Estimation of detectability limits in EELS with Monte Carlo simulations

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Electron energy loss spectroscopy (EELS) is an effective method for studying the composition and electronic structure of materials in the transmission electron microscope (TEM) [1]. However, there has been very few Monte Carlo (MC) simulations of EELS spectra. This paper presents computation of EELS detection limits using MC simulations based on optical data models to generate EELS spectra [2]. The basic component of an optical data model is the optical oscillator strength (OOS), from which the energy loss function can be derived. In this work, the LEEPS code of Fernández-Varea *et al.* [2] was adapted to perform simulations of EELS spectra.

Huber et al [3] reported a decrease of edge to the background ratio for NiO as the specimen thicknesses (t) increases. For the MC simulation of NiO EELS spectra, the OOS of NiO was built by combining of optical data [4] and X-ray photoelectric cross section [5] (Fig. 1a). The consistency of obtained OOS was checked by means of Bethe sum rule. Several simulations for different specimen thicknesses at a beam energy (E_0) of 200 keV were performed as presented in Fig. 1.b. The probe illumination and collection angles used in the simulations were 9 and 18 mrad respectively, equal to the condition of experimental collected spectra. The jump ratio, the maximum (I_{max}) to minimum intensity (I_{min}) at ionization edge, was the quantity chosen to compare experimental data and simulation results. Generally, MC simulations reproduced the experimental data with acceptable accuracy (Fig 1.c). Discrepancies between the present simulation results and experiment are likely due to slight differences in the experiment and simulation conditions, combined with approximations underlying the OOS and the extrapolation of the Bethe surface.

We have also studied the effect of composition on the signal quality of ionization edges of Al-Cu alloy by MC simulation. The OOS for Al-Cu alloy was built using the OSSs of pure Al and copper and combining them based on Bragg's additivity rule. Simulated EELS spectra are presented in Fig. 2, for different compositions and sample thicknesses. The signal-to-noise ratio was defined as $SNR=(I_{max}-I_{min})/(2I_{min})^{1/2}$, where I_{max} and I_{min} are the intensities above and below the edge. Simulation results of the kind presented in Fig. 3 may help to select the sample thickness giving the best SNR. For the specimen at 100nm thickness with high concentration of Cu, SNR shows some decrease suggesting that for very thick specimens the detectability limit of heavier element in EELS spectra decreases.

References

[1] R . Egerton, Rep. Prog. Phys**.** **72** (2009) 016502.

[2] J M Fernández-Varea *et al*, Nucl. Instrum. and Meth. B **108** (1996) 35-50.

[3] Huber *et al*, "Relative Sensitivity of XEDS vs EELS in the AEM ", Late Breaking Poster, M&M 2010, Portland.

[4] Parmigiani *et al*, Solid State Communications **96** (1995) 161-165.

[5] C T Chantler *et al*, NIST Standard Reference Database 66, 2005.

