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A Discrete Dislocation Dynamics Model for Nano-crystalline Materials

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The strength of polycrystalline materials generally increases with decreasing grain size as it approaches micron to sub-micron length scales. This “smaller is stronger” effect can be explained by the Hall-Petch relationship based on dislocation pile-ups against the grain boundaries. However, as the grain size approaches the tens of nanometer regime, the so-called inverse Hall-Petch relationship has been observed. Previous studies revealed that in nano-crystralline materials, grain boundary activities could dominate over plasticity induced by lattice dislocations, highlighting the importance to consider not only dislocation activities, but also grain boundary activities and their interactions with dislocations. We therefore adapt the 2D discrete dislocations dynamics (DDD) approach to include dislocation glide, dislocation nucleation within grains, grain boundary sliding, dislocation adsorption at grain boundaries, dislocation emission from grain boundaries, and dislocation transmission across grain boundaries. The objective is to predict the mechanical behavior of nano-crystalline materials using a single DDD framework.

Keywords: Discrete dislocation dynamics, polycrystals, grain boundaries, plasticity