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Modeling of Dislocation-Grain Boundary Interaction and Scale-Dependent Mechanical Properties of Metal Polycrystals

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Abstract (300 words)

Scale dependent characteristics of mechanical properties of metal polycrystals are well known and summarized in the form of Hall-Petch relation. In recent years, there have been extensive research efforts to model such effects into the theory of continuum mechanics. Among them, an introduction of the concept of plastic strain gradient, or more directly the concept of the geometrically necessary dislocations, into the framework of the theory has been made and Hall-Petch type relation of plastic flow stress level was successfully reproduced. On the other hand, scale dependent characteristics of the yield stresses are not yet captured and left to be explored.

In this communication, we first focus our attention on the initial movement of dislocation(s) that expand from a Frank-Read source and its interaction with grain boundaries. To simulate such process, we use a dislocation dynamics simulation technique, and find the minimum resolved shear stress for the FR source to emit at least one closed loop. When the grain size is large enough compared to the size of FR source, the minimum resolved shear stress levels off to a value, but when the grain size is close to the size of FR source, the minimum resolved shear stress shows a sharp increase. This result is modeled into the expression of the critical resolved shear stress of slip systems which is used in the continuum mechanics based crystal plasticity analyses of six-grained polycrystal model. Results of the crystal plasticity analyses show a distinct increase of yield stress for specimens with smaller mean grain diameter. Scale dependent characteristics of the yield stress and its relation to some control parameters are discussed.