A phase field dislocation dynamics model for a bicrystal interface system: an investigation into dislocation slip transmission across cube-on-cube interfaces

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Abstract

In this work, we present a phase field dislocation dynamics formulation designed to treat a system comprised of two materials differing in moduli and lattice parameters that meet at a common interface. We apply the model to calculate the critical stress τ_{crit} required to transmit a perfect dislocation across the bimaterial interface with a cube-on-cube orientation relationship. The calculation of τ_{crit} accounts for the effects of: 1) the lattice mismatch (misfit or coherency stresses), 2) the elastic moduli mismatch (Koehler forces or image stresses), and 3) the formation of the residual dislocation in the interface. Our results show that the value of τ_{crit} associated with the transmission of a dislocation from material 1 to 2 is not the same as that from material 2 to 1. Dislocation transmission from the material with the lower shear modulus and larger lattice parameter tends to be easier than the reverse and this apparent asymmetry in τ_{crit} generally increases with increases in either lattice or moduli mismatch or both. In efforts to clarify the roles of lattice and moduli mismatch, we construct an analytical model for τ_{crit} based on the formation energy of the residual dislocation. We show that path dependence in this energetic barrier can explain the asymmetry seen in the calculated τ_{crit} values. Significantly, it reveals that τ_{crit} scales with $\frac{a^{(2)}G^{(2)}}{a^{(1)}+a^{(2)}} \left(\frac{a^{(1)}}{a^{(2)}} - \frac{G^{(1)}}{G^{(2)}} \right)^2$, where G is the shear modulus, a is the lattice parameter, and the superscripts (1) and (2) indicate quantities for material 1 and material 2, respectively.

Keywords:

dislocations, crystal plasticity, metallic material

1. Introduction

In recent years, two-phase or nanolayered metals have received much attention due to reports of superior strength and ductility in ambient and extreme temperatures (Misra et al., 2005; Zheng et al., 2014; Mara and Beyerlein, 2014; Nizolek et al., 2015). As in any metal, their plastic deformation behavior and strength are governed by the motion of dislocations, which are generated when the material is mechanically deformed. However, unlike traditional or coarser-grained metals, the nanoscale dimensions (grain sizes less than 100 nm) of these metals result in activation of unique deformation mechanisms, such as partial dislocation mediated plasticity, twinning, and grain boundary sliding, that can drastically impact the overall material strength response of these metals (Van Swygenhoven et al., 1999a,b; Yamakov et al., 2004; Farkas et al., 2005; Chen et al., 2003; Van Swygenhoven et al., 2004; Schiøtz and Jacobsen, 2003; Vo et al., 2008; Shan et al., 2004; Liao et al., 2003; Yamakov et al., 2003). Further complexity is added when these nanoscale materials are layered creating two-phase or multiphase composite systems (Chu et al., 2013). The exceptional properties of these nanolayered metals can be attributed to the interaction of dislocations with the bimetal

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interfaces (Embury and Hirth, 1994; Werner and Stüwe, 1985; Wang et al., 2008; Martinez et al., 2014; Beyerlein et al., 2015b). Unfortunately, there are still gaps in understanding in the dominant dislocation-interface interactions, and how these interactions are impacted by changes in grain size, temperature, loading conditions, etc. Moreover, this lack of understanding has made it difficult to develop predictive, physically informed models. Such a capability would provide a better understanding of dislocation-interface interactions and also aid in the design of even stronger and more robust multiphase nanolayered metals than those realized today.

One particular dislocation-interface mechanism is slip transmission, i.e., the transmission of a dislocation across the interface from one material into another. The critical threshold stress, τ_{crit} that must be overcome for slip transmission occur can be several orders of magnitude greater than the Peierls barrier that the same dislocation would overcome in order to glide in its habit glide plane (Rao and Hazzledine, 2000; Misra et al., 2005; Hoagland et al., 2004). This ability of interfaces to act as obstacles to dislocation motion contributes to the exceptional strength of two-phase nanomaterials. Hence, due to its importance, many modeling and experimental studies have been carried out to understand how interface properties affect τ_{crit} . Modeling efforts vary widely over length scale, ranging from continuum mechanics models to simple geometric models to atomistic simulations (Chu et al., 2013; Mayeur et al., 2013; Hoagland et al., 2002, 2004; Koehler, 1970; Pacheco and Mura, 1969; Shehadeh et al., 2007; Wang et al., 2008). From this body of work, it can be appreciated that τ_{crit} is not the same for all bimaterial interfaces and is sensitive to the orientation relationship, lattice parameter mismatch, and moduli mismatch across the interface. These trends inspire the idea that materials can be optimized via bimetal interface design.

Early continuum mechanics models studied the effect of image forces, present due to moduli mismatch, on τ_{crit} (Koehler, 1970; Pacheco and Mura, 1969), by predicting the stress fields on dislocations within a finite distance from the interface ($\sim 2b$). The interfaces modeled were nearly coherent so that the lattice mismatch and resulting misfit strains were negligible. In two-phase bimetal systems, the difference in line energy ($\sim Gb^2$) of the dislocation in material 1 versus material 2 can cause an asymmetry in τ_{crit} , such that dislocations prefer to transmit from material 1 to 2 when the dislocation has the lower line energy in material 2. By considering the stress state when a dislocation interacts with these image forces, Koehler estimated that the stress required to bring the dislocation to the interface in the non-preferred direction, that is, when originating from the softer material, scales as $G^{(1)}(G^{(2)} - G^{(1)})/(G^{(2)} + G^{(1)})$ (Koehler, 1970). On this basis, it was suggested that τ_{crit} for a dislocation to transmit from the softer to the stiffer material would scale in the same way.

Because continuum scale models are applicable to larger length scales, they do not explicitly account for any microscopic considerations of the bimetal system, such as differences in lattice parameter or in crystallographic orientation between the two adjoining materials. At least two effects can arise from such finer length-scale differences. First, making the mismatched lattices coherent in order to have a fully bonded interface can induce a misfit strain field and/or create misfit dislocations in the interface (Frank and van der Merwe, 1949; Shoykhet et al., 1998; Matthews and Blakeslee, 1974; Chu et al., 2013), which can affect the lattice dislocation attempting to transmit across the interface. Second, the value of the Burgers vector of the lattice dislocation, which scales with the lattice parameter, changes as it transmits from material 1 to material 2. A residual dislocation gets deposited at the interface during the slip transmission event and serves as an energetic penalty to transmission.

The effects of differences in crystallographic orientation (or misorientation) across the interface on τ_{crit} have been captured by many geometric models. Much of the earlier work on slip transmission involved experimental characterization and development of geometric based criteria for whether the dislocation was prone to crossing the interface (Livingston and Chalmers, 1957; Lim and Raj, 1985; Misra and Gibala, 1999; Werner and Prantl, 1990; Lee et al., 1990; Robertson et al., 1989). The basic idea behind these criteria is that the more aligned the two slip systems are on either side of the interface, the more likely transmission will occur. The better alignment of slip plane results in a smaller Burgers vector value of the residual dislocation formed in the interface; therefore, it is the more favorable formation pathway. On this basis, τ_{crit} is expected to scale as the self-energy of the residual dislocation (Misra and Gibala, 1999; Lim and Raj, 1985; Ma et al., 2006) and be even higher in the event that the transmission leaves a step in the interface (Hoagland et al., 2002; Henager Jr. and Hoagland, 2004). Furthermore, these models studied the resolved shear stresses that drive the dislocations to move. They found that slip transmission is more likely to occur when the local stress states in the adjoining crystals were sufficient to push the dislocation into one side of the interface and out of the other side (Lee et al., 1990; Misra and Gibala, 1999).

