Journal of the Mechanics and Physics of Solids 73 (2014) 228–241

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

Stability of ideal fcc twin boundaries

T.W. Wright *, N.P. Daphalapurkar, K.T. Ramesh

Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD 21218, USA

ARTICLE INFO

Article history:
Received 22 March 2014
Received in revised form
12 September 2014
Accepted 19 September 2014
Available online 2 October 2014

Keywords:
Twinning
Elastic materials
Stability and bifurcation
Variational calculus
Molecular dynamics

ABSTRACT

Ideas from continuum mechanics are used to derive an elastic stability inequality for a boundary between two different materials under quasi-static, homogeneous conditions. The terms in this inequality are interpreted for the case of an ideal twinning plane between two variants of a face-centered cubic material. High quality potentials for Ni and Cu are used in molecular dynamics calculations to calibrate relevant energies and displacements near the twinning plane. It is found that in comparison with direct molecular dynamics calculations the inequality predicts the critical stress that initiates movement of the twinning plane in Ni within 1.9% and within 1.3% for Cu. Although the predicted and calculated critical stresses are only upper bounds for the more realistic case of an imperfect boundary, the calculations give considerable insight into the interplay of energies that lead to boundary motion.

1. Introduction

In face-centered cubic (fcc) metallic materials with nanoscale grain sizes twinning on {111} planes may compete with dislocations as a mechanism for plastic deformation, e.g., see Zhu et al. (2012). Under sufficient shear traction in favored directions the twinning plane can move through the crystal lattice, remaining more or less parallel to the original plane. This is accomplished by atoms in a plane adjacent to the twinning plane that jump from current potential wells into neighboring wells in their own plane. By doing so, they restore the full fcc symmetry to the starting twinning plane, but cause the plane of jumping atoms to become the new twinning plane. Thus motion of an fcc twin boundary in its normal direction is a consequence of atoms jumping laterally to new wells. In general not all parts of the jumping plane move simultaneously, but rather "ledges," which are partial dislocations, develop where lattice defects or favorable fluctuations occur, or alternatively the ledges are emitted from grain boundaries, (Zhu et al., 2012). A ledge can then race across the old twinning plane, leaving an advancing twinning plane in its wake. Twin boundary motion thus follows the instability of one configuration and the attempt to find a more favorable configuration. The ledges cause local stress concentrations that move along the twinning plane under sufficient continued loading.

A homogeneous or ideal twinning plane without preexisting ledges or other defects is a simpler configuration to understand than one with ledges, etc., but which still gives considerable insight into the initiation of twin boundary motion and its underlying causation, namely, the interplay of various energies in the neighborhood of the twinning plane. This

* Corresponding author.
E-mail address: tim4906@comcast.net (T.W. Wright).

http://dx.doi.org/10.1016/j.jmps.2014.09.007
0022-5096/

paper will examine only the stability of a single homogeneous twinning plane, which determines the ideal shear strength of a twin boundary. The more complex issue of stability of a twinning plane with ledges will be left for the future.

To estimate the critical stress (ideal shear strength) that initiates motion of a twinning plane through the crystal lattice we examine the elastic stability of a preexisting uniform twin boundary using standard continuum concepts, supplemented by further information from molecular dynamics. First we review the criterion for continuum stability of a small uniformly loaded volume of a homogeneous material. Next we extend the analysis to two small volumes of different materials, joined to each other by a flat plane that independently carries energy. The same analysis that yields the volumetric criterion for stability, now gives an extra condition for stability of the joining plane. In our model problem the two materials are two twin variants of the same fcc material, joined by the twinning plane, which exists in a hexagonal close packed (hcp) configuration with respect to the adjacent planes of atoms in each of the fcc twin variants. Under quasi-static shear loading molecular dynamics can compute the constant state of stress, as well as the energy density in the twinning plane itself and in each plane parallel to it in the two fcc variants (see Appendix A). This approach also requires an account of displacements in the neighborhood of the twinning plane prior to instability. Molecular dynamics also supplies this information.

The problem now is to reconcile the continuum description and the information obtained from molecular dynamics. An elementary argument suggests a simple scaling relation between the critical shearing stress for twinning plane instability (the start of plane migration) and three elementary physical properties; elastic shear modulus, stacking fault energy, and spacing between {111} planes. Detailed molecular dynamic (MD) calculations yield reasonably good estimates of the actual critical stresses. A scatter plot between actual and scaling stresses in several fcc materials verifies the rough validity of the scaling relation.

