Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Simulation of electron-energy-loss spectra including both diffraction and solid-state effects[1] MICAH PRANGE, MARK OXLEY, Vanderbilt University and ORNL, MARIA VARELA, ORNL, STEPHEN PENNYCOOK, ORNL and Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University and ORNL — Aberration-corrected scanning transmission electron microscopes yield probe-position-dependent electron-energy-loss spectra (EELS) that can potentially provide spatial mapping of the underlying electronic states. EELS calculations, however, typically describe excitations by a plane wave travelling in vacuum, neglecting diffraction and interference effects. Here we report the development and initial application of a methodology that combines a full electronic-structure calculation with beam propagation in a thin film. The simulations are based on PAW plane-wave calculations of the excitation spectrum of the material and Bloch wave simulations of the probe propagation.

[1]This work was supported in part by DOE grant no. DE-FG02-09R46554 (MPP, MPO, STP), by the DOE Basic Energy Sciences (SJP,MV,STP) and by the McMinn Endowment at Vanderbilt University (STP).

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Date submitted: 11 Nov 2011 Electronic form version 1.4