Finally, at the lowest lengths scales, molecular dynamics (MD) simulations and atomically informed meso-scale micromechanical models (Hoagland et al., 2002, 2004; Rao and Hazzledine, 2000; Anderson et al., 1999; Anderson

and Li, 1995; Shehadeh et al., 2007; Wang et al., 2008) have also been employed to study slip transmission across a bimetal interface. Since atomic-scale methods resolve the individual atoms in the crystal lattice, the core region of the dislocation can be modeled. During transmission, observations of core spreading within the interface plane, changes in stacking fault width, and separate transmissions of leading and trailing partials are reported. They indicate that in addition to the mismatch in linear elastic moduli and crystallographic orientation, many other factors can significantly impact τ_{crit} , such as the coherency (or misfit) strains generated due to lattice mismatch at the interface, interactions with misfit dislocations lying in the interface, or the effects of nonlinear elastic moduli at the interface. Furthermore, unlike continuum or geometric based models, atomic-scale based techniques can account for changes in the dislocation core structure as the dislocation attempts to traverse the interface (Hoagland et al., 2002; Henager Jr. and Hoagland, 2004; Rao and Hazzledine, 2000). It has been shown that mechanisms for transmission can depend on the atomic structure of the interface. For instance, for coherent or semi-coherent interfaces in face-centered cubic (fcc) bicrystals, the core of an fcc dislocation can extend into a leading and trailing partial, where the leading transmits first followed by the trailing partial (Hoagland et al., 2002, 2004). The cores of full or partial dislocations of screw character attempting to transmit can instead spread in the interface (Rao and Hazzledine, 2000; Anderson and Li, 1995), hindering its transmission. For incoherent interfaces, such as Cu-Nb, the cores of incoming dislocations tend to spread for those interface characters that are weak in shear, again, making it difficult for the dislocation to transmit (Wang et al., 2008). However, for another Cu-Nb interface with a different crystallographic character that has a much higher shear resistance, the core of an incoming dislocation tends to remain compact making it easier to transmit (Beyerlein et al., 2012).

From the above assessment of modeling efforts, a need arises for a meso-scale modeling tool that can capture many of these effects occurring across the atomic to meso-scale length scales, but also inform the larger length scale continuum and geometric methods. Such a tool would be expected to assess multiple discrete dislocation loops, possibly moving across many interfaces of differing crystallography and spacing. Kinetics would be simulated over longer periods of time and stress states and strain rates closer to those realized in actual strained crystals than those attainable with atomistic methods. Toward this end, we advance a meso-scale technique, called phase field dislocation dynamics (PFDD), for mechanically deformed crystals in which discrete dislocations and grain boundaries and interfaces can be modeled explicitly. The fundamental framework of the PFDD model is energy-based, hence it determines the motion and configuration of individual dislocations by minimizing the total system energy. By not explicitly accounting for atomic motions and interactions, much larger crystal sizes and longer time scales (on the order of seconds) can be assessed. This allows the model to treat interesting deformation phenomena operating in the meso-scale regime. In its original formulation, PFDD has been applied to study dislocation motion in single-phase fcc crystals. Over the years, its formulation has been extended to treat polycrystals, grain boundary sliding, and dislocation nucleation from grain boundaries (Cao et al., 2015; Koslowski et al., 2011; Hunter and Beyerlein, 2014b). In efforts to recover some atomic-scale physics, its formulation has been extended to permit incorporation of the energetics of atomic-scale dislocation cores from density functional theory (DFT) calculations to study partial dislocation nucleation and deformation twinning (Hunter et al., 2014; Hunter and Beyerlein, 2014b,a, 2015). Most recently, PFDD has been advanced to treat two-phase metals (Lei et al., 2013).

In this work, we develop a bimaterial interface model within the PFDD framework and use it to simulate a slip transmission event, wherein a perfect dislocation originating in one crystal crosses the bimetal interface to the other crystal differing in elastic modulus and lattice parameter. Model development includes extending the bimaterial PFDD formulation to account for the local energy terms in the interface region that are involved when a dislocation directly interacts with the bimaterial interface. The calculations aim to determine the minimum or critical resolved shear stress τ_{crit} required for the dislocation to successfully transmit through a completely intact interface. To this end, we extend the PFDD model to account for the effects of: 1) the stresses induced at the interface due to the lattice mismatch (coherency stresses), 2) the elastic moduli mismatch (Koehler forces), and 3) the formation energy of the residual dislocation. In the examples presented, both crystals have an fcc crystal structure, form an interface at their mutual (001) plane, and have a cube-on-cube orientation relationship. A wide range of fcc/fcc bimaterial systems with low lattice mismatch ($< 3.5\%$) is considered.

The set of simulations presented here reveal an asymmetry in τ_{crit} with respect to the slip transmission pathway. In most cases, τ_{crit} is higher when the dislocation transmits from a softer to stiffer material and from a material with a larger lattice parameter, a . Further, composite systems with low lattice and moduli mismatch, like Au-Ag, tend to have a small asymmetry, whereas systems with much larger lattice and moduli mismatch, like Cu-Ni and Al-Pt, have a

strong asymmetry. To achieve a better understanding of the role of lattice and moduli mismatch, we develop analytical expressions for the energy required to form a residual Burgers vector in the interface and the critical transmission stress associated with it. We show that the formation energy of the residual dislocation exhibits path dependence and can explain the asymmetry in τ_{crit} . Significantly, the analysis reveals that τ_{crit} strongly scales with $\frac{a^{(2)}G^{(2)}}{a^{(1)}+a^{(2)}} \left(\frac{a^{(1)}}{a^{(2)}} - \frac{G^{(1)}}{G^{(2)}} \right)^2$, where G is the shear modulus, a is the lattice parameter, and the superscripts (1) and (2) indicate quantities for material 1 and material 2, respectively.

2. Methodology

Phase field dislocation dynamics (PFDD) is a model that predicts the motion of individual dislocations in crystals (Wang et al., 2001; Koslowski et al., 2002; Koslowski, 2007, 2010; Hunter et al., 2011; Hunter and Beyerlein, 2014b). The basic framework of this model relies on the evolution of phase field variables (also called order parameters), which are scalar variables that vary in space and time. In PFDD, a phase field variable $\xi^\alpha(\mathbf{x}, t)$ is assigned to each active slip system α in the crystal. Its value is used to track the sign and the number of dislocations that cross the slip plane at position $\mathbf{x}$ and time t (Koslowski et al., 2002; Hunter and Beyerlein, 2014b). Where and when a dislocation belonging to slip system α has slipped, the phase field variable ξ^α increments by one (positive integer increments correspond to positively signed dislocations and likewise negative integer increments correspond to negatively signed dislocations). For un-slipped regions, the phase field variable equals zero. So called active phase field variables refer to times and locations where the phase field variable is non-zero and dislocations have slipped. The slip displacement caused by the motion of only one dislocation is $\xi^\alpha b$, where ξ^α equals one and b is the value of the Burgers vector of the dislocation belonging to slip system α .

In this work, plasticity is mediated by the motion and interactions of lattice dislocations (as opposed to other inelastic mechanisms such as grain boundary sliding or deformation twinning). The plastic strain, ϵ^p , is, therefore, directly dependent on the active phase field variables as given by (Koslowski et al., 2002):

$$\epsilon_{ij}^p(\mathbf{x}, t) = \frac{1}{2} \sum_{\alpha=1}^N \xi^\alpha(\mathbf{x}, t) \delta_\alpha \left(s_i^\alpha m_j^\alpha + s_j^\alpha m_i^\alpha \right), \quad (1)$$

where N is the number of slip systems, $\mathbf{s}^\alpha$ is the direction of the Burgers vector, $\mathbf{m}^\alpha$ is the slip plane normal, and δ_α is a Dirac distribution supported on the slip plane α . The evolution of these phase field variables under loading is governed by the minimization of the total system energy E through use of a Ginzburg-Landau equation (Wang et al., 2001; Koslowski et al., 2002; Hunter and Beyerlein, 2014b).

