Motion of grain boundaries incorporating dislocation structure

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Energetic and dynamic properties of grain boundaries play vital roles in the mechanical and plastic behaviors of polycrystalline materials. We developed a continuum model for the dynamics of low angle grain boundaries in two dimensions incorporating both the motion of grain boundaries and the dislocation structure evolution on the grain boundaries. The long-range elastic interaction is included to maintain a stable dislocation structure during the evolution. These evolutions of the grain boundary and its dislocation structure are able to describe both normal motion and tangential translation of the grain boundary and grain rotation due to both coupling and sliding. Since the continuum model is based upon dislocation structure, it naturally accounts for the grain boundary shape change during the motion and rotation of the grain boundary by motion and reaction of the constituent dislocations. Using the derived continuum grain boundary dynamic model, simulations are performed for the dynamics of circular and non-circular two dimensional grain boundaries, and the results are validated by discrete dislocation dynamics simulations.