Equilibrium shape and dislocation nucleation in strained epitaxial islands

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The shape and size of strained epitaxial islands in a Stranski-Krastanow growth process has been a subject of intense experimental and theoretical studies due to its relevance for fabrication of semiconductor nanostructures [1]. The optimal size and shape result from a delicate balance of energy lowering through strain relaxation and energy cost through extra surface energies. Previous work on equilibrium shape of coherent islands have used simple predefined faceted shapes in analytical calculations based on continuum elasticity theory [2]. We study numerically the equilibrium shape and dislocation nucleation of epitaxial islands with a two-dimensional atomistic model, using interatomic potentials of Lennard-Jones type. The phase diagram for the equilibrium island shapes as a function of island size and lattice misfit with the substrate is obtained. We have also investigated the energy barrier and transition path for transition between different shapes of the islands and for dislocation nucleation in initially coherent islands using a method introduced recently, based on a systematic search of the transition paths for activated events [3]. It is found that dislocations can nucleate spontaneously at the edges of the adsorbate-substrate interface above a critical size.

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