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Partitioning of elastic distortions at a semicoherent heterophase interface between anisotropic crystals

A.J. Vattré[a,*] and M.J. Demkowicz[b]

[a]CEA, DAM, DIF, F-91297 Arpajon, France

[b]Department of Materials Science and Engineering, MIT, Cambridge, MA 02139, USA

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Abstract—Bicrystals containing semicoherent interfaces exhibit distortions produced by the superposition of coherency strains and the elastic strain fields of interface Volterra dislocations. Using an approach that combines the quantized Frank–Bilby equation with anisotropic elasticity theory, this residual elastic state is computed for semicoherent heterophase interfaces formed by face- and body-centered cubic crystals. Elastic distortions are found to be unequally partitioned between the neighboring anisotropic materials. For any given heterophase interface, these distortions determine the coherent reference state within which the Burgers vectors of the interfacial dislocations are defined.

Keywords: Semicoherent heterophase interfaces; Anisotropic elasticity; Partitioning of distortions; Misfit dislocation structures

1. Introduction

Interfaces in polycrystalline solids have a profound effect on numerous physical properties, including mechanical behavior [1], electrical conductivity [2] and point defect sink efficiency [3]. One of the longest-standing challenges in materials science is the prediction of these properties from interface structure [4]. However, due to the shear variety and complexity of interfaces in solids [5,6], linking engineering material performance and design with interfacial structure continues to be a difficult task [7,8]. Here, we show how to predict the partitioning of elastic distortions between the neighboring crystals in semicoherent interfaces. Accurate prediction of elastic distortions is required to determine the elastic strain energy of interfaces and to assess elastic interactions between interfaces and extrinsic defects, such as point defects or dislocations.

Semicoherent interfaces have non-uniform structures comprised of misfit dislocations [5,9]. The strain state produced by these interface dislocations accommodates the attendant coherency strains such that the superposed strain fields vanish at long range. Moreover, the rotation state associated with the dislocations must be consistent with the prescribed interface misorientation in bicrystals [10–13]. All these elastic fields are partitioned between the adjacent solids in a manner that depends on their stiffness constants [12,13].

For interfaces formed by isotropic crystals with identical elastic constants, the elastic distortions (strains and rotations) are equally partitioned between each crystal [10,12]. However, for anisotropic bicrystals with dissimilar moduli, the partitioning of strains and rotations is far more complex. The unequal rotational partitioning at two-phase interfaces has been described in Ref. [14], though without considering the general case when both strains and rotations are unequally partitioned.

We have developed a computational method for predicting misfit dislocation patterns in semicoherent heterophase interfaces by combining the quantized Frank–Bilby equation (qFBE) with anisotropic elasticity theory [13]. We used this method to analyze elastic fields near tilt and twist grain boundaries as well as near pure misfit heterophase interfaces [13]. We also discussed the consequences of selecting incorrect coherent reference states and showed that it leads to non-zero far-field stresses as well as far-field rotations inconsistent with prescribed misorientations [8]. Finally, we showed that the strain energies of different dislocation patterns consistent with the qFBE may be used as a criterion for finding the most likely structures of semicoherent interfaces [8,15].

In this paper, we expand on our study of semicoherent heterophase interfaces comprising two sets of dislocations and formed along closest-packed planes in face- and body-centered cubic (fcc/bcc) metals [8]. We show that elastic distortions, i.e. strains as well as tilt and twist rotations, are in general unequally partitioned at such interfaces. The correct partitioning of these fields determines the coherent reference state for which the bicrystal of interest is free of far-field

* Corresponding author; e-mail: aurelien.vattre@cea.fr

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strains. Using these results, we compute and analyze the stress fields generated by misfit dislocation patterns for the Cu/Nb system in the Nishiyama–Wassermann (NW) [16,17] and Kurdjumov–Sachs (KS) [18] orientation relations (ORs). We also determine the dislocation structure (i.e. the Burgers vectors, spacings and line directions) in lowest strain energy solutions of the qFBE along a specific transformation pathway between the NW and KS ORs.