In following sections, the PFDD model is further developed to calculate the critical stress τ_{crit} to pass a dislocation across the interface of the bicrystal. In Section 2.1 the relationship between the motion and interaction of dislocations and the differences in elastic moduli is presented. Sections 2.2 and 2.3 describe how PFDD accounts for local interface effects such as differences in lattice parameters and formation of residual dislocations, and how they connect to the overall formulation for dislocation motion.

2.1. PFDD for a bimaterial system

The basic model geometry treated here is a bicrystal comprised of two fcc crystals joined at a single common interface. The volumes of the two crystals are equal. The crystals differ in their elastic moduli and lattice parameters. Notationally, properties of these two materials will be indicated by superscripts (1) and (2). The interface has a known crystallographic character, described by the crystallographic plane of each crystal corresponding to the interface plane and the orientation relationship of the two crystals.

For each fcc crystal in the bicrystal, the preferred slip planes and slip directions belong to the family of $\{111\} \langle 110 \rangle$ slip systems. Accordingly, the model has 12 phase field variables, $\alpha = 1 \dots 12$. The same 12 phase field variables are used for the entire bicrystal system. For instance, the phase field variable associated with the (111)[10 $\bar{1}$] slip system is the same variable whether in material 1 or material 2. It is the same order parameter but evaluated at two different positions $\mathbf{x}$. With the phase field variables known, Equation 1 is used to calculate ϵ^p in each crystal.

The difference in elastic moduli at the bimaterial interface creates an internal stress field, which in studies of bilayered composites is often referred to as the Koehler force (Koehler, 1970). In the inhomogeneous PFDD model,

recently presented by Lei et al. (2013), this image force caused by the moduli mismatch is calculated by making use of Eshelby's equivalent inclusion method (Mura, 1987). In this method, an inhomogeneous system consisting of a matrix containing inhomogeneities is replaced with a homogeneous system comprised of the matrix and an eigen- or virtual strain, ϵ^v that is non-zero in regions where the inhomogeneity existed. For the bimaterial system considered in this work, the inhomogeneous system is made up of the matrix material, material 1, and a single inhomogeneous region that is material 2. The equivalent homogeneous system is comprised fully of material 1 with a virtual strain that is non-zero and evolved throughout the simulation in the region where material 2 should be. Henceforth, calculation of ϵ^v will be described in the context of the particular two-phase bicrystal geometry of interest here and we refer the reader to Lei et al. (2013) for the basic formulation.

The total system energy E is the sum of two primary contributions, E^{strain} and E^{core} (Koslowski et al., 2002; Lei et al., 2013):

$$E = E^{strain} + E^{core}. \quad (2)$$

E^{strain} represents the strain energy stored within the system and E^{core} is the energy barrier encountered by dislocations as they move through the crystal lattice (i.e., the Peierls barrier). In this work, the total energy of the system E is a function of the virtual strain $\epsilon^v(\mathbf{x}, t)$ and phase field variables $\xi^\alpha(\mathbf{x}, t)$, which account for the motion of the dislocations leading to ϵ^p . The relationship between E^{strain} and E^{core} and $\epsilon^v(\mathbf{x}, t)$ and phase field variables $\xi^\alpha(\mathbf{x}, t)$ are described next.

For a system that has inhomogeneities, E^{strain} can be written in terms of the energy of the equivalent, homogeneous system, E^{eq} plus the difference in energy, ΔE between the inhomogeneous and homogeneous systems. The complete E^{strain} can be expressed as (Lei et al., 2013)

$$E^{strain} = E^{eq} + \Delta E = \frac{1}{2} \int C_{ijkl}^{(1)} (\epsilon_{ij}(\mathbf{x}) - \epsilon_{ij}^0(\mathbf{x})) (\epsilon_{kl}(\mathbf{x}) - \epsilon_{kl}^0(\mathbf{x})) d^3\mathbf{x} - \frac{1}{2} \int_2 (C_{ijmn}^{(1)} \Delta S_{mnpq}(\mathbf{x}) C_{pqkl}^{(1)} + C_{ijkl}^{(1)}) \epsilon_{ij}^v(\mathbf{x}) \epsilon_{kl}^v(\mathbf{x}) d^3\mathbf{x}, \quad (3)$$

where $\epsilon_{ij}(\mathbf{x})$ is the total strain. The first integral for E^{eq} is taken over the whole domain (materials 1 and 2), and the second integral for ΔE is taken over material 2 only. In Equation 3, the strain ϵ_{ij}^0 is defined as:

$$\epsilon_{ij}^0(\mathbf{x}) = \begin{cases} \epsilon_{ij}^p(\mathbf{x}) & \text{if } \mathbf{x} \in \text{material 1} \\ \epsilon_{ij}^p(\mathbf{x}) + \epsilon_{ij}^v(\mathbf{x}) & \text{if } \mathbf{x} \in \text{material 2.} \end{cases} \quad (4)$$

In addition, we define $C_{ijkl}^{(1)}$ and $C_{ijkl}^{(2)}$ as the stiffness tensors in materials 1 and 2, respectively. $\Delta S_{mnpq}(\mathbf{x}) = (C_{mnpq}(\mathbf{x}) - C_{mnpq}^{(1)})^{-1}$ is only defined in material 2, where $C_{mnpq}(\mathbf{x})$ is a stiffness tensor defined as:

$$C_{mnpq}(\mathbf{x}) = \begin{cases} C_{mnpq}^{(1)} & \text{if } \mathbf{x} \in \text{material 1} \\ C_{mnpq}^{(2)} & \text{if } \mathbf{x} \in \text{material 2.} \end{cases} \quad (5)$$

Using stress equilibrium and the principle of superposition, we have the following expression for the total strain $\epsilon_{ij}(\mathbf{x})$ (Lei et al., 2013):

$$\epsilon_{ij}(\mathbf{x}) = \bar{\epsilon}_{ij}^0 + \oint \hat{G}_{jk}(\mathbf{k}) k_i k_l C_{klmn}^{(1)} \hat{\epsilon}_{mn}^0(\mathbf{k}) e^{ikx} \frac{d^3k}{(2\pi)^3} + S_{ijkl}^{(1)} \sigma_{kl}^{ap}, \quad (6)$$

where the super-posed ($\hat{\cdot}$) stands for the Fourier transformation, $G_{ki}(\mathbf{x})$ is the elastic Green's function, k_i is the wave number vector, $\oint$ represents the principal value of the integral, $\bar{\epsilon}_{ij}^0 = \frac{1}{V} \int \epsilon_{ij}^0(\mathbf{x}) d^3\mathbf{x}$ is the average stress-free strain and V is the volume of the computational domain, $S_{ijkl}^{(1)}$ is the compliance tensor in material 1, and σ_{ij}^{ap} is the externally applied stress. Substituting Equations 4 and 6 into Equation 3 allows us to express the E^{strain} in terms of the plastic and virtual strains (Lei et al., 2013):

$$\begin{aligned}
E^{strain} &= E^{eq} + \Delta E \\
&= \frac{1}{2} \int \hat{A}_{mnuv}(\mathbf{k}) (\hat{\epsilon}_{mn}^v(\mathbf{k}) + \hat{\epsilon}_{mn}^p(\mathbf{k})) (\hat{\epsilon}_{uv}^{v*}(\mathbf{k}) + \hat{\epsilon}_{uv}^{p*}(\mathbf{k})) \frac{d^3 k}{(2\pi)^3} \\
&\quad - \frac{V}{2} S_{ijkl}^{(1)} \sigma_{ij}^{ap} \sigma_{kl}^{ap} - \sigma_{ij}^{ap} \int (\epsilon_{ij}^v(\mathbf{x}) + \epsilon_{ij}^p(\mathbf{x})) d^3 x \\
&\quad - \frac{1}{2} \int_2 (C_{ijmn}^{(1)} \Delta S_{mnpq}(\mathbf{x}) C_{pqkl}^{(1)} + C_{ijkl}^{(1)}) \epsilon_{ij}^v(\mathbf{x}) \epsilon_{kl}^v(\mathbf{x}) d^3 x,
\end{aligned} \tag{7}$$

where $\hat{A}_{mnuv}(\mathbf{k}) = C_{mnuv}^{(1)} - C_{kluv}^{(1)} C_{ijmn}^{(1)} \hat{G}_{ki}(\mathbf{k}) k_j k_l$. The first three terms constitute the internal strain energy: the first integral describes that from elastic interactions including dislocation-dislocation interactions, the second from the externally applied stress σ_{ij}^{ap} , and the third from the interaction energy between σ_{ij}^{ap} and the plastic and virtual strains. The final integral accounts for elastic strain energy due to the presence of the inhomogeneity, which generates an internal stress state due to the difference in elastic moduli between the two bicrystals.

