Effects of size-dependent island-edge barriers on submonolayer nucleation, utilizing a modified Union-Find-Delete algorithm

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Abstract

The effects of size-dependent island-edge barriers on submonolayer nucleation are studied via kinetic Monte Carlo simulations of a simplified model of epitaxial thin-film growth. Standard nucleation theory predicts an exponent $\chi = i/(i+2)$ (where i is the critical island size) relating the island density N at a fixed coverage θ to the ratio between diffusion rate D and the deposition rate F, $N \sim (D/F)^{-\chi}$. In contrast, Attachment Limited Aggregation (ALA) assumes that a barrier to attachment to islands leads to a higher prediction of $\chi = 2i/(i+3)$. The viability of ALA as an explanation for recent experimental values of χ greater than 1 is examined. Regimes with a critical island size, i, of 1 and 3 are simulated, along with two cases of a barrier to monomer attachment. In the first case, a size-independent barrier for attachment of a diffusing monomer to another monomer or island is assumed, while in the second case, there is only a barrier for attachment to islands larger than a given size S. Our results support a previous conjecture that barriers to island attachment extend the transient regime of island nucleation. Additionally, it appears that size-dependent barriers lead to the onset of island coalescence at a lower coverage θ as well as a shortened aggregation regime. However, our results do not indicate that barriers to monomer attachment increase the value of χ. In the first case, corresponding to a island-size independent monomer attachment barrier, we find that the exponent χ is seen to decrease with the inclusion of a barrier to any attachment. With a size-dependent barrier to attachment, there is no clear observed trend in the values of χ with varying S. These results do not support ALA alone as the explanation for the unusually high values of χ observed in experimentally.