Runnels, Brandon; Beyerlein, Irene J.; Conti, Sergio; Ortiz, Michael

A relaxation method for the energy and morphology of grain boundaries and interfaces.

(English) Zbl 1482.74022


Summary: The energy density of crystal interfaces exhibits a characteristic “cusp” structure that renders it non-convex. Furthermore, crystal interfaces are often observed to be faceted, i.e., to be composed of flat facets in alternating directions. In this work, we forge a connection between these two observations by positing that the faceted morphology of crystal interfaces results from energy minimization. Specifically, we posit that the lack of convexity of the interfacial energy density drives the development of finely faceted microstructures and accounts for their geometry and morphology. We formulate the problem as a generalized minimal surface problem couched in a geometric measure-theoretical framework. We then show that the effective, or relaxed, interfacial energy density, with all possible interfacial morphologies accounted for, corresponds to the convexification of the bare or unrelaxed interfacial energy density, and that the requisite convexification can be attained by means of a faceting construction. We validate the approach by means of comparisons with experiment and atomistic simulations including symmetric and asymmetric tilt boundaries in face-centered cubic (FCC) and body-centered cubic (BCC) crystals. By comparison with simulated and experimental data, we show that this simple model of interfacial energy combined with a general microstructure construction based on convexification is able to replicate complex interfacial morphologies, including thermally induced morphological transitions.

MSC:
74A50 Structured surfaces and interfaces, coexistent phases
74N05 Crystals in solids

Full Text: DOI

References:
graphs (2000), Oxford University Press · Zbl 0957.49001
[7] Bollmann, W., Crystal Defects and Crystalline Interfaces (1970), Springer-Verlag
[8] Bulatov, V. V.; Reed, B. W.; Kumar, M., Grain boundary energy function for fcc metals, Acta Mater., 65, February, 161-175 (2014)


[21] Herring, C., Some theorems on the free energies of crystal surfaces, Phys. Rev., 82, April, 87-93 (1951) - Zbl 0042.23201


[23] Li, J., Disclination model of high angle grain boundaries, Surf. Sci., 31, June, 12-26 (1972)


[29] Read, W.; Shockey, W., Dislocation models of crystal grain boundaries, Phys. Rev., 78, 3, 275 (1950) - Zbl 0037.13303


[34] Taylor, J. E.; Cahn, J. W., Shape accommodation of a rotating embedded crystal via a new variational formulation, Interfaces Free Bound., 9, 4, 493 (2007) - Zbl 1132.82302


[37] Tschopp, M. A.; McDowell, D. L., Structures and energies of \(\Sigma = 3\) asymmetric tilt grain boundaries in copper and aluminium, Philos. Mag., 87, August, 3147-3173 (2007)


[41] Wolf, D., Correlation between the energy and structure of grain boundaries in b.c.c. metals I. Symmetrical boundaries on the (110) and (100) planes, Philos. Mag. Part B, 59, June, 667-680 (1989)


This reference list is based on information provided by the publisher or from digital mathematics libraries. Its items are heuristically matched to zbMATH identifiers and may contain data conversion errors. It attempts to reflect the references listed in the original paper as accurately as possible without claiming the completeness or perfect precision of the matching.