Last, we describe E^{core} , the energy expended as dislocations glide through the crystal lattice by breaking and reforming atomic bonds. This energy term is directly dependent on the active phase field variables, but not the virtual strain. Non-zero, non-integer values of the phase field parameter represent the dislocation line, i.e., where the core lies. E^{core} is non-zero in these regions because it represents the region in which the atomic bonds are breaking in order to translate a dislocation. In contrast, non-zero, integer values of the phase field parameter represent perfect Burgers vector translations, i.e., where a perfect dislocation has slipped. Therefore, E^{core} is zero in these regions because the atomic bonds have already been reformed. As in prior works (Wang et al., 2001; Koslowski et al., 2011; Lei et al., 2013), we model the Peierls potential as a sinusoidal function. A sinusoidal function is considered suitable since it exhibits a periodicity that follows the regular atomic lattice of a cubic crystal structure. Using this model, the expression for E^{core} is given by:

$$E^{core} = \sum_{\alpha=1}^N \int B \sin^2(\pi \xi^\alpha(\mathbf{x})) \delta_\alpha d^3 x, \tag{8}$$

where B defines the magnitude of the energy barrier. Here we use a model from Ortiz and Phillips (1999), which relates B to the properties of the material as follows:

$$B = \left(\frac{1}{2\pi}\right)^2 \frac{1}{d} C'_{ijkl} b_i b_k m_j m_l, \tag{9}$$

where $\mathbf{b}$ is Burgers vector, $\mathbf{m}$ is slip plane normal, d is the inter-planar spacing distance between two adjacent (111) planes, and C'_{ijkl} is the stiffness tensor in the local coordinate system (x' , y' , z') of the slip system of the active phase field variable. In the present calculations, we assume elastic isotropy and slip plane normal points to z direction. With this, B simplifies to:

$$B = \left(\frac{1}{2\pi}\right)^2 \frac{1}{d} C_{i3k3} b_i b_k, \tag{10}$$

where as before, C_{ijkl} is the stiffness tensor in global coordinate system (x, y, z). Tables 1 and 2 in Section 3 lists the values of B in units of mJ/m^2 used in the present calculations. Consequently in the bicrystal model, E^{core} will depend on whether the dislocation is moving in material 1 or material 2.

At every time increment, the phase field variables and virtual strain are determined by minimization of the total energy in the system, E . As in prior work, minimization is carried out using the following set of time-dependent Ginzburg-Landau (TDGL) kinetic equations (Wang et al., 2001; Koslowski et al., 2002; Lei et al., 2013):

$$\begin{aligned}
\frac{\partial \xi^\alpha(\mathbf{x}, t)}{\partial t} &= -L \frac{\delta E(\xi, \epsilon^v)}{\delta \xi^\alpha(\mathbf{x}, t)} \text{ in materials 1 and 2,} \\
\frac{\partial \epsilon_{ij}^v(\mathbf{x}, t)}{\partial t} &= -K \frac{\delta E(\xi, \epsilon^v)}{\delta \epsilon_{ij}^v(\mathbf{x}, t)} \text{ in material 2,}
\end{aligned} \tag{11}$$

where L is a kinetic coefficient that defines the time scale of the simulation, and K is a material constant related to material 2. The phase field variables are associated with plasticity and these evolve in the entire domain in order to account for plasticity throughout the system. In contrast, the virtual strain evolves only within the region of inhomogeneity (material 2 in the bicrystal model). Outside of this region, the virtual strain is zero. For the simulations discussed in the sections below, we assume quasi-static loading. Hence we are mainly concerned with the equilibrium state at the end of each time step, even though a time-dependent equation is used for system evolution. Equilibrium is reached when the left-hand side of Equation 11 becomes 0. Thus, the equilibrium state is independent of parameters L and K . Numerically, this criterion is achieved through iteration over the total system energy. Convergence is reached when the error in the total system energy is less than 10^{-7} .

With the solution for the phase field variables and virtual strain, the mechanical stress and strain fields and location of the dislocations in the entire system are then determined. However, local interface effects still have not been accounted for. In the next two sections we present extensions of the PFDD model to account for misfit stresses/strains at the interface, and the energy required to form a residual dislocation in the interface during a slip transmission event.

2.2. Accounting for the misfit strain at the bimaterial interface

In the bicrystal material model of interest here, the lattice parameters $a^{(1)}$ and $a^{(2)}$ of material 1 and material 2 will generally not be equal. A lattice parameter mismatch at the interface generates a localized misfit strain as the atoms must distort in the region near the interface in order to attain a coherent interface. The misfit stress corresponding to this strain is equal in magnitude but opposite in sign in material 1 and material 2 in order to maintain equilibrium. The material with the larger lattice parameter is in compression, while the material with the smaller lattice parameter is in tension. Atomic-scale calculations on Cu-Ni interfaces with a cube-on-cube orientation relationship have indicated that the resulting misfit strain (and stress) is maximum at the interface (Hoagland et al., 2002) and decays rapidly to zero over several lattice spacings (Shoykhet et al., 1998). As such, the localized stress and strain state caused by the lattice misfit at the interface can be sufficient to affect the motion of dislocations attempting to cross the interface. However, they are not likely to affect dislocations gliding far from the interface.

In the PFDD model individual atomic positions are not modeled, and therefore, to account for the lattice mismatch, we add the misfit strain to the formulation of the total system energy. In doing so, it is important to specify the type of bimaterial interfaces being modeled. In the examples to follow, we consider a bicrystal containing an interface with a cube-on-cube orientation relationship and a (001) interface plane. With a cube-on-cube orientation relationship, the same axes in crystals 1 and 2 are parallel and the slip planes and slip directions are continuous across the interface. The expression we employ to calculate the misfit strain best applies to this particular interface crystallography. Moreover, it assumes that the bimaterial system has a low lattice parameter mismatch (approximately $< 3.5\%$) such that the interfaces are either coherent or semi-coherent with widely spaced misfit dislocations with coherent regions in between. Consequently, the PFDD simulation results presented in later sections would best apply to dislocations attempting to cross the coherent regions of the semi-coherent interface. (Although later in Section 3.2, we will also use the model to consider a case where the lattice mismatch is much greater.)