In Section 2 we briefly describe the methodology for determining the reference states by combining the qFBE with anisotropic elasticity theory for fcc{111}/bcc{110} interfaces in the NW OR as well as in ORs that differ from the NW by an in-plane twist rotation. Section 3 deals with partitioning of elastic distortions for specific interfaces: Cu/Nb, Ag/V and Cu/Mo interfaces in the NW and KS ORs. We show that spurious elastic fields arise when an incorrect reference state is selected. When the correct reference state is determined, the approach is used to find the dislocation pattern with minimum local elastic energy between the NW and KS ORs. Section 4 provides a summary of our main conclusions.

2. The reference and natural states

The concept of reference and natural states of an interface is depicted in Fig. 1. The natural state contains an interface formed by joining two crystals with prescribed misorientation and interface planes as well as vanishing far-field strains [13]. This state is related to a single-crystal, coherent reference state by uniform displacement gradients ${}_{\text{fcc}}\mathbf{F}$ and ${}_{\text{bcc}}\mathbf{F}$, which map the reference state to the natural state [12,13], as shown in Fig. 1(a). In the reference state, the interface is coherent, i.e. the two adjacent materials that meet at the interface are rotated and strained such that they are in perfect registry with each other across the $\hat{\boldsymbol{X}}-\hat{\boldsymbol{Z}}$ interface plane after bonding. In general, these displacement gradients entail interface misorientations that have both tilt and twist components [5,9,12]. In the natural state, the interface along the $\hat{\boldsymbol{x}}-\hat{\boldsymbol{z}}$ plane is not coherent, but rather semicoherent due to the presence of misfit dislocations.

We focus on atomically sharp fcc{111}/bcc{110} interfaces in NW and in-plane twisted-NW ORs containing two periodic arrays of infinitely long, straight and uniformly spaced dislocations [13]. In the NW OR, one of the ⟨110⟩ directions in an fcc {111} plane lies parallel to the ⟨100⟩ direction in a bcc {110} plane [16,17]. The in-plane twisted-NW ORs considered here differ from the NW OR only by a twist rotation of one crystal (here, the bcc material) with respect to the adjacent (fcc) crystal about the axis normal to the interface.

To determine the unique reference states that meet the condition of vanishing far-field strains and prescribed misorientation for such interfaces, we follow a three-step procedure:

① The dislocation content $\boldsymbol{B}$ of an interface, intersected by a probe vector $\boldsymbol{p}$ contained within the interface plane as illustrated in Fig. 1(b), is described by the qFBE [5,19,20]:

$$\boldsymbol{B}=\sum_{i=1}^{2}\left(\frac{\boldsymbol{n}\times\boldsymbol{\xi}_i}{d_i}\cdot\boldsymbol{p}\right)\boldsymbol{b}_i=\left({}_{\text{fcc}}\mathbf{F}^{-1}-{}_{\text{bcc}}\mathbf{F}^{-1}\right)\boldsymbol{p}=\mathbf{T}\boldsymbol{p} \tag{1}$$

Here, $\boldsymbol{n}$ is the unit vector normal to the interface, $\boldsymbol{\xi}_i$ is the line direction of the i^{th} set of dislocations, d_i is the spacing and $\boldsymbol{b}_i$ is the corresponding Burgers vector. As discussed in Ref. [13], the O-lattice vectors $\boldsymbol{p}_i^{\text{o}}$, and therefore the geometries of interface dislocations (line directions and spacings), are independent of the choice of the reference state. Thus, following previous investigators [21–23], we initially select the fcc crystal as the reference state within which three Burgers vectors are selected. Approaches stemming from Bollmann's O-lattice theory [22] may then be used to compute $\boldsymbol{n}, \boldsymbol{\xi}_i$ and d_i [24,25] from the O-lattice vectors $\boldsymbol{p}_i^{\text{o}}$, defined by $\boldsymbol{b}_i=\mathbf{T}\boldsymbol{p}_i^{\text{o}}$ with $\boldsymbol{p}_1^{\text{o}}\neq\boldsymbol{p}_2^{\text{o}}$. Because fcc {111} planes contain three $a/2\langle110\rangle$-type Burgers vectors, three dislocation geometries comprised of two arrays of parallel dislocations (with no local reactions at nodes) are possible in these interfaces [23].

