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Large-scale Molecular Dynamics Simulations of Glancing Angle **Deposition**¹ BRADLEY HUBARTT, XUEJING LIU, JACQUES AMAR, University of Toledo — While a variety of methods have been developed to carry out atomistic simulations of thin-film growth at small deposition angles with respect to the substrate normal, due to the complex morphology as well as the existence of multiple scattering of depositing atoms by the growing thin-film, realistically modeling the deposition process for large deposition angles can be quite challenging. Accordingly, we have developed a computationally efficient method based on the use of a single graphical processing unit (GPU) to carry out molecular dynamics (MD) simulations of the deposition and growth of thin-films via glancing angle deposition. Using this method we have carried out large-scale MD simulations, based on an embedded-atom-method potential, of Cu/Cu(100) growth up to 20 monolayers for deposition angles ranging from 50° to 85° and for both random and fixed azimuthal angles. Our results for the thin-film porosity, roughness, lateral correlation length, and density vs height will be presented and compared with experiments. Results for the dependence of the microstructure, grain-size distribution, surface texture, and defect concentration on deposition angle will also be presented.

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