

Grain Size “Softening” in Nanocrystalline Materials Using a Discrete Dislocation Dynamics Approach

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Abstract

When the grain size in polycrystalline materials is reduced to the nanometer length scale (nanocrystallinity), observations from experiments and atomistic simulations suggest that the yield strength decreases (softening) as the grain size is decreased. This is in contrast to the Hall-Petch relation observed in larger sized grains. The now classical discrete dislocation dynamics (DDD) approach has several limitations when one attempts to model nanocrystalline systems. Firstly, typical lattice dislocation density in nanometer-sized grains would mean that the average distance between dislocations is greater than the grain size, so there would likely be little to no pileups and the Hall-Petch theory would collapse. Secondly, even if an artificially high dislocation or dislocation source density is used in a DDD simulation, the grain boundaries typically only act as obstacles, and there is no additional mechanism that could possibly result in an inverse Hall-Petch effect. Atomistic simulations allow us to observe the various stress relief mechanisms at the grain boundaries of nanocrystalline systems. We incorporated some of these mechanisms (grain boundary sliding, dislocation emission from junctions, etc.) into the DDD framework and obtained the smaller is weaker relationship observed in these nanocrystalline materials. Analyses of the DDD results also lend further insight on the possible mechanisms that lead to the inverse Hall-Petch effect.

Keywords: Discrete dislocation dynamics; nanocrystalline; Hall-Petch