Molecular dynamics simulation of nano-scale metallic bilayer thin film growth

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The interfacial features and the growth morphology of the metallic bilayer system are quantitatively investigated by molecular dynamics simulation. Fe on Ni(100) system has shown intermixing and formation of an intermetallic compound. However, characteristics such as layer coverage function and mixing length are observed to differ from other ferromagnetic/non-ferromagnetic metallic bilayer systems. The different intermixing behavior can be successfully explained in terms of cohesive energy, lattice matching and local acceleration effect. It can be clearly seen that the intermixing is rather insensitive to the change of the initial kinetic energy of adatoms, but largely dependent on the substrate temperature and orientation of the Ni substrate.