Kinetically driven island morphology in growth on strained Cu (100)v

Indiras Khatri, Ehsan H Sabbar, Jacques G Amar

Abstract:

We study the effects of strain on the monomer and dimer diffusion mechanisms and island morphology during the growth of Cu on a biaxially strained Cu(100) substrate. We find an approximately linear dependence of the activation barriers on strain. In particular, while hopping is favored for compressive and/or small (<2%) tensile strain, for greater than 2% tensile strain, the exchange mechanism is favored. We then present the results of temperature-accelerated dynamics simulations of submonolayer growth at 200 K. For the case of 2% compressive strain we find that, as in previous kinetic Monte Carlo simulations of Cu/Ni(100) growth, the competition between island growth and multi-atom relaxation ("pop-out") events leads to an island morphology with a mixture of open and closed steps. At slightly higher coverage, island coalescence then leads to elongated islands. However, annealing leads to a significant decrease in the number of open steps. In contrast, for the case of 8% tensile strain, only one large strongly anisotropic island is formed. Surprisingly, we find that despite the large strain, the island anisotropy is not due to energetics but is instead due to anisotropic attachment barriers that favor the exchange-mediated attachment of monomers to corners over close-packed step-edges. An explanation for the asymmetry in attachment barriers is provided. Our results provide a new general kinetic mechanism for the formation of anisotropic islands in the presence of isotropic diffusion and tensile strain.