of the EMCD effect of a (spin-polarized) Cobalt single crystal. For that simulation, full elastic scattering calculations were performed to accurately describe the interference terms that are the origin of the EMCD signal. It is evident that the results are in excellent agreement with previously published experimental data [5].
References

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Figure 1. Comparison of the simulated ELNES intensity before applying broadening using the Telnes.3 component of WIEN2k and our software package “bw” with suppressed elastic scattering.

Figure 2. Simulation (left) and measurement (right) of an EMCD experiment on a crystalline, 20 nm thick Co sample using a systematic row condition including the (1 0 0) diffraction spot. Life-time and spectrometer broadening are taken into account in the simulated data. The features in the range of approximately 790-795 eV in the simulated data stem from artefacts in the density of states produced by WIEN2k. Note that the experimental data is inherently superimposed on a background that is not reproduced by WIEN2k. The experimental data is taken from [5].