For this misfit strain calculation, we first consider a local coordinate system (x_1, x_2, x_3) lying in the interface plane as shown in Figure 1. For an interface with a cube-on-cube orientation relationship, the assumption of plane stress in the plane of the interface can be appropriately adopted. This leads to the following basic formulation of the misfit strain is (Hoagland et al., 2002):

Figure 1: Schematic showing the local coordinate system, (x_1, x_2, x_3) , in the interface region between two materials used in the derivation of the misfit strain.

$$\begin{aligned}\epsilon_{ij}^{mis,loc}(\mathbf{x}) &= \begin{pmatrix} \epsilon_{11}^{(1)} & 0 & 0 \\ 0 & \epsilon_{22}^{(1)} & 0 \\ 0 & 0 & \epsilon_{33}^{(1)} \end{pmatrix} \cdot \left(1 - \frac{d(\mathbf{x})}{d^{(1)}}\right), & \mathbf{x} \in \text{material 1} \\ \epsilon_{ij}^{mis,loc}(\mathbf{x}) &= \begin{pmatrix} \epsilon_{11}^{(2)} & 0 & 0 \\ 0 & \epsilon_{22}^{(2)} & 0 \\ 0 & 0 & \epsilon_{33}^{(2)} \end{pmatrix} \cdot \left(1 - \frac{d(\mathbf{x})}{d^{(2)}}\right), & \mathbf{x} \in \text{material 2}\end{aligned}\quad (12)$$

where $d(\mathbf{x})$ is the normal distance from the interface to a point $\mathbf{x}$ in the material and $d^{(1)}$ and $d^{(2)}$ are the limiting values of $d(\mathbf{x})$ beyond which the misfit strain becomes negligible in material 1 and material 2, respectively. While any form for the decay of the misfit strain can be implemented, as a simplifying assumption, we model the variation in misfit strain normal to the interface in Equation 12 as linear.

In the local coordinate system, the misfit strain components in Equation 12 can be written as (Hoagland et al., 2002, 2004; Wang et al., 2003):

$$\begin{aligned}\epsilon_{11}^{(1)} = \epsilon_{22}^{(1)} &= \frac{C_{eff}^{(2)}(a^{(2)} - a^{(1)})}{C_{eff}^{(1)}a^{(2)} + C_{eff}^{(2)}a^{(1)}}; & \epsilon_{33}^{(1)} &= \frac{-2\nu^{(1)}\epsilon_{11}^{(1)}}{1 - \nu^{(1)}} \\ \epsilon_{11}^{(2)} = \epsilon_{22}^{(2)} &= \frac{C_{eff}^{(1)}(a^{(1)} - a^{(2)})}{C_{eff}^{(1)}a^{(2)} + C_{eff}^{(2)}a^{(1)}}; & \epsilon_{33}^{(2)} &= \frac{-2\nu^{(2)}\epsilon_{11}^{(2)}}{1 - \nu^{(2)}}\end{aligned}\quad (13)$$

where $C_{eff}^{(c)} = \frac{E^{(c)}}{1-\nu^{(c)}}$, $E^{(c)}$ is the Young's modulus, and $\nu^{(c)}$ is the Poisson's ratio for $c = 1$ and 2 . The $\epsilon_{11}^{(c)}$ and $\epsilon_{22}^{(c)}$ are the in-plane normal strain components in the x_1 and x_2 directions, and $\epsilon_{33}^{(c)}$ is the out-of-plane normal strain component, normal to the interface plane in the x_3 direction (see Figure 1). The elastic moduli near the interface are set equal to the bulk elastic moduli. We note that the PFDD model does allow for variation in the elastic moduli, hence, $C_{eff}^{(c)}$ could be replaced by a better estimate should such a measurement or calculation become available.

To incorporate the local misfit strain into the PFDD bicrystal model, we transform it into the global coordinate system via:

$$\epsilon_{ij}^{mis}(\mathbf{x}) = R_{ik}R_{jl}\epsilon_{kl}^{mis,loc}(\mathbf{x}), \quad (14)$$

where R is the transformation matrix from the local interface coordinate system (x_1, x_2, x_3) to the global one (x, y, z) , as shown schematically in Figure 1.

Under an assumption of additive decomposition of strain, the misfit strain is added to the total strain, $\epsilon_{ij}(\mathbf{x})$, presented in Equation 6. The new total strain then becomes:

$$\epsilon_{ij}(\mathbf{x}) = \bar{\epsilon}_{ij}^0 + \int \hat{G}_{jk}(\mathbf{k}) k_i k_l C_{klmn}^{(1)} \hat{\epsilon}_{mn}^0(\mathbf{k}) e^{ikx} \frac{d^3 k}{(2\pi)^3} + S_{ijkl}^{(1)} \sigma_{kl}^{ap} + \epsilon_{ij}^{mis}(\mathbf{x}). \quad (15)$$

The strain energy is revised by inserting the modified total strain in Equation 15 into Equation 3, which gives

$$\begin{aligned} E^{strain} &= E^{eq} + \Delta E \\ &= \frac{1}{2} \int \hat{A}_{mnuv}(\mathbf{k}) (\hat{\epsilon}_{mn}^v(\mathbf{k}) + \hat{\epsilon}_{mn}^p(\mathbf{k})) (\hat{\epsilon}_{uv}^{v*}(\mathbf{k}) + \hat{\epsilon}_{uv}^{p*}(\mathbf{k})) \frac{d^3 k}{(2\pi)^3} \\ &\quad - \frac{1}{2} \int C_{ijkl}^{(1)} \epsilon_{ij}^{mis}(\mathbf{x}) \epsilon_{kl}^{mis}(\mathbf{x}) d^3 \mathbf{x} - C_{ijkl}^{(1)} \int (\epsilon_{ij}^v(\mathbf{x}) + \epsilon_{ij}^p(\mathbf{x})) \epsilon_{kl}^{mis}(\mathbf{x}) d^3 \mathbf{x} \\ &\quad - \frac{V}{2} S_{ijkl}^{(1)} \sigma_{ij}^{ap} \sigma_{kl}^{ap} - \sigma_{ij}^{ap} \int (\epsilon_{ij}^v(\mathbf{x}) + \epsilon_{ij}^p(\mathbf{x})) d^3 \mathbf{x} + \int S_{ijkl}^{(1)} \sigma_{ij}^{ap} \epsilon_{kl}^{mis}(\mathbf{x}) d^3 \mathbf{x} \\ &\quad - \frac{1}{2} \int_2 (C_{ijmn}^{(1)} \Delta S_{mnpq}(\mathbf{x}) C_{pqkl}^{(1)} + C_{ijkl}^{(1)}) \epsilon_{ij}^v(\mathbf{x}) \epsilon_{kl}^v(\mathbf{x}) d^3 \mathbf{x}. \end{aligned} \quad (16)$$

The misfit strain results in additional contributions to the energy, which are found in the second and third lines above. The second and third integral terms in the second line describe the strain energy associated with the misfit strain. The additional integral term in the third line accounts for the interaction between the external applied stress and misfit strain. We note that the misfit strain is non-zero only within a localized volume close to the interface.

2.3. Energy associated with forming an interfacial residual dislocation

In this section, we further extend the PFDD formulation to include the formation energy of the residual dislocation that is left behind after the dislocation passes across the bimaterial interface. Before presenting the new formulation, we believe it worthwhile to describe in the context of the PFDD framework how the Burgers vector of the transmitting dislocation and value of the active phase field variable will change during the transmission process. Consider the schematic system presented in Figure 2, which shows the steps involved in the transmission of a perfect dislocation from the donor material (material 1) to the recipient material (material 2) across an interface. Since the interface has a cube-on-cube orientation relationship, this active slip system is the same in both materials. Accordingly only the phase field variable associated with this slip system will be active. Henceforth, we will drop the superscript α , which was used previously to distinguish a slip system among many. The displacement caused by the motion of a dislocation at a point in material 1 and a time t is $b^{(1)}\xi(\mathbf{x}, t)$, where $\mathbf{b}^{(1)}$ is the Burgers vector of the dislocation in material 1 and $\xi = 1$ in regions that have been slipped. Likewise, the displacement caused by the motion of a dislocation on the same slip system but at a point in material 2 and at time t is $b^{(2)}\xi(\mathbf{x}, t)$, where $\mathbf{b}^{(2)}$ is the Burgers vector in material 2 and $\xi = 1$. Thus, while the lattice parameters a and Burgers vectors $\mathbf{b}$ in materials 1 and 2 are different, the phase field variable ξ and its value associated with dislocation glide ($\xi(\mathbf{x}, t) = 1$) are the same. Consequently when this dislocation transmits from material 1 to material 2 across the interface, its Burgers vector changes from $\mathbf{b}^{(1)}$ to $\mathbf{b}^{(2)}$, but the phase field variable ξ does not change and moreover equals 1 at points where this dislocation has traveled.

