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**Temperature-dependence of Ni+Al co-deposition on NiAl(110): Atomistic-level modeling of deviations from perfect alloy ordering** YONG HAN, DAPENG JING, BARIS UNAL, P.A. THIEL, J.W. EVANS, Institute for Physical Research and Technology; Departments of Chemistry, MSE, Mathematics, Physics and Astronomy; Ames Lab, ISU, Ames, Iowa 50011 — Stoichiometric co-deposition of Ni and Al on NiAl(110) for high enough temperatures (below the order-disorder transition for NiAl) must produce near-perfect alloy islands and overlayers. However, at 300K, island structure is far from perfectly ordered and depends strongly on the deposition protocol (e.g., simultaneous vs. sequential). Realistic atomistic-level modeling of this non-equilibrium behavior must provide an accurate description of not just alloy thermodynamics (through adatom adsorption and interaction energies), but also of diffusion kinetics (for adatom attachment-detachment at and transport along island edges). This is achieved by multi-site lattice gas modeling with DFT input for adsorption and interaction energies for adatoms both at adsorption sites and at transition states for hopping [T. Duguet, Y. Han et al., Proc. Nat. Acad. Sci. 107 (2010) Special Issue on Surface Chemistry; Y. Han et al., submitted (2010)]. Model analysis by KMC simulation shows a transition from poor alloy order at 300K to almost perfect order at 600K.

Yong Han
Institute of Physical Research and Technology,
Iowa State University, Ames, Iowa 50011

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