Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

STEM-EELS calculations including both fine structure and diffraction[1] M.P. PRANGE, M.P. OXLEY, Vanderbilt University, S.J. PENNYCOOK, Oak Ridge National Lab, S.T. PANTELIDES, Vanderbilt University —
Electron energy loss spectroscopy in scanning transmission electron microscopy (STEM-EELS) probes electronic excitations with high spatial and energy resolution. Interpretation of the spectra requires accurate treatment of both the diffraction of the electron probe and the electronic excitation of the sample. We present a theory of core loss STEM-EELS based on a detailed calculation of the mixed dynamic form factor (MDFF) using DFT which informs a Bloch wave treatment of the probe/sample interaction. No dipole approximation is made. The probe diffraction is computed using the Bloch wave method which includes the microscope geometry, multiple elastic, and thermal diffuse scattering. We illustrate the method with calculations of complex oxide materials.

[1]This work was supported by DOE grant DE-FG02-09ER46554 (M.P., M.P.O., S.T.P.) and by DOE BES Mater. Sci. and Eng. Div. (S.J.P.).

M.P. Prange
Vanderbilt University

Date submitted: 28 Dec 2010 Electronic form version 1.4