

Abstract Submitted
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Shape transitions in strained Cu islands on Ni(100): kinetics versus energetics¹ YUNSIC SHIM, JACQUES AMAR, University of Toledo — We examine the shape transition from compact to ramified islands observed in submonolayer Cu/Ni(100) growth. Recently, it has been argued that this transition is not due to a growth instability but can be understood in terms of energetic arguments. In order to determine the responsible mechanisms we have carried out energetics calculations as well as temperature-accelerated dynamics (TAD) and kinetic Monte Carlo (KMC) simulations. Our results indicate that the shape transition cannot be explained by equilibrium arguments, but is instead due to kinetic effects which are mediated by strain. In particular, by calculating the relevant line-tension and strain energies, we find that the equilibrium critical island-width is at least four orders of magnitude larger than the experimentally observed arm-width. In contrast, our TAD simulations indicate that unexpected concerted motions occurring at step edges are responsible. The energy barriers for these concerted motions decrease with increasing island size and appear to saturate for islands larger than 300 - 400 atoms. By including these strain-induced kinetic processes in our KMC simulations of island-growth, we have been able to explain both the temperature- and coverage-dependence of the island morphology.

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