

Abstract Submitted  
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**Atomistic Mechanism of Catalyzed Growth of Silicon Nanowire**

SEUNGHWA RYU, Physics Department, Stanford University, WEI CAI, Mechanical Engineering Department, Stanford University — Understanding the growth mechanism of semiconductor nanowire(NW) from catalyzed droplet is important for better control of the shape and growth speed of NWs by chemical vapor deposition through the Vapor-Liquid-Solid (VLS) process. To accurately describe the interatomic interaction between gold and silicon atoms, we developed a Au-Si binary potential based on modified embedded-atoms method (MEAM), which is benchmarked against the experimental binary phase diagram and mixing enthalpy. Advanced sampling method is employed to obtain the critical island at the liquid(Si Au alloy) - solid(silicon nanowire) interface. The dependence of the nucleation rate of the critical island on temperature and Si supersaturation is compared with experimentally observed NW growth rate and conditions of growth anomalously such as kinking.

Seunghwa Ryu  
Physics Department, Stanford University

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