Kinetics of Facile Bilayer Island Formation for Ag on NiAl(110)

J.W. EVANS, YONG HAN, D.-J. LIU, BARIS UNAL, F. QIN, D. JIN, C.J. JENKS, P.A. THIEL, Iowa State University — STM studies reveal that deposition of Ag on NiAl(110) at 127 K and above leads to bilayer-by-bilayer growth of a nearly-strain-free film with Ag(110) structure [1]. This growth mode is attributed to Quantum Size Effects (QSE) associated with electron confinement in the Ag film. Our focus here is on analysis the initial nucleation and growth of bilayer Ag(110) islands on NiAl(110) which is facile even at 127K despite requiring uphill transport of Ag. DFT analysis for supported Ag films determines adatom adsorption energies (which display QSE), interaction energies, and various relevant diffusion barriers. Kinetic Monte Carlo simulation of an atomistic lattice-gas model incorporating these energies highlights the role of strongly anisotropic interactions in facilitating bilayer island formation.


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