Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Molecular Dynamics Simulation of Nanostructured Thin Film Growth X.W. ZHOU, D.A. MURDICK, J.J. QUAN, B. GILLESPIE, H.N.G. WADLEY, University of Virginia, R. DRAUTZ, D.G. PETTIFOR, University of Oxford — Properties of nanostructured films are sensitive to atomic defects. Molecular dynamics (MD) simulations of growth can reveal defect formation mechanisms that are difficult to explore using other approaches. There are mainly two challenges. First, nanostructures often utilize different materials with metallic, ionic and covalent bondings. The MD must hence use an interatomic potential transferable to different local bonding environments encountered during growth. Secondly, growth is simulated by randomly adding atoms on the surface. The interatomic potential must hence accurately predict surface properties under various surface configurations. The newest MD approaches have begun to enable the growth simulation for a wide range of materials. The embedded atom method (EAM) potential was successfully used to simulate the growth of giant magnetoresistance metal multilayers. Our integrated EAM and charge transfer ionic potential is transferable between metallic and ionic materials and has been successfully used to simulate the growth of spin tunnel junction multilayers. Stillinger-Weber, Tersoff, and our analytical bond order potentials are compared for simulating covalent semiconductor growth.

X.W. Zhou
University of Virginia

Date submitted: 04 Dec 2004 Electronic form version 1.4