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Lecture Title:
Interpretation and Prediction of Nanostructural Evolution Based on First-Principles Studies

Abstract:

Self-assembly has been ingeniously used in nature, such as the formation of beautiful snowflakes. However, our present understanding is still too shallow to achieve such complex process. By using *ab initio* kinetic Monte Carlo simulation, we can uncover some of the building regulations of the surface-based nanostructures down to atomic-scale. In this talk, I will first introduce a one-, two-, and three-dimensional Ehrlich-Schwoebel (ES) barrier in kinetics-driven growth. Within this framework, I will show how one can control the island shape, the island instability, and the film roughness. Furthermore, I will discuss a novel concept: a true upward adatom diffusion on metal surface, which is beyond the traditional Ehrlich-Schwoebel (ES) barrier model.

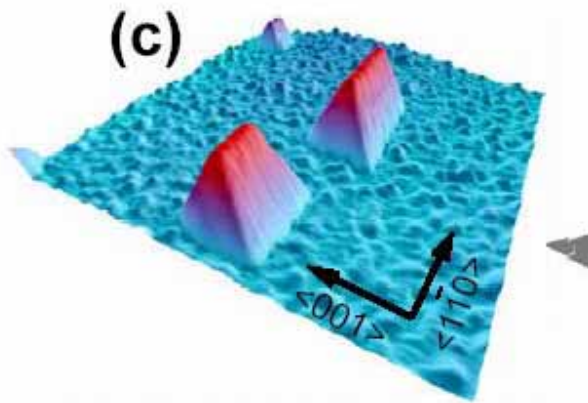


Figure 1 Bimodel growth in Al (110) homoepitaxy.