In order to conserve mass, the Burgers vectors must also be conserved. Hence, a residual dislocation is left at the interface with a Burgers vector $\mathbf{b}^r = \mathbf{b}^{(2)} - \mathbf{b}^{(1)}$ after the dislocation has transmitted into material 2. The value of the phase field variable ξ associated with the displacement caused by the residual dislocation is non-zero. It is also not expected to be integer-valued as it would be for a lattice dislocation, since the residual dislocation is not a full dislocation belonging to any slip system of either material 1 or material 2. Moreover, the residual dislocation lies not in either material 1 or material 2, but in an interface region. As shown in Figure 2, the interface region in the bicrystal model is a volume comprised of two planes, the interface plane contributed by material 1 and the interface plane contributed by material 2, and has surface area S and width w . Let $\mathbf{x}^{(I)}$ be the subset of points $\mathbf{x}$ located along

Figure 2: A schematic of a fcc/fcc bimaterial system with cube-on-cube orientation and a single coherent interface. The interface surface region width is denoted as w . The schematic shows a single edge dislocation transmit through the interface region leaving a residual dislocation in the interface. On the planes bounding the interface we distinguish the phase field variables on the donor and recipient sides as $\xi^{(1)}$ and $\xi^{(2)}$, respectively.

the interface plane contributed by material 1 and $\mathbf{x}^{(I2)}$ be the subset of points along the interface plane contributed by material 2.

When the residual dislocation has formed, the net displacement caused by the residual dislocation $\mathbf{u}_r$ is given by

$$\mathbf{u}_r = \xi^{(2)} \mathbf{b}^{(2)} - \xi^{(1)} \mathbf{b}^{(1)}, \quad (17)$$

where $\xi^{(1)}$ is short form for $\xi(\mathbf{x}^{(I1)})$ and likewise $\xi^{(2)}$ is short for $\xi(\mathbf{x}^{(I2)})$. Note, these are not separate or different phase field variables from ξ introduced earlier.

Formation of a residual dislocation will add an additional energy term, E^{res} , to the total system energy giving

$$E = E^{strain} + E^{core} + E^{res}. \quad (18)$$

E^{res} is non-zero in the event that a dislocation transmits from material 1 to material 2 across the interface.

The displacement $\mathbf{u}_r$ will give rise to tractions $\boldsymbol{\tau}^{(1)}$ and $\boldsymbol{\tau}^{(2)}$ on both the material 1 and material 2 side of the interface. The energy E^{res} associated with formation of the residual is given by:

$$E^{res} = \int_S |\boldsymbol{\tau}^{(1)} \cdot \mathbf{u}_r^{(1)} - \boldsymbol{\tau}^{(2)} \cdot \mathbf{u}_r^{(2)}| dS. \quad (19)$$

The distortions in each material caused by the residual dislocation are given by

$$\beta_{ij}^{(c)} = \xi^{(c)} s_i^{(c)} m_j^{(c)}, \quad c = 1, 2 \quad (20)$$

and the stress $\sigma_{ij}^{(c)}$ generated by the plastic distortion $\beta_{ij}^{(c)}$ is approximated by:

$$\sigma_{ij}^{(c)} = C_{ijkl}^{*(c)} \cdot \text{sym}(\beta_{kl}^{(c)}) = C_{ijkl}^{(c)} \cdot \epsilon_{kl}^{(c)}, \quad c = 1, 2 \quad (21)$$

where $\epsilon_{ij}^{(c)}$ is the symmetric part of $\beta_{ij}^{(c)}$. We have made a very simple approximation that $\sigma_{ij}^{(c)}$ is directly related to $\epsilon_{ij}^{(c)}$ through a non-linear modulus for the interface $C_{ijkl}^{*(c)}$. Finally, the tractions are given by:

$$\tau_i^{(c)} = \sigma_{ij}^{(c)} \cdot n_j, \quad (22)$$

where $\mathbf{n}$ is the interface normal.

Values for $C_{ijkl}^{*(c)}$ are not generally known for the coherent and semi-coherent interfaces considered here. Consistent with an assumption we made earlier with the misfit strains in Equation 13, we equate $C_{ijkl}^{*(c)}$ with the elastic moduli $C_{ijkl}^{(c)}$ of the donor and recipient materials. With this substitution, Equation 21 becomes

$$\sigma_{ij}^{(c)} = C_{ijkl}^{(c)} \cdot \epsilon_{kl}^{(c)}. \quad (23)$$

2.4. Implementation into the PFDD algorithm

To simulate the transmission process in time, the total system energy E defined in Equation 18 is minimized using the pair of TDGL kinetic equations presented in Equation 11. The result provides the phase field variables $\xi^\alpha(\mathbf{x})$ and virtual strain $\epsilon_{ij}^v(\mathbf{x})$, from which the mechanical stress and strain fields and location of the dislocations in the entire system are determined. The active phase field variables and virtual strain components are solved using the lattice Greens function fast fourier transform (FFT) (Frigo and Johnson, 1997, 1998) at discrete grid points in a cubic grid with a spacing of the lattice parameter. Since the formulation presented in the above sections is reduced to perfect dislocations, one slip system will be active in the simulations discussed below. Hence, only one order parameter is solved for at each grid point throughout the system. In material 2, however, the 9 components of the virtual strain are also solved for. This results in solving for one degree of freedom at each point in material 1 and 10 degrees of freedom everywhere in material 2. The degrees of freedom increases with the number of active slip systems. The implementation of the PFDD framework used for simulations here is serial, with simulation times on the order of an hour. In comparison to atomistic methods, the computation time is much less for similar systems sizes hence, time scales and loading rates similar to those used in experiments can be accessed. A parallel version of the model has been used in previous studies (Hunter et al., 2013; Hunter and Beyerlein, 2014b; Hunter et al., 2014; Hunter and Beyerlein, 2015) and is described in detail by Hunter et al. (2010).

The contributions of the residual dislocation energy E^{res} and misfit energy evolve only in the localized region near the interface, whereas the remaining terms evolve everywhere. To account for the effects of the localized energy contributions when minimizing the total system energy, a sub-cycling approach is employed. At each time increment, we evolve the TDGL equations for the bulk regions and local interface region separately and alternately until the terms have fully equilibrated, after which we proceed to the next time step. Generally, for the interfaces considered here, the local and bulk energy states equilibrate after only a few (1-5) sub-cycles, and hence the efficiency of the PFDD algorithm is not significantly compromised by the additional sub-cycling. Moreover, when the dislocation is far from the interface, before or after it has transmitted, the local energy state at the interface is not evolving and equilibrium between the bulk and local regions of the system is reached with little to no sub-cycling.

2.5. Initial simulation conditions

Figure 3 shows the basic bicrystal model geometry for all PFDD simulations to follow. Consistent with the assumptions mentioned in our presentation of the PFDD formulation, the bicrystal joins two fcc crystals of different materials at a single interface plane. As shown, the orientation relationship of the interface is cube-on-cube and the interface plane (red plane) is the mutual (100) plane of materials 1 and 2.

