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Modeling of nanoscale graphite superlattices and its applications[1]

REZA ROCK, University of Delaware, WING TAT PONG, Materials Science and Engineering Laboratory, NIST — The study of superlattices on graphite surfaces by scanning tunneling microscopy is hampered by the lack of a method for reproducibly creating these superlattices for laboratory study. Computer models have been used to simulate these structures using the Moire pattern mechanism as the cause for superlattices. However, it is difficult to perform quantitative analyses using this simple model because the calculated corrugation amplitude of the atomic lattice is unrealistically large compared to the amplitude of the superlattice. We made the modeling results more useful and realistic by averaging the surface profile within an optimum radius around each data point. This has the effect of simulating the finite sharpness of a tunneling tip. The averaging radius controls the ratio of the atomic corrugation to the superlattice corrugation, and can be adjusted to achieve more realistic simulation results. With this model, it is now possible to perform useful analyses on the cross sections of the model superlattices. We present analyses of the layer coefficient ideality, impact of the angle of misorientation of the top graphite layer on superlattice corrugation, attenuation factor, and coexisting superlattices.

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