Abstract Submitted
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First-Principles Calculations of Off-Normal LEEM Reflectivity Spectra of Few Layer Graphene[1] JOHN MCCLAIN, Integrated Applied Mathematics, University of New Hampshire, KARSTEN POHL, JIAN-MING TANG, Department of Physics and Materials Science Program, University of New Hampshire — We present calculations of the off-normal low-energy electron specular reflectivity spectra of few layer graphene (FLG) systems using our first-principles theoretical approach that leverages the self-consistent scattering potentials produced by density-functional theory [1]. Our Bloch wave matching approach, which replaces the traditional analysis using multiple scattering off muffin-tin potentials, admits a straightforward handling of non-normal incident beams. Our calculated off-normal spectra for free-standing FLG reveal the shifting of the characteristic thickness-dependent oscillations in reflectivity found for energies between 0 and 7 eV in normal-incidence low-energy electron microscopy (LEEM) spectra. We also find shifts in other peaks and new features for incoming beams with in-plane momentum far from Γ. We compare the spectra to features in the in-plane band structure of FLG and to available experimental LEEM and LEED data for FLG on metallic and semiconductor substrates. We discuss modeling reflection for small deviations from normal incidence, as well as the possibility of accessing novel spectra features using wide-angle scattering. [1] McClain et al., arXiv.1311.2917.

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