② For interfaces in the NW OR, we define a transformation pathway that continuously adjusts the reference state from the strain-free state of the fcc crystal present at the interface to that of the adjacent bcc crystal. For all reference states along this path, we use the method described in Refs. [13,8] to compute the superposition of the uniform coherency strains, $\mathbf{E}_{\text{c}}$, needed to maintain perfect registry and the far-field strain fields produced by the Volterra dislocation arrays, $\mathbf{E}_{\text{dis}}^{\infty}$. In the correct reference state, these quantities cancel and the total far-field strain field $\mathbf{E}_{\text{tot}}$ vanishes in both upper fcc ($\hat{\boldsymbol{y}}>0$) and lower bcc ($\hat{\boldsymbol{y}}<0$) materials:

$$\lim_{\hat{\boldsymbol{y}}\to\pm\infty}\mathbf{E}_{\text{tot}}(\hat{\boldsymbol{x}},\hat{\boldsymbol{y}},\hat{\boldsymbol{z}})=\mathbf{0}\Longleftrightarrow\begin{cases}{}_{\text{fcc}}\mathbf{E}_{\text{tot}}^{\infty}={}_{\text{fcc}}\mathbf{E}_{\text{c}}+{}_{\text{fcc}}\mathbf{E}_{\text{dis}}^{\infty}=\mathbf{0}\\ {}_{\text{bcc}}\mathbf{E}_{\text{tot}}^{\infty}={}_{\text{bcc}}\mathbf{E}_{\text{c}}+{}_{\text{bcc}}\mathbf{E}_{\text{dis}}^{\infty}=\mathbf{0}\end{cases} \tag{2}$$

These requirements restrict the choice of reference states to a single specific one [13], for which the far-field rotation state in the NW OR is consistent with the given crystallographic character (interface plane and misorientation).

To find the reference state for interfaces differing from those in the NW OR by an in-plane twist angle θ, a second pathway is defined by rotating the previously determined reference state in the NW OR from 0 to θ. Along this second path we find that the rotated reference state for which Eqs. (2) are satisfied also yields far-field rotations consistent with the in-plane prescribed twist misorientations.

③ Using the correct reference states for all ORs, we compute the short-range interface strains and stresses that arise from the incomplete cancellation of the coherency and Volterra dislocation fields near the interfaces. We also compute the interface elastic energy as a surface integral over a unit cell, A, of the misfit dislocation pattern:

$$\gamma_{\text{elastic}}=\frac{1}{2A}\iint_{A}\boldsymbol{\sigma}_{\text{tot}}(\hat{\boldsymbol{x}},0,\hat{\boldsymbol{z}})\boldsymbol{n}\cdot\Delta\boldsymbol{u}_{\text{dis}}(\hat{\boldsymbol{x}},\hat{\boldsymbol{z}})\,dS \tag{3}$$

Here, $\boldsymbol{\sigma}_{\text{tot}}\boldsymbol{n}$ is the traction vector produced at the interface and $\Delta\boldsymbol{u}_{\text{dis}}$ is the disregistry vector produced by the two sets of misfit dislocations [13]. We limit the domain of integration to parts of the interface unit cell that are not within a pre-determined cutoff distance r_0 of the dislocation cores. We have previously described how this elastic strain energy may be used to determine the likeliest interface misfit dislocation configurations whenever the qFBE (Eq. (1)) admits multiple solutions [8,15], so this point will not be discussed further in the present work. However, in this paper we will illustrate the complex distribution of the short-range stress fields that arise near fcc/bcc interfaces as a result.