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Crystal plasticity analysis of deformation behavior of nanocrystalline nickel

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ABSTRACT

Nanocrystalline (NC) metals with grain sizes <100 nm have attracted a lot of attention in the materials science field for more than a few decades because of their ultra-high strength and hardness. Various experimental and computational studies indicate that dislocation-mediated plasticity prevails in NC metals when the grain size is larger than ~10 nm. Recent molecular dynamics (MD) simulations have found that dislocation-mediated plasticity in NC fcc metals is predominantly determined by dislocation propagation rather than nucleation and nucleation is the rate-limiting process. However, most of the earlier micromechanics models for NC metals have ignored this key feature. In this study, we have developed a statistical model to analyze the distribution of the critical resolved shear stresses (CRSS) associated with propagating a dislocation, from its grain boundary source, across the grain, *t* propagate, of a given size. We have incorporated this CRSS distribution into a 3D crystal plasticity model to study the stress–strain response of NC Nickel. The influences of grain size, dominant texture, and GB interactions are all considered in this study. From our study, we find that the distribution of *t* propagate is very asymmetric and follows the generalized extreme value distribution. By considering the distribution of *t* propagate, the simulation results from the crystal plasticity model can capture the key experiment trends observed for the strength of NC Ni: the strength increases with decreasing grain size following the Hall–Petch relationship. In addition, our simulation results predict a strong connection between the grain size and heterogeneity of plastic deformation in NC Ni.