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Modeling the complex evolution of self-assembled quantum dots¹

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In heteroepitaxy, misfit strain often leads to spontaneous formation of islands. Such islands have attracted great interest as “self-assembled quantum dots”. The growth of these quantum dots is remarkably rich, exhibiting alloy intermixing, island coarsening, trench formation, and even spontaneous *lateral* motion of islands. Islands also interact with topographic features on the substrate, providing a means for controlling the position of quantum dots. The diverse experimental observations provide an ideal opportunity to test and extend our theoretical understanding of growth at the nanoscale. We find that much of the complexity arises because there is a strong thermodynamic driving force for intermixing (to increase entropy and reduce strain energy) as well as for morphological evolution (to reduce strain energy); but this evolution must occur under the kinetic constraint of diffusion occurring only at the surface. Simulations of such constrained evolution directly reproduce many of the observed phenomena [Y. Tu and J. Tersoff, Phys. Phys. Lett. 98, 096103 (2007)].

¹Work done in collaboration with Yuhai Tu