Stress-dependence of generalized stacking fault energies

Predrag Andric , Binglun Yin , W.A. Curtin

PII: S0022-5096(18)30575-1
DOI: https://doi.org/10.1016/j.jmps.2018.09.007
Reference: MPS 3438

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 3 July 2018
Revised date: 21 August 2018
Accepted date: 5 September 2018

Please cite this article as: Predrag Andric , Binglun Yin , W.A. Curtin , Stress-dependence of generalized stacking fault energies, *Journal of the Mechanics and Physics of Solids* (2018), doi: https://doi.org/10.1016/j.jmps.2018.09.007

Stress-dependence of generalized stacking fault energies

Predrag Andric, Binglun Yin, W.A. Curtin
Laboratory for Multiscale Mechanics Modeling
Ecole Polytechnique Fédérale de Lausanne
CH-1015 Lausanne, Switzerland

Abstract

The energy associated with shearing of planes of atoms in a crystal is the generalized stacking fault energy (GSFE). It is a crucial material property for describing nanoscale plasticity phenomena in crystalline materials, such as dislocation dissociation, nucleation, and twinning. The dependence of the GSFE on applied stress normal to the stacking fault has been suggested to influence such phenomena. Here, the stacking fault stress dependence is analyzed through (i) the generalized stacking fault potential energy (GSFE) and (ii) the generalized stacking fault enthalpy (GSFH). At an imposed shear displacement, there is also an associated inelastic inter-planar normal displacement around the fault. Extensive molecular statics simulations with interatomic potentials and/or first principle calculations in Ni, Cu, Al and Mg reveal that GSFE and inelastic normal displacement both increase with tensile stress. An increasing GSFE contradicts long-standing wisdom and previous studies. Positive inelastic normal displacement coupled to the applied normal stress decreases the GSFH, but is not useful for general mechanics problems. The existence of the inelastic displacement can lead to incorrect measurements of the GSFE and GSFH in finite systems loaded by an applied strain. Application of the GSFE and the inelastic normal displacement to both fcc dissociation distance versus applied normal stress and crack tip dislocation emission under mixed Mode II/I loading show very good agreement with direct simulations. In general, "opening softening" effects are not universal, and so the analysis of any particular nanomechanics problem requires precise implementation of the combination of GSFE and inelastic normal displacement rather than the GSFH.

Keywords: Generalized Stacking Fault Energy, Molecular Statics, First Principle Calculations, Opening Softening, Dislocations.