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Channeling Effects in High Angular Resolution Electron Spectroscopy

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Momentum-transfer resolved electron spectroscopy, a technique for examining the electronic structure of materials, requires the use of detectors accepting a small range of momentum transfers. High angular resolution electron channeling electron spectroscopy (HARECES), in which one measures the variation of a spectroscopic signal with illumination angle, is one such experimental technique [1]. When detectors with small acceptance angles are used in conjunction with crystalline specimens, it is necessary to consider the channeling behaviour of the fast electrons both before and after inelastic scattering to adequately describe the signals produced. Results from such an experiment, looking at the energy loss about the oxygen *K*-shell edge in NiO, are shown in Fig. 1.

Using oxygen *K*-shell core-loss in NiO as a case study, we examine channeling in HARECES, through both exploratory simulations and direct comparison with experimental data. The roles of the effective nonlocality of the ionization interaction [2], the channeling of both incident and scattered electrons (so-called double channeling), and the sample thickness will be described [3]. The thickness dependence of the energy-integrated cross section, which thus emphasizes the role of channeling, is shown in Fig. 2(a) for the double channeling model. The best comparison between the experimental data and the simulation is shown in Fig. 2(b), and the importance of the double channeling is evident.

Preliminary results of combining channeling simulations with a cluster calculation approach to calculating the energy loss fine structure [4] are shown in Fig. 3. Possible implications of the fast electron channeling on the fine structure recorded will be discussed.

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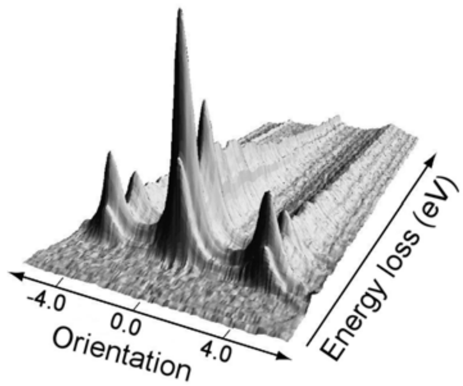

FIG. 1. Surface plot of the orientation dependence (in units of Bragg angles) of the oxygen K-shell energy loss fine structure from NiO along the <200> systematic row. The incident beam energy was 200 keV. The detector semi-angle was 0.2 mrad. The tilt step size was 0.25 mrad.

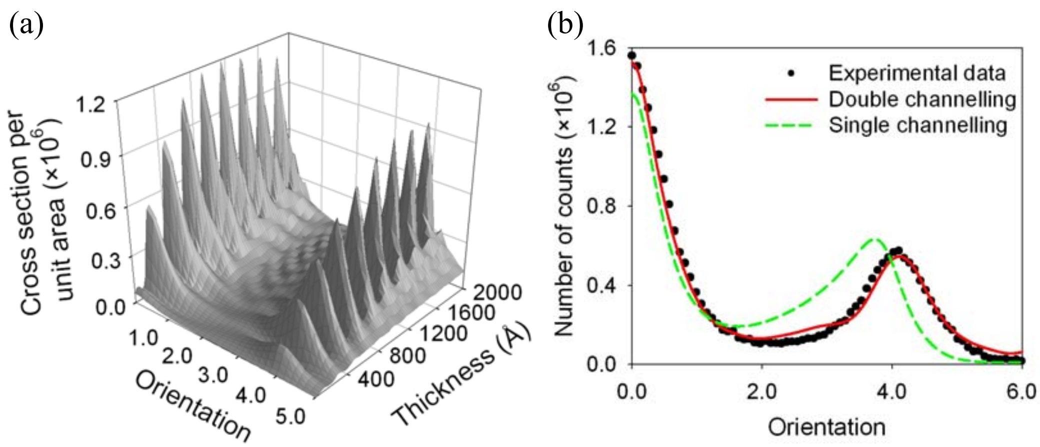

FIG. 2. (a) Double channeling simulation of the orientation dependence of the integrated energy loss spectrum (100 eV window above threshold) as a function of thickness. (b) Best comparison with theory, obtained assuming a wedge-like crystal varying in thickness between 450 Å and 570 Å.

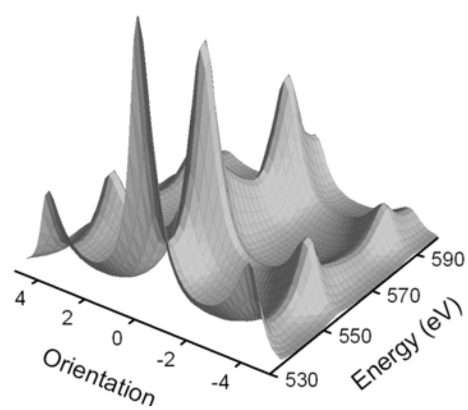

FIG. 3. Preliminary simulation of the full NiO HARECES data set accounting for the electron channeling.

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