Mechanism of stacking fault formation in metal(100) heteroepitaxial growth

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Abstract:

Strain in metal(100) heteroepitaxial thin-film growth can lead to a variety of effects such as the formation of stacking faults (SFs). To gain a better understanding we have carried out temperature-accelerated dynamics (TAD) simulations of the submonolayer growth of Cu islands on a biaxially strained Cu substrate at 200 K. In the case of 4% compressive strain we find that SF formation occurs with a morphology very similar to the structures found experimentally in Cu/Ni(100) growth. We also find that islands play a key role by lowering the barrier for vacancy formation. In particular, once two substrate vacancies are formed and diffuse to form the appropriate configuration this leads to the formation of a SF in both the substrate and island. While the activation barrier for SF formation is very high, due to the presence of a large number of low-frequency vibrational modes, the saddle-point entropy is large while the corresponding Vineyard prefactor is more than 10 orders of magnitude larger than is typical of atomic processes in fcc metals. Similarly, an analysis of the entropy of the SF state indicates that the reverse prefactor is much smaller, while the free energy of this state is lower than that of the initial state.