

ATOMISTIC SIMULATION OF DISLOCATION ACTIVITIES IN THIN METAL FILMS

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The overall strength of a thin metal film bonded to a stiff substrate is controlled to a large extent by the interface constraint. This is manifested by the experimentally measured high flow stress that can be carried by films on a substrate compared to the case of free-standing films. The substrate confinement effect is typically reasoned from the energy consideration involving the formation misfit dislocations at the film/substrate interface. However, there is a general lack of experimental evidence of misfit dislocations in recent electron microscopy examinations of aluminum and copper films. In this study we invoke atomistic modeling to provide a mechanistic rationale for the substrate effect in thin-film strength. Molecular statics simulations were carried out using the pair potential model for copper. The tensile stress-strain response is modeled for the free-standing and substrate-bonded films. It is found that the formation and glide of dislocations readily occur in the stretched free-standing film, inducing slip steps at both surfaces of the film. The existence of an interface with the substrate constrains the dislocation motion in the film and restricts the slip steps to only the free surface. The propensity of film plasticity is dictated by the capability of atoms to slide along the interface. The higher flow stress in the substrate-constrained film, compared to the free-standing film, can be correlated with the dislocation activities obtained from the atomistic simulation. The propensity of dislocation core spreading near the interface is also examined.