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A general and predictive model of anisotropic grain boundary energy and morphology for polycrystal-level simulations BRANDON RUNNELS, University of Colorado Colorado Springs, IRENE BEYERLEIN, Los Alamos National Laboratory, SERGIO CONTI, University of Bonn, MICHAEL ORTIZ, California Institute of Technology — In this work, a new model for anisotropic GB energy and morphology is formulated that is fast, general, dependent on only three material parameters, and is verified by comparison with more than 40 MD and experimental datasets for (a)symmetric, tilt/twist, FCC/BCC materials, as well as experimental measurements. A relaxation algorithm is presented that is able to efficiently compute the optimal facet pattern and corresponding relaxed energy. Finally, the GB model is implemented as an interface model in a polycrystal simulation to observe the effects of GB in conjunction with elastic and plastic deformation. The simulations are compared with those using an isotropic GB model, and the effect of the GB isotropy on the bulk properties and microstructure is determined. The results have applications towards, e.g., improved polycrystal simulations, understanding void nucleation, and GB engineering.

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