For these simulations, periodic boundary conditions are applied. The domain size for all simulations is $64a^{(c)} \times 2a^{(c)} \times 64a^{(c)}$ ($c=1,2$) in the x , y , and z ($[\bar{1}10]$, $[11\bar{2}]$, and $[111]$ in Figure 3a) directions, respectively. We have found that this domain size with a resolution of the lattice parameter, $a^{(c)}$, is sufficiently large such that the image dislocations arising from the periodic boundary conditions do not affect dislocation motion or slip transmission behavior. Since our interests lie in the crossing of one interface, slip transmission is only considered across the central (red) interface plane in Figure 3. The other interfaces in neighboring periodic cells do not account for any of the local interface energy terms, and hence the energy barrier for slip transmission is very large and these interfaces can be considered as impenetrable.

The schematic in Figure 3 also shows the slip system for the edge and screw oriented dislocations that will attempt to cross the interface. The slip plane is the blue, (111) plane and the slip direction is $[\bar{1}10]$. The dislocations are straight and due to periodic boundary conditions, infinite in length. For the cube-on-cube (100) interface, it is expected that during transmission, the dislocations will maintain the same slip plane and direction on both sides of the interface.

To determine the critical stress τ_{crit} required to transmit a dislocation through the interface, the dislocation is initially placed in the donor material and driven toward the interface by an applied uniform shear stress (σ_{xz} for the edge orientation, and σ_{xy} for the screw orientation) (see Figure 3). Once the dislocation reaches the interface, the applied stress is incrementally increased until the stress is just large enough to cause the dislocation to transmit through the interface into the recipient material. From this critical applied stress, the resolved shear stress for the slip system shown in Figure 3 is calculated. Henceforth, we call this resolved shear stress the critical transmission stress,

τ_{crit} .

Figure 3: A schematic of the PFDD simulation set-up for an initial (a) edge dislocation and (b) screw dislocation in a fcc/fcc bimaterial system with a (100) interface (red plane). In both cases, a constant shear stress is applied to initiate dislocation motion.

Table 1: Lattice constant (in Å), cubic elastic constants (units of GPa), the effective (isotropic) shear and Young's moduli (units of GPa) and Poisson's ratio, and core energy amplitude (mJ/m²) used in the PFDD simulations, where $G^{eff} = 0.5 * (C_{11} - C_{12})$, $E^{eff} = 2G^{eff}(1 + \nu^{eff})$, and $\nu^{eff} = 0.5 * C_{12}/(C_{12} + G^{eff})$ (Hirth and Lothe, 1982).

Material	a (Å)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	G^{eff} (GPa)	E^{eff} (GPa)	ν^{eff}	B (mJ/m ²)
Copper	3.61	168.4	121.4	75.4	23.5	66.7	0.419	620.4
Nickel	3.52	246.5	147.3	127.4	49.6	136.3	0.374	933.4

3. PFDD Slip Transmission Results

3.1. The Cu-Ni system

First, we consider a Cu-Ni bicrystal. Cu and Ni differ by 2.5% in their lattice parameter, and by approximately 50% in their effective Young's modulus and shear modulus. Therefore, we expect that the virtual strain, misfit strain, and residual dislocation, left in the interface after the transmission process, will be non-negligible. Table 1 presents the material parameters used in the PFDD simulations.

We begin with the simulation of the transmission of a perfect edge dislocation from Cu to Ni. Figure 4 shows snapshots of the PFDD simulation for this case. The dislocation line direction ($[11\bar{2}]$ for an edge dislocation) points out of the plane of the page. The color represents the value of the phase field variable, where green corresponds to a value of 1 and are areas slipped by the perfect edge dislocation. The critical stress for transmission is calculated to be 2.58 GPa. In Figure 4c, we see the formation of a residual dislocation in the interface (red point), which is an edge dislocation and is expressed with a non-integer value of the phase field variable. We note that because the dislocation is moving from the material with the larger Burgers vector (Cu) to a material with a smaller Burgers vector (Ni), the fractional component of the phase field variable that represents the residual dislocation is greater than one. Conservation of the Burgers vector requires that a residual dislocation b^r forms with a Burgers vector magnitude given by $b^{Cu} = b^r + b^{Ni}$ where b^r should equal to 0.0064 nm according to the values presented in Table 1. The value of the residual Burgers vector b^r in Figure 4c is 0.0064 nm, as expected.

As introduced earlier, the volume around the interface affected by the misfit strain is defined by $d^{(1)}$ and $d^{(2)}$. The maximum misfit strain occurs at the interface and decays relatively rapidly with distance from the interface. In the foregoing simulation, $d^{(c)} = 8a^{(c)}$ for $c = 1, 2$, a choice that is made based on prior atomic-scale simulations for this

Figure 4: A straight, edge dislocation crossing from Cu to Ni. The black line is the interface between Cu and Ni. The edge dislocation initially traverses through the Cu (a) before meeting the Cu-Ni interface (b). In the final frame (c), the dislocation slips across the interface and through the recipient material, leaving a residual Burgers vector (red color). Frames (d), (e), and (f) show the evolution of the phase field order parameter (blue dashed line) and its derivative (red solid line) across the midline of the glide plane. In these figures, the interface is located at $48a^{(c)}$. The applied stress of 2.58 GPa is also the critical stress required for slip transmission.

Cu-Ni interface (Hoagland et al., 2002). These MD simulations also suggested that the spatial variation of misfit strain is non-linear, unlike the linear form of the decay used here. Because the misfit strain field is highly localized and short-ranged and its maximum occurs at the interface, we suspect that details of its variation with distance away from the interface may have a relatively small effect on τ_{crit} . In an attempt to quantify its influence, we calculate τ_{crit} for an edge dislocation from Cu to Ni, while varying $d^{(1)}$ and $d^{(2)}$ independently and systematically within the range of $3a - 13a$. We find that $d^{(1)}$ and $d^{(2)}$ only mildly affects the motion of the dislocation as it approaches the interface and negligibly affects dislocation motion after transmission and τ_{crit} . Hence, hereinafter, in the following PFDD simulations for all material systems, we set $d^{(c)} = 8a^{(c)}$.

We repeated the simulation in Figure 4 with a screw dislocation originating in Cu. As expected from the conservation of the Burgers vector, the magnitude of the residual Burgers vector left in the interface is the same as that left by an edge dislocation, 0.0064 nm. However the residual dislocation has screw character. The simulation finds $\tau_{crit} = 2.22$ GPa, which is slightly lower than that for the edge case. Theoretically, the edge and screw dislocation line energies per unit length differ by $1/(1 - \nu)$ (Hirth and Lothe, 1982). Accordingly, the transmission of a screw dislocation could be easier than that of an edge dislocation since the residual screw dislocation left in the interface during transmission of the screw will have a lower self-energy than the residual edge dislocation left after transmission of the edge.

In the cases presented thus far, the dislocation originated in Cu (donor) and transmitted to Ni (recipient). We repeated the simulations for the reverse path, with the dislocation being driven to transmit from Ni to Cu. Figure 5 shows the evolution of an edge dislocation crossing from Ni to Cu. We find that $\tau_{crit} = 5.36$ GPa is significantly higher than in the previous simulation of an edge dislocation transmitting from Cu to Ni. For the case of a screw

Figure 5: A straight, edge dislocation crossing from Ni to Cu. The edge dislocation is initially located in Ni (a), meets the Ni-Cu interface (b), and transmits through the interface into the Cu (c). Frames (d), (e), and (f) show the evolution of the phase field order parameter (blue dashed line) and its derivative (red solid line) across the midline of the glide plane. In these figures, the interface is located at $48a^{(c)}$. The applied stress of 5.36 GPa is also the critical stress required for slip transmission.

dislocation crossing from Ni to Cu, $\tau_{crit} = 4.69$ GPa, again higher than that for the screw dislocation to take the reverse transmission path. In this case the recipient material has the smaller shear modulus and larger Burgers vector (or lattice parameter). Hence, the fractional value of the phase field variable that represents the residual dislocation is less than one (appears as a blue-green point in Figure 5c).

