A Kinetic Monte Carlo Study of Effects of Adatom-Adatom Repulsive Interactions on Nucleation and Growth of Nanoclusters

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The effects of adatom-adatom repulsive interactions on nucleation and growth of nanoclusters have been studied using Kinetic Monte Carlo computer simulations. The dependence of nanocluster density on the mobility (movement) and coverage of adatoms is analyzed. Several sets of data on nanocluster density are obtained for different models of growth corresponding to repulsive adatom-adatom interactions of different ranges and strengths. The different roles played by different groups of adatoms based on their time of deposition (stages of growth) are closely examined. This study shows that while the presence of repulsive interactions between adatoms generally increases the density of nanoclusters, the impact on the density's dependence on coverage is especially profound. Specifically, it was discovered that the presence of such interactions dramatically changed the roles played by the adatoms deposited in later stages of growth, from mostly aggregation to existing nanoclusters to critically contributing to the formation of new nanoclusters. As a result, nucleation continues to occur at late stages of growth and the density of nanoclusters increases with coverage, with the extent of delayed nucleation dependent on the range and strength of repulsive interactions. The impact of this study on our understanding of the theory of nucleation and growth of nanoclusters, the quality of thin films grown in an experiment, and potential applications in areas such as catalysis, magnetic storage, and spintronics will be discussed.

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