INTRINSIC DEFORMATION SCALE-EFFECTS IN METALS

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Abstract

Several advances in computational mechanics methods are required to realize the goals of Integrated Computational Materials Science and Engineering. These include proper multi-scale representation of material heterogeneities as well as corresponding, characteristic length-scales. Scale effects can be quantified and validated using lower scale, physics-based models. These can be systematically verified experimentally to develop scale dependent analysis methods to inform modeling of microstructure heterogeneities. Recent experiments have shown strong size effects in metal micro-pillars with dimensions below ~100 micro-meters. This size dependent behavior is consistent with deformation occurring below a characteristic dislocation correlation length. Micro-scale dislocation evolution simulations exhibit the same behavior and reveal the mechanistic source of strengthening (and stochastic flow) at theses scales. In this work, large scale atomistic and dislocation dynamics simulations are used to assess the aspects of ensemble hardening in simple metals. Atomistic simulations illustrate the effects of cross slip on full 3-d simulations of forest hardening. The work hardening rates of micro pillars, uniaxial loaded along <100>, <110>, and <111>, are calculated using dislocation dynamics simulations. Simulations include dislocation intersection cross slip which enhances the rapid increase in dislocation density. Analyses of the evolving dislocation ensembles, including the formation of strong dislocation heterogeneities are reviewed.