Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Computational Models for Catalyzed Growth of Si Nanowire. SEUNGHWA RYU, Department of Physics, Stanford University, WEI CAI, Department of Mechanical Engineering, Stanford University — We present molecular simulation models for the growth of silicon nanowires from gold catalyst particles. Because the number of atoms involve in this process is above 1000, it is infeasible to use ab initio models. Hence our first step is to develop an interatomic potential model for Au-Si using the modified embedded-atoms method (MEAM) framework. For the first time, we computed the Au-Si phase diagram entirely from the interatomic potential. The melting points are computed from free energy methods with uncertainties less than 1K. Molecular simulation of the interaction between the gold nanoparticle with the Si substrate and Si NW is presented.

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Date submitted: 27 Nov 2007 Electronic form version 1.4