A multiple-mechanism-based model for prediction of yield strength in crystals

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Abstract

The size dependent plastic deformation in nanocrystalline materials on small scales has received intensive research in the past two decades. Various strain gradient plasticity models have been established that capture well the-smaller-the stronger phenomenon. In those models, the grain boundaries and surfaces have been assumed either explicitly or implicitly to barriers to dislocation motion. However, the accumulated experiments and simulations have revealed the-smaller-the-softer phenomenon for some polycrystals when the grain size shrinks to several nanometers. The mechanisms underlying are still not very clear but may be related to the grain boundary mediated processes. Meanwhile, many experiments have discovered the deformation mechanisms such as grain boundaries and surfaces as sources/sinks for dislocations, and grain boundaries sliding may be active during the plastic deformation of nanocrystals. Thus, to capture the deformation of crystals at small scales, different mechanisms should be taken into account. To this end, in this work, a model for crystal plasticity has been developed to allow for strain gradient effect, surface/interface as dislocation sources/sinks and grain boundary sliding. It is achieved in an energetic manner. Based on the model, a bicrystal under plane constrained deformation has been considered. It has been revealed that the yield strength increases with grain size when it is within tens of nanometers and otherwise exhibits the usual the-smaller-the-stronger behavior. And such size dependent yield strength can be attributed to the different active dominant deformation mechanism at different size range.

Keywords: multiple mechanism, crystal plasticity, energetic approach, yield strength, size effect