

Abstract Submitted  
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**Graphite Superlattices Simulation Software and its Research Applications**<sup>1</sup> REZA ROCK, Chemical Engineering, University of Delaware, PHILIP W.T. PONG, Metallurgy Division, National Institute of Standards and Technology — Superlattices are commonly observed on graphite surfaces when imaged using scanning tunneling microscopy. There is, however, currently no reproducible laboratory method to create these superlattices in a controlled fashion for study. A simple model has been used to simulate graphite superlattices using the Moiré interference pattern assumption. However, it is difficult to perform quantitative analyses on the output data from this simple model because the corrugation amplitude of the atomic lattice is comparable to that of the superlattice. We have developed an averaging algorithm to filter the output to rectify this problem, yielding a more realistic simulated surface. The parameters for this filter were optimized and the simulation results are much more realistic and similar to actual STM measurements. A MATLAB program utilizing this algorithm with graphical user interface to simulate graphite superlattices was developed. Coexisting superlattices, superlattices surrounding a screw dislocation, one-dimensional fringes resulting from Moiré patterns and other variable-periodicity superlattices were modeled and analyzed.

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