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The Effects of Dynamical Electron Scattering on Electron Energy-Loss Near-Edge Structure

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Aberration correction has allowed routine imaging of complex materials systems at near Ångstrom resolution or better in the scanning transmission electron microscope (STEM). Improved instrumentation and stability has also permitted routine atomic-resolution electron energy-loss spectroscopy (EELS) providing both chemical mapping and information about local electronic states via the core-loss near edge structure. However, while instrumentation has advanced rapidly, the theoretical tools required for quantitative interpretation of atomic resolution energy loss near edge structure (ELNES) have lagged somewhat behind.

Density functional theory (DFT) calculations of ELNES are usually based on X-ray absorption codes, and at best assume plane wave incidence (1). Simulation of STEM EELS images, based on dynamical scattering theory, have correctly accounted for the evolution of the incident electrons through the specimen but isolated atomic models have described core-shell ionization (2). While useful for chemical mapping, such calculations contain no information about local empty states in the crystal, and hence no ELNES information. We have recently presented a formulation that combines DFT with dynamical scattering theory, providing a robust theoretical framework within which to examine the electronic structure of complex materials (3).

This presentation will examine probe position dependent ELNES, both from equivalent atomic positions and the mixing of spectra from atoms in different local electronic environments. In addition, the effects of dynamical diffraction on ELNES as a function of probe size will be discussed.

1. Buczko R, Duscher G, Pennycook S, Pantelides S. Physical review letters. 2000;85(10):2168.
2. Allen LJ, Findlay SD, Oxley MP, Rossouw C. Ultramicroscopy. 2003;96(1):47-64.
3. Prange MP, Oxley MP, Varela M, Pennycook SJ, Pantelides ST Physical Review Letters. 2012;109(24).
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