Abstract Submitted
for the SES07 Meeting of
The American Physical Society

Dynamics of crystal nucleation and growth from large scale simulations[1] LUJIAN PENG, Dept. of Materials Science, University of Tennessee, JAMES MORRIS, RACHEL AGA, Oak Ridge National Laboratory, Y.C. LO, National Sun Yat-Sen University, Kaohsiung, Taiwan 804, Republic of China — In previous work, we showed that when simulation size effects and transient nucleation theory were considered, crystal nucleation times from simulations could be predicted using classical theory. We have now extended this to the Lennard-Jones system. Homogeneous crystal nucleation is simulated by large-scale molecular dynamics. We study nucleation dynamics as a function of system size and temperature. We present quantitative comparisons between our results and classical nucleation theory. This is done without parameter fitting, using interfacial free energies and other properties calculated from separate equilibrium simulations.

[1]This research has been sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy under contract with DE-AC05-00OR-22725 with UT-Battelle.

James Morris
Oak Ridge National Laboratory

Date submitted: 17 Aug 2007 Electronic form version 1.4