A Quantitative Characterization of Thermally Excited Ripples in Graphene

DONALD PRIOUR, JR, University of Missouri, Kansas City — In the framework of an atomistic model, we calculate the amplitude and typical wavelength of undulations in graphene sheets with length scales similar to those encountered in experiment. As part of a quantitative treatment, bond bending and stiffness constants are fixed by appealing to phonon frequency dispersion curves measured experimentally and from \textit{ab initio} electronic structure calculations. Equilibrium thermodynamic quantities, such as mean square atomic deviations and the average length scale (i.e. the typical “wavelength”) of graphene ripples, are calculated in the context of statistical mechanical Monte Carlo simulations. Thermally induced rippling is examined for suspended graphene, as well as graphene in the presence of a substrate, where the attractive coupling of atomic species to the substrate layer is modeled with a Lennard-Jones potential. The contribution of quenched substrate disorder to undulations in the graphene sheet relative to the component of graphene ripples due purely to thermal fluctuations is studied by examining graphene sheets bound to substrates with various levels of intrinsic positional disorder.