SAND2015-9158C

A diffuse interface model of grain boundary faceting

F. Abdeljawad[1], D. L. Medlin[2], J. A. Zimmerman[2], K. Hattar[1], S. M. Foiles[1]

[1] *Sandia National Laboratories, Albuquerque, NM, 87185 USA*

[2] *Sandia National Laboratories, Livermore, CA, 94551 USA*

(Dated: October 15, 2015)

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.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.