Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Parallel temperature accelerated dynamics simulations of vacancy formation in low temperature Cu/Cu(100) growth YUNSIC SHIM, VALERY BOROVIKOV, JACQUES G. AMAR, University of Toledo, BLAS P. UBERUAGA, ARTHUR F. VOTER, Los Alamos National Laboratory — While molecular dynamics simulations may be used to study thin-film growth at very low temperatures and at very high deposition rates, in order to study growth over time scales close to experiment, accelerated dynamics simulations are needed. Here we present the results of parallel temperature-accelerated dynamics simulations of low-temperature Cu/Cu(100) growth carried out using our recently developed parallel temperature-accelerated dynamics (parTAD) method, in order to understand recent X-ray diffraction experiments showing a surprisingly large vacancy concentration in Cu(100) growth at low temperature. In general, we find that, due to the existence of increased surface relaxation and activated events, the vacancy concentration obtained in our parTAD simulations is smaller than the corresponding concentration obtained in molecular dynamics (MD) simulations. The dependence of compressive strain and vacancy concentration, as well as the surface roughness and morphology, on growth temperature and deposition angle will also be discussed and compared with experiments.

Yunsic Shim
University of Toledo

Date submitted: 27 Nov 2007 Electronic form version 1.4