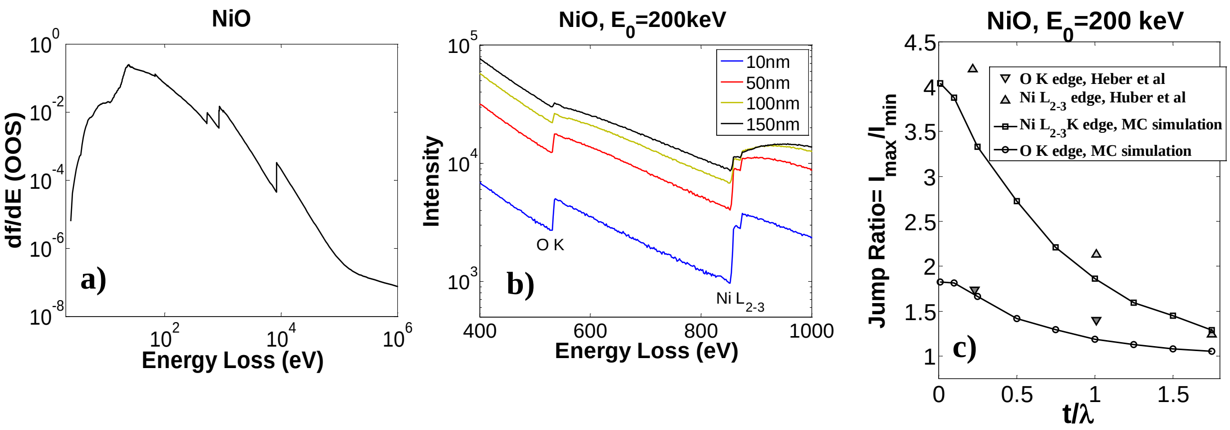

Figure [1] *a) Composite OOS for NiO resulting from a combination of dielectric data and photoelectric cross section b) Simulated EELS spectra for NiO at E_0=200 keV and different specimen thicknesses c) Comparison between jump ratios obtained from MC simulations and from the measurements of Huber et al [3].*

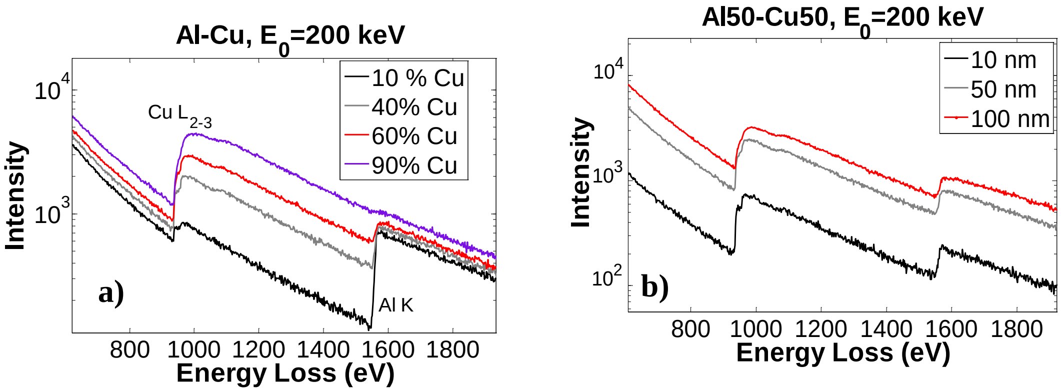

Figure [2] *a) Simulated EELS spectra by MC simulations for Al-Cu alloy at different compositions of Al and Cu b) Simulated EELS spectra for Al50-Cu50 alloy at different thicknesses. The probe illumination and collection solid angle were 5 and 10 mrad, respectively.*

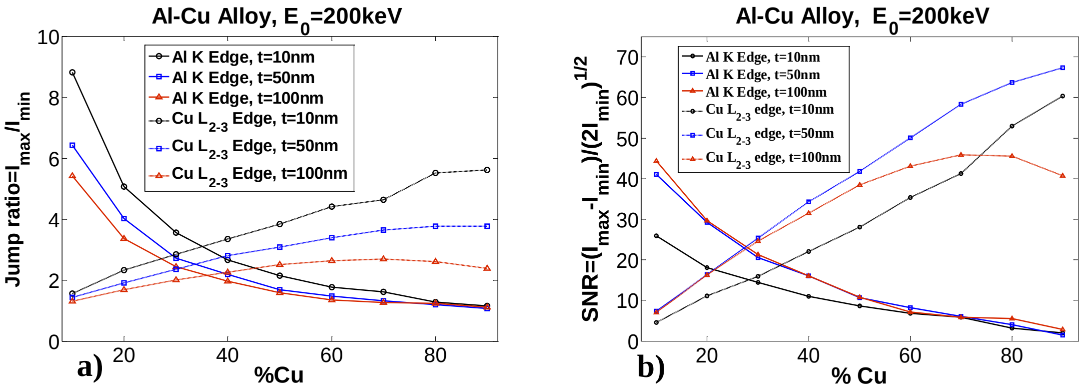

Figure [3] *a) Jump ratios and b) SNR for Al K edge and Cu $L_{2\text{-}3}$ edge for targets with different thicknesses and compositions*