Interpretation and prediction of nanostructural evolution based on first-principles studies

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Pattern formation and decay in the early stage of growth is fundamental to many materials physics and chemistry. Understanding the complex interplay between factors that influence the evolution of surface-based nanostructures can be challenging. Computer simulation will play an important role in providing insight. 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 to control the island shape, the island instability, and the film roughness efficiently. 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. This process offers new indications as how to use ab initio kinetic Monte Carlo simulation can uncover some of the building regulations of the evolution mechanism down to atomic-scale.