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A diffuse interface model of grain boundary faceting¹ FADI ABDELJAWAD, DOUGLAS MEDLIN, JONATHAN ZIMMERMAN, KHALID HATTAR, STEPHEN FOILES, Sandia National Laboratories — Incorporating anisotropy into thermodynamic treatments of interfaces dates back to over a century ago. For a given orientation of two abutting grains in a pure metal, depressions in the grain boundary (GB) energy may exist as a function of GB inclination, defined by the plane normal. Therefore, an initially flat GB may facet resulting in a hill-and-valley structure. Herein, we present a diffuse interface model of GB faceting that is capable of capturing anisotropic GB energies and mobilities, and accounting for the excess energy due to facet junctions and their non-local interactions. The hallmark of our approach is the ability to independently examine the role of each of the interface properties on the faceting behavior. As a demonstration, we consider the $\Sigma 5$ $\langle 001 \rangle$ tilt GB in iron, where faceting along the $\{310\}$ and $\{210\}$ planes was experimentally observed. Linear stability analysis and numerical examples highlight the role of junction energy and associated non-local interactions on the resulting facet length scales. On the whole, our modeling approach provides a general framework to examine the spatio-temporal evolution of highly anisotropic GBs in polycrystalline metals.

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