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Low-Energy Electron Reflectivity of Two-dimensional Materials

QIN GAO, PATRICK MENDE, NISHTHA SRIVASTAVA, MICHAEL WIDOM, RANDALL FEENSTRA, Carnegie Mellon University — Based on density functional theory, we develop a self-consistent description of low-energy electron reflectivity spectra of both free-standing thin films and thin films on substrates. Our approach utilizes wavefunctions for a thin multilayer slab together with wavefunctions of bulk substrate, if any [1, 2]. Our results compare well with experimental data for graphene on SiC and on various metallic substrates. From our modelling, we find that the minima of reflectivity arise from states with wavefunctions localized *between* the graphene layers, rather than on the layers as previously suggested [3]. The energies of the reflectivity minima are sensitive to the layer spacing between graphene and substrate; thus our method also provides a way to determine the layer spacing by comparing with the experimental reflectivity curve. A simple method is also proposed for inclusion of inelastic effects (electron absorption) in the computed reflectivity spectra, and is applied to graphene and hexagonal boron nitride (h-BN) on various substrates [4].

- [1] R. M. Feenstra, N. Srivastava, Q. Gao, M. Widom, G. Diaconescu, T. Ohta, G. L. Kellogg, J. T. Robinson and I. V. Vlassiuk, Phys. Rev. B 87, 041406(R) (2013).
[2] N. Srivastava, Q. Gao, M. Widom, R. M. Feenstra, S. Nie, K. F. McCarty and I. V. Vlassiuk, Phys. Rev. B 87, 245414 (2013). [3] H. Hibino, H. Kageshima, F. Maeda, M. Nagase, Y. Kobayashi, and H. Yamaguchi, Phys. Rev. B 77, 075413 (2008). [4] Q. Gao, P. C. Mende, M. Widom, and R. M. Feenstra, submitted (2014).

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