Type of presentation: Poster

IT-5-P-2735 Quantitative Position-Averaged Core-Loss Scattering in STEM

Zhu Y.[1], Dwyer C.[2]

[1]Monash Centre for Electron Microscopy (MCEM) and Department of Materials Engineering, Monash University, VIC 3800, Australia, [2]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, and Peter Grunberg Institute, Forschungszentrum Julich, D-52425 Julich, Germany

Email of the presenting author: ye.zhu@monash.edu

With the rapid development in core-loss spectroscopic mapping in the scanning transmission electron microscope (STEM), it raises the need for the quantitative interpretation of core-loss intensity and map contrast. However, a quantitative interpretation of atomic-resolution chemical maps is not straightforward due to the dynamical scattering of the electron probe. The effect of dynamical scattering on core-loss maps bears similarities to its effect on annular-dark-field (ADF) images. Dynamical-scattering calculations are thus required to interpret both the core-loss map and ADF image intensities on a quantitative level.

Based on recent progresses on quantitative STEM imaging and inelastic multislice simulations, we have performed a quantitative comparison between experimental position-averaged core-loss scattering from *K*-, *L*- and *M*-shells of various elements and simulations based on a single-particle description of the core-loss process. The materials we studied include single-crystal Si, LaB_6, $SrTiO_3$, and $LaAlO_3$. To facilitate a direct comparison free of adjustable or compensating parameters, we compare absolute scattering cross-sections for zone-axis-aligned crystals whose thicknesses have been measured independently using convergent electron beam diffraction (CBED). Our study of the position-averaged scattering avoids the complexity and any errors associated with evaluating the effects of aberrations and source size. Experimental results are compared with simulations that include an accurate description of multiple elastic and thermal-diffuse scattering both prior and subsequent to the core-loss events (double-channelling). In order to exclude any pronounced solid-state effects, which are not included in our simulations, we have considered discrete-continuum transitions that are at least 30 eV above edge onsets. The results show that the double-channelling simulations based on a single-particle model quantitatively predict the position-averaged scattering from *K*-shells, as well as that from *L*-shells in some cases (Si-$L_{2,3}$). On the other hand, limitations of the single-particle picture are clearly revealed by the discrepancies in the case of M-shells (La-$M_{4,5}$). Our results represent a critical step towards quantitatively predicting the absolute intensity and contrast in core-loss chemical maps with nano- or even atomic-resolution.

Acknowledgement: This work was supported by the Australian Research Council (ARC) grant DP110104734. The FEI Titan at Monash Centre for Electron Microscopy was funded by the ARC Grant LE0454166.

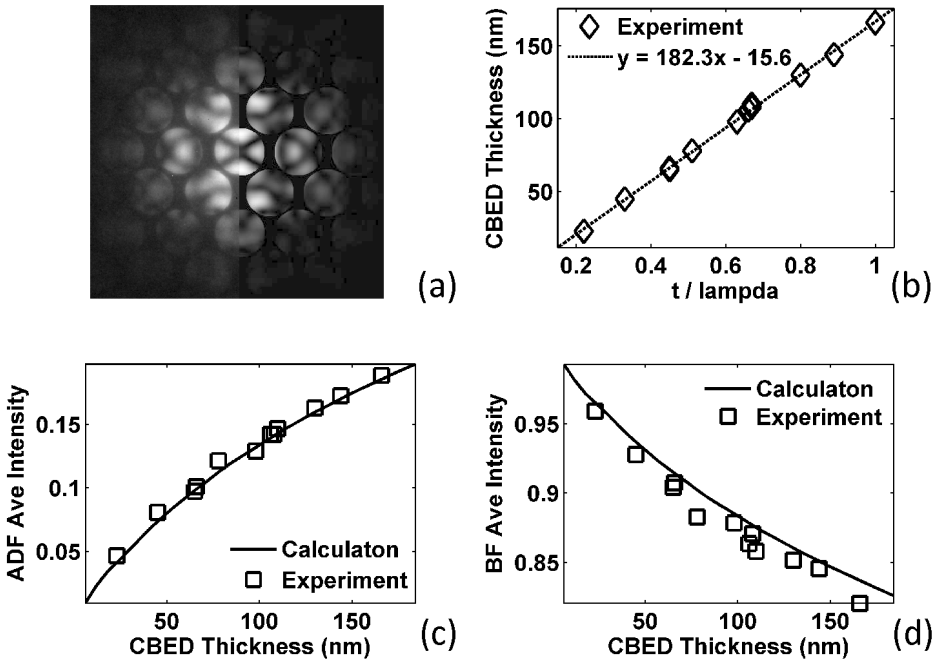

Fig. 1: (a) Experimental (left) and Bloch-wave simulated (right) PA-CBED pattern from 108 nm [110] Si. (b) PA-CBED determined thickness versus t/λ on [110] Si. (c-d) Experimental and simulated (c) ADF and (d) BF average intensities as a function of PA-CBED determined thickness on [110] Si.

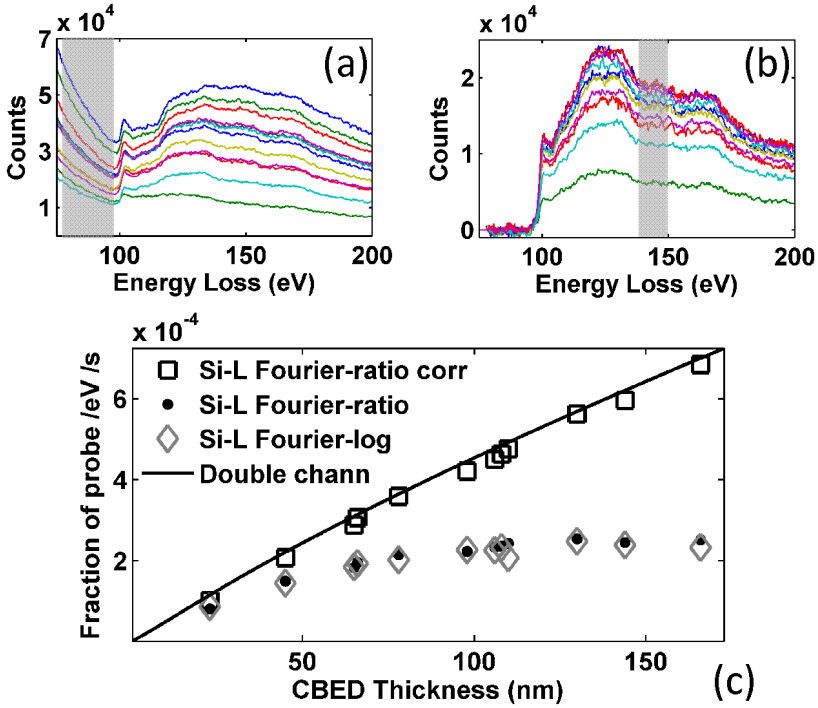

Fig. 2: (a) Raw EEL spectra showing Si-L edge at different thickness. (b) Background-subtracted Si-L2,3 edge. The average intensity in the region highlighted in gray was compared to simulation. (c) Experimental (scattered) and simulated double-channelling (line) Si-L2,3 edge intensity at 45 eV above the edge onset.