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Atomistic Mechanism of Catalyzed Growth and Termination of Silicon Nanowire SEUNGHWA RYU, Physics, Stanford University, WEI CAI, Mechanical Engineering, Stanford University — Understanding the growth mechanism of semiconductor nanowire from catalyzed droplet is important for better control of the shape and growth speed of nanowires 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 nanowire growth rate. The termination of Si nanowire growth is investigated from Au-crystal nucleation inside the liquid droplet at the tip of nanowire.

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