MD calculations also provide all the energies and displacements needed to verify and clarify the continuum criterion for stability; see the Appendix A for a brief description of the computational problem. Although molecular dynamics can estimate the critical stress for this particular problem, continuum mechanics in tandem with molecular dynamics gives added depth and insight concerning changes to energetic relationships that would be next to impossible to discern from molecular dynamics alone.

2. Review of stability for bulk material

A theoretical study of the stability of bulk material has been discussed by Hill and Milstein (1977) and by Milstein and Hill (1979). Wang et al. (1995) also gave a derivation of the conditions for loss of stability in a uniformly strained homogeneous crystal and remarked that "The spirit of our analysis here may be compared to a virtual work argument." In fact, a virtual work argument, posed here in the conventional language of nonlinear continuum mechanics, verifies that statement and further clarifies the nature of the possible mechanical instabilities.

Consider a small volume of material that is stress free in an initial configuration, $\boldsymbol{X}$, and that experiences uniform, static stresses and deformations in an equilibrated configuration given by $\boldsymbol{x}(\boldsymbol{X})$ (Refer to Fig. 1). The constant deformation gradient is given by $\boldsymbol{F}=\partial\boldsymbol{x}/\partial\boldsymbol{X}$, and the constant Cauchy stress is denoted by $\bar{\boldsymbol{t}}$. Next imagine that the small volume of material is deformed further to a neighboring equilibrium configuration given by $\boldsymbol{y}=\boldsymbol{y}(\boldsymbol{X})$. The additional small displacement is denoted $\delta\boldsymbol{u}=\boldsymbol{y}-\boldsymbol{x}$, the deformation gradient is $\boldsymbol{F}+\delta\boldsymbol{F}=\partial\boldsymbol{y}/\partial\boldsymbol{X}$, and consequently $\delta\boldsymbol{F}=\partial(\delta\boldsymbol{u})/\partial\boldsymbol{X}$. The Green strain is $\boldsymbol{E}=\frac{1}{2}(\boldsymbol{F}^T\boldsymbol{F}-\boldsymbol{I})$, and to first order the strain increment is $\delta\boldsymbol{E}=\frac{1}{2}(\delta\boldsymbol{F}^T\boldsymbol{F}+\boldsymbol{F}^T\delta\boldsymbol{F})=\frac{1}{2}[\{(\delta\boldsymbol{u})_{,\boldsymbol{X}}\}^T\boldsymbol{F}+\boldsymbol{F}^T(\delta\boldsymbol{u})_{,\boldsymbol{X}}]$, where $(\delta\boldsymbol{u})_{,\boldsymbol{X}}$ denotes $\partial(\delta\boldsymbol{u})/\partial\boldsymbol{X}$ or $\partial(\delta u_i)/\partial X_\alpha;\quad i=1,2,3\,,\ldots,\quad \alpha=1,2,\ldots$. The increment of strain relative to the deformed configuration then is defined as $\delta\boldsymbol{e}=\boldsymbol{F}^{-T}\delta\boldsymbol{E}\boldsymbol{F}^{-1}$, or in Cartesian coordinates this increment of strain is given by the familiar expression

$$\delta e_{ij}=\frac{1}{2}\left(\frac{\partial(\delta u_i)}{\partial x_j}+\frac{\partial(\delta u_j)}{\partial x_i}\right)=\frac{1}{2}(\delta u_{i,j}+\delta u_{j,i}). \tag{1}$$

The stress measure that is work conjugate to the Green strain is the symmetric Piola–Kirchoff stress, $\boldsymbol{T}$. If the Helmholz energy per unit mass is given by $\psi(\boldsymbol{E},T)$, where T is temperature (considered to be constant from here on), then

$$\boldsymbol{T}=\rho_0\frac{\partial\psi}{\partial\boldsymbol{E}}. \tag{2}$$

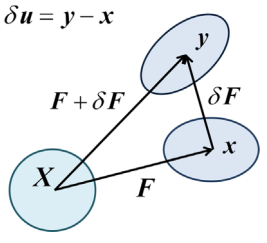

Fig. 1. The geometry of finite elastic deformation with an additional incremental deformation.