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Quantitative model of heterogeneous nucleation and growth of SiGe quantum dot molecules[1] HAO HU, FENG LIU, Department of Materials Science and Engineering, University of Utah, FENG LIU TEAM — We develop a quantitative theoretical model for heterogeneous nucleation and the growth of a quantum dot molecule — a few islands "strain bonded" by a pit in heteroepitaxy of thin films, in contrast to homogeneous nucleation and growth of isolated strain islands on the surface. We use a multiscale approach combining continuum model with first-principles calculation, and show that the critical size and energy barrier for island nucleation next to a pit is substantially reduced with the increasing pit size, but the reduction approaches an upper bound of ∼85% and ∼72% for the size and barrier, respectively. Our model also predicts a self-limiting effect on island growth, resulting from an intriguing interplay between island-pit attraction and island-island repulsion, that drives the island size to increase linearly with the pit size, which explains a long-standing puzzle of experimental observation.

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