Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First-Principles Modeling of Low-Energy Electron Diffraction of Few Layer Graphene[1] JOHN MCCLAIN, University of New Hampshire, JIEBING SUN, Michigan State University, JAMES HANNON, IBM Thomas J Watson Research Center, KARSTEN POHL, JIAN-MING TANG, University of New Hampshire — We present calculations of the low-energy electron microscopy (LEEM) spectra of few layer graphene (FLG) systems using our newly developed theoretical approach based on density-functional theory (DFT). The traditional analysis using multiple scattering off muffin-tin potentials is replaced with a Bloch wave matching approach using self-consistent potentials via DFT to better describe the LEEM spectra, especially in the low energy range. Our calculated results for free-standing FLG exhibit oscillations in reflectivity for energies between 0 and 7 eV, in good agreement with the experimental LEEM spectra of FLG observed on various substrates. The number of oscillations is correlated to the number of graphene layers, a fact often used to determine the number of graphene layers in a sample region. We have calculated FLG on Ni(111)-(1x1) and find that the FLG features dominate those of the bare Ni(111) when two graphene layers are added, as seen in experiments. Our results show that the valleys in the LEEM spectra due to graphene appear only with more than one graphene layer, consistent with our results for free-standing FLG.

[1]We acknowledge funding support from NSF DMR-1006863.

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Date submitted: 09 Nov 2012 Electronic form version 1.4