Multiscale simulations of oblique-incidence Cu/Cu(100) epitaxial growth[1] V. BOROVIKOV, Y. SHIM, J.G. AMAR, University of Toledo — We present an improved method for multiscale simulations of homoepitaxial growth of metal thin films in which the effects of oblique incidence on the deposition process may be accurately taken into account. Our method combines a kinetic Monte Carlo (KMC) simulation for the thermal surface diffusion with a small scale molecular-dynamics simulation of every deposition event, in order to account correctly for both shadowing as well as the detailed atom-surface interaction of depositing atoms. To speed-up the simulations, that are very time consuming computationally, we have utilized a parallel algorithm that involves simultaneous depositions in different areas of the surface along with parallel kinetic Monte Carlo. Simulation results for the growth of Cu/Cu(100) at 160 and 200 K are presented and compared with both ordinary KMC simulations and experiments. Results will be presented for the case of both normal incidence as well as oblique angle incidence.

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Date submitted: 30 Nov 2005   Electronic form version 1.4