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Fine Structure of Core Loss Excitations in EELS by Monte Carlo Simulation

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Electron energy loss spectroscopy (EELS) gives useful information about the electronic structure and composition of materials. The combination of optical data models for describing electron energy losses with Monte Carlo (MC) simulation provides a versatile method to improve the analysis of EELS spectra [1]. The optical oscillator strength (OOS) is the main input for the optical data models [1]. In this study OOSs were obtained by combining optical properties calculated from density functional theory (DFT) and X-ray photoelectric data. Figure 1a shows the calculated energy loss function of NiO performed by WIEN2k code [2]. NiO is a strongly correlated system; hence in the DFT calculation we used the new modified Becke-Johnson (mBJ) exchange potential [3] and the local density approximation (LDA) correlation potential [2]. In comparison with the generalized gradient approximation (GGA), the new exchange potential gives results in better agreement with experimental data. Figure 1b shows the calculated OOS obtained by a combination of data from our DFT calculation and X-ray photoelectric data [4], and applying Bethe sum rule.

Fine structure of core loss excitation in EELS gives valuable information about atomic bonds and their electronic structure. Using X-ray photoelectric data cannot provide enough resolution to study the effect of parameters of experimental EELS such as thickness and collection semi-angle on the fine structure of core loss excitations in MC simulations. Hence, the fine structure was included in the MC simulated EELS spectra through a new approach. The OOS was refined using the experimental EELS spectra. After background removal from experimental data [5] and applying a single scattering approach for thin specimen the OOS with fine structure was obtained. The obtained OOS can be normalized by comparison to the area under the edges from the OOS obtained from X-ray photoelectric data and thereafter it can be replaced in the original OOS presented in Figure 1b. The same approach was used for the simulated shape of edges obtained from DFT calculations; however in this case is not necessary to use the single scattering approach. As another approach, the height of added experimental edges was fixed equal to the height of edges obtained from the X-ray photoelectric data. The LEEPS code [6] was adapted to perform MC simulation of EELS spectra of NiO for different thicknesses. Generally, all these three methods predict the effect of thickness on the shape of core loss edges well by introduction of background signal as observed in Figure 2. Thus with the proposed approaches the fine structure of edges can be simulated through the refined OOS and using it for MC simulations.

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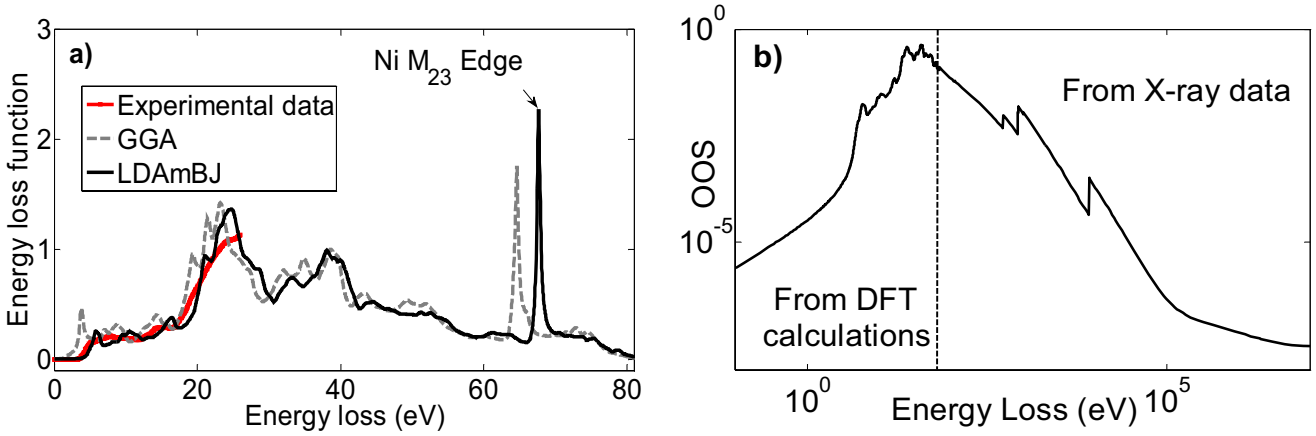

FIG.1. a) Comparison of the energy loss function, of NiO calculated using GGA and LDA with mBJ exchange-correlation potential with experimental data [7]. b) OOS of NiO calculated by combination of optical data calculated from DFT calculations and X-ray photoelectric cross section [4]. The dashed line indicates the 65eV.

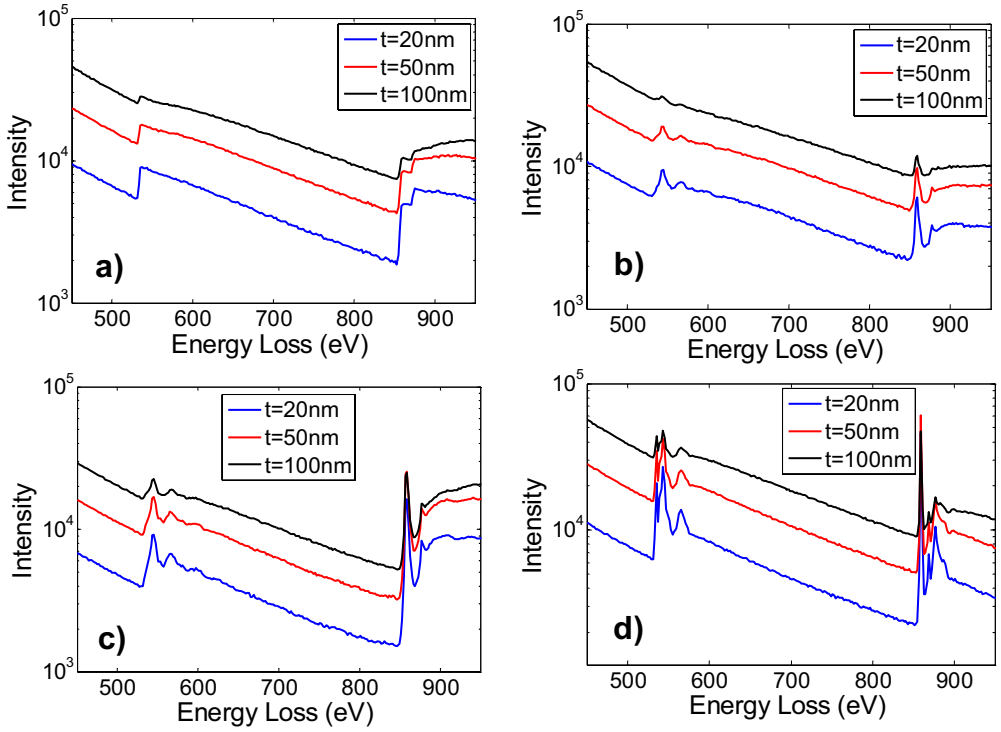

FIG. 2. Fine structure MC simulations of O K and Ni L_{2-3} edges using four methods: a) X-ray photoelectric data b) fixed height experimental data c) normalized experimental data d) normalized DFT simulation data for different thicknesses (t).

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