A Simulation-Based Study of Nanocluster Growth through Deposition and Surface Diffusion

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The growth of new materials based on the self-assemblage of individual atoms is one of the most promising methods for achieving nanofabrication at the atomic scale. To achieve this goal requires understanding the growth processes at the atomic level. With the invention of STM (Scanning Tunneling Microscope) and similar techniques, it is now possible to examine a given structure with atomic resolution. However, despite decades of efforts, researchers are still far from understanding the connections between the motion of individual atoms and the structure grown. The focus of this study is to identify the roles played by individual atoms in the nanocluster growth processes. The results of computer simulations of nanocluster growth of vapor-based deposition and surface diffusion under various conditions provide convincing evidence that the behavior of adatoms is strongly influenced by time of deposition. The study examines the factors that impact the growth of a large nanocluster, nucleation sites on a biased surface, and cluster density.

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