MULTISCALE MODELING AND SIMULATIONS OF DEFECTS IN CRYSTAL

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ABSTRACT

We develop a multiscale continuum model to describe the interface structure in crystalline material such as FCC metals. The interface structure for twist, tilt and misfit grain boundaries are described by the dislocation network. The model incorporates both the anisotropy elasticity of each grain in crystalline materials and the molecular dynamics calculation informed interaction between two bulks, i.e., the nonlinear generalized stacking-fault energy. The equilibrium structures are obtained from the numerical simulations of the force balance differential equations. We apply this approach to determine the structure and energetics of twist, tilt and general grain boundaries. We also investigated the dislocation structure in heterogeneous crystalline material. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

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