Atomistic Mechanisms of Orientation and Temperature Dependence in Gold-Catalyzed Silicon Growth

Yanming Wang[1,2] , Adriano Santana[3] and Wei Cai[1]

[1] *Department of Mechanical Engineering, Stanford University, CA, USA*
[2] *Research Laboratory of Electronics, Massachusetts Institute of Technology, MA, USA*
[3] *Beijing Computational Science Research Center, Beijing, China*

Gold-catalyzed vapor-liquid-solid (VLS) growth is widely used in the synthesis of silicon-based low-dimensional nano-structures. However, growth anomalies are often observed [1, 2], whose formation is believed to highly depend on the growth orientation and temperature, but a complete understanding has not been achieved yet. In this talk, we present a systematic study on the orientation and temperature dependences in the VLS process [3], by means of long molecular dynamics (MD) simulations up to 100 ns using an MEAM potential that well reproduces the binary phase diagram [4]. The Si growth velocities are extracted from the simulations under various conditions for ⟨110⟩ and ⟨111⟩ orientations respectively. Our data suggest a linear dependence of the growth velocity on the Si supersaturation for ⟨110⟩ growth, in contrast to a non-linear dependence for ⟨111⟩ growth (Figure 1). By analyzing the surface morphologies, this difference is linked to the continuous growth mechanism on {110} substrate and the island nucleation controlled growth on {111} substrate (Figure 1). Furthermore, we find that the ⟨111⟩ growth in our MD simulations operates in the regime where the nucleation rate is higher than the island expansion rate. This is traced to the formation of a gold saturated monolayer above the nucleated Si island, impeding its further growth. Also, it is found that the temperature dependent atom activity near the {111} interface is lower, explaining the smaller growth velocity of the {111} surface than that of the {110} surface.

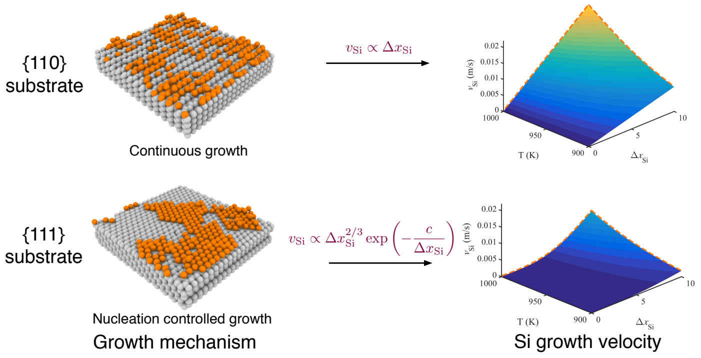

Figure 1. Growth interface morphologies (left) and growth velocities plotted as functions of temperature and Si supersaturation (right) for {110} and {111} substrates.

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