Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Atomistic Mechanism of Kinking in the Vapor-Liquid-Solid Growth of Silicon Nanowires SEUNGHWA RYU, WEI CAI, Stanford University — Understanding the atomistic growth mechanism of semiconductor nanowires from the catalytic droplet is important for better control of the shape and orientation of nanowires deposited through the Vapor-Liquid-Solid (VLS) process. Kinking is a frequently observed event, in which the nanowire suddenly changes the growth orientation. This behavior is usually undesirable, but can also be explored to grow nanowires of complex shapes if it can be controlled. Unfortunately, the atomistic origin of kinking is not well understood. We employ advanced sampling methods to compute the probability of the orientation change during VLS growth. Several growth directions and nanowire diameters are simulated at 1000 K. The simulation uses a recently developed Au-Si inter-atomic potential fitted to the experimental binary phase diagram.

Seunghwa Ryu
Stanford University

Date submitted: 28 Nov 2010 Electronic form version 1.4