Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Multiscale simulations of oblique-incidence Cu/Cu(100) epitaxial growth[1] V. BOROVIKOV, Y. SHIM, J.G. AMAR, University of Toledo — We present the results of multiscale simulations of oblique-incidence Cu/Cu(100) epitaxial multilayer growth carried out in order to explain the experimentally observed ripple formation at large deposition angles with respect to the substrate normal. Our method combines a kinetic Monte Carlo (KMC) simulation for the thermal surface diffusion with a small-scale one-atom molecular dynamics (MD) simulation of every deposition event, in order to account correctly for shadowing as well as the short-range and long-range attraction of depositing atoms to the surface. These simulations are particularly challenging both because of the existence of significant finite-size effects at large deposition angles, as well as because of the computational time required to simulate the deposition process, and therefore an efficient algorithm for carrying out parallel simulations of deposition will be described. The relative importance of shadowing and long-range attraction, as well as the dependence of the surface morphology on such parameters as the Ehrlich-Schwoebel barrier, edge- and corner-diffusion, and deposition flux will be discussed. Preliminary results in which both the substrate atoms and the depositing atom undergo molecular dynamics in the final stages of deposition will also be presented for comparison.

[1]Supprted by ACS PRF and NSF

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Date submitted: 02 Dec 2006 Electronic form version 1.4