For both dislocation characters, we see an asymmetry in τ_{crit} with respect to the direction of slip transmission. Transmission from Cu to Ni is easier than from Ni to Cu. Transmission from the softer to the stiffer material and from the larger to smaller Burgers vector is favored.

In prior MD studies of slip transmission across coherent interfaces, the magnitude and sign of the in-plane component of misfit stress was shown to play a dominating role in slip transmission (Hoagland et al., 2004). In our Cu-Ni simulation, the in-plane component of misfit stress is +1890 MPa and -1890 MPa in the Ni and Cu sides, respectively, at the interface where its value achieves a maximum. When the misfit stress is resolved onto the glide plane of the dislocation in Ni that is approaching the interface, we find that it is negative (being -772 MPa) and thus resists dislocation motion. When resolved onto a dislocation approaching the interface from the Cu side +772 MPa, it is positive and aids its approach. In the case of Cu-Ni, the misfit stress would lead to an asymmetry in the interaction of a moving dislocation with the interface.

3.2. Critical threshold stress dependencies for other fcc/fcc systems

In this section, we use the model to calculate τ_{crit} for the same cube-on-cube (001) interface for a range of fcc/fcc composite systems. Table 2 lists the material parameters for the other systems studied. Consistent with the formulation of the misfit strain and energy in Section 2.2, these two-phase systems studied have a low lattice parameter mismatch

Table 2: Lattice constant (in Å), cubic elastic constants (units of GPa), the effective (isotropic) shear and Young's moduli (units of GPa) and Poisson's ratio, and core energy amplitude (mJ/m²) used in the PFDD simulations, where $G^{eff} = 0.5 * (C_{11} - C_{12})$, $E^{eff} = 2G^{eff}(1 + \nu^{eff})$, and $\nu^{eff} = 0.5 * C_{12}/(C_{11} + G^{eff})$ (Hirth and Lothe, 1982).

Material	a (Å)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	G^{eff} (GPa)	E^{eff} (GPa)	ν^{eff}	B (mJ/m ²)
Aluminum	4.05	107.3	60.9	28.3	23.2	63.2	0.362	473.3
Gold	4.08	192.9	163.8	41.5	14.6	42.5	0.459	758.0
Platinum	3.92	346.7	250.7	76.5	48.0	136.3	0.420	1385.6
Silver	4.09	124.0	93.4	46.1	15.3	43.7	0.430	510.0

Table 3: Critical transmission stress (in GPa) for all systems tested as calculated with the bimaterial PFDD model. Percent lattice mismatch is also shown.

System ($a^{(1)} > a^{(2)}$)	τ_{crit} (GPa)					Lattice Mismatch
	Edge	Screw	System ($a^{(2)} > a^{(1)}$)	Edge	Screw	
Al/Pt	2.34	2.19	Pt/Al	5.33	4.54	3.3 %
Cu/Ni	2.58	2.22	Ni/Cu	5.36	4.69	2.5 %
Ag/Al	1.70	1.45	Al/Ag	2.48	2.20	0.98 %
Au/Al	1.64	1.38	Al/Au	2.55	2.20	0.74 %
Ag/Au	1.70	1.40	Au/Ag	2.20	1.47	0.24 %

(approximately $\leq 3.5\%$), such that the bimaterial interface is either coherent or semi-coherent. Among them, Al-Pt has the greatest and Ag-Au the least lattice and moduli mismatch.

To examine the effect of lattice and moduli mismatch on donor-recipient asymmetry, the PFDD calculations were carried out for slip transmission in both directions. Table 3 shows the resulting τ_{crit} values. In all cases, transmission of an **edge dislocation is harder than a screw dislocation** with all else being equal (including transmission pathway). As seen earlier in the Cu-Ni case, the resistance against transmission is higher when moving from a material with a smaller a to one with a larger a . With the exception of Ag-Au, the resistance to slip transmission is higher when the dislocation is moving from the stiffer to softer material.

To take a closer look at the effects of the lattice mismatch, Figure 6 plots the maximum misfit stress at the interface resolved onto the incoming gliding dislocation for both edge and screw transmissions. Overall, we observe that the greater the lattice mismatch, the larger τ_{crit} . This trend, however, does not apply in all cases. Pt-Al has the largest lattice mismatch, see Table 3, but Ni-Cu has the largest τ_{crit} . Ni-Cu has a larger moduli mismatch than Pt-Al. Evidently, while the misfit stress has a dominant effect, so does the moduli mismatch.

Koehler (1970) and also Pacheco and Mura (1969) proposed that τ_{crit} scales with the moduli mismatch in the case of $G^{(2)} > G^{(1)}$. According to their continuum mechanics model, when $G^{(2)} > G^{(1)}$, τ_{crit} for the transmission of screw dislocations scale as $G^{(1)}(G^{(2)} - G^{(1)})/(G^{(2)} + G^{(1)})$. In Figure 7 we test our PFDD results for τ_{crit} against this scaling factor exclusively for screw dislocations and only in cases of $G^{(2)} > G^{(1)}$. **For the few points we test, the calculated values of τ_{crit} do not contradict this scaling law.** In particular, it finds that τ_{crit} for Cu-Ni should be higher than Al-Pt. However, PFDD finds that $G^{(2)} > G^{(1)}$ is the easier transmission pathway in all cases except the Au-Ag system. Clearly, there are competing effects impacting making it difficult to determine a clear scaling effect for τ_{crit} .

Our analysis of the calculated τ_{crit} shows that both lattice and moduli mismatch are key variables and can give rise to a donor-recipient asymmetry in τ_{crit} . It then becomes of interest to understand why τ_{crit} depends not only on the absolute differences in **$a^{(e)}$ and $G^{(e)}$** across the interface, but also on which material the dislocation originates and which material receives it. Simply put, how does τ_{crit} scales **with $a^{(2)}$, $a^{(1)}$, $G^{(2)}$, and $G^{(1)}$** ? It is not readily obvious from the calculation. In its calculation of τ_{crit} , the PFDD simulation couples many effects, such as the line energies of the participating dislocations, interactions of the residual dislocation with the other dislocations, the misfit stress, and the image forces, and the energetic barrier required to form the residual dislocation.

One could take into account the combined effect of the lattice and moduli mismatch by examining the change in

Figure 6: PFDD results for τ_{crit} versus the maximum misfit stress resolved on the slip plane for transmission of an edge (a) and screw (b) oriented perfect dislocation.

Figure 7: The critical transmission stress, τ_{crit} calculated by the PFDD model for screw dislocations versus the scaling factor $G^{(1)}(G^{(2)}-G^{(1)})/(G^{(2)}+G^{(1)})$ where $G^{(2)} > G^{(1)}$ proposed by Koehler (1970) and Pacheco and Mura (1969).

Figure 8: The critical transmission stress associated with the direction of easier transmission, τ_{crit}^{easy} , plotted against the self-energy of the residual Burgers vector, $G_{point} |\mathbf{b}^r|^2$, where G_{point} is the shear modulus of the material into which residual dislocation Burgers vector points following slip transmission of an edge dislocation.

self-energy of the dislocation, which would certainly lead to a donor-recipient asymmetry. With the strain energy per unit length of a dislocation proportional to $G b^2$, a dislocation in Cu would have the lower and the dislocation in Ni the higher self-energy. On this basis, it could be argued that transmission from Ni to Cu would be favored since the dislocation would be able to lower its self-energy. However, according to the PFDD simulation results, transmission from Ni to Cu is not favored compared to the reverse from Cu to Ni.

Another concept that considers the effects of lattice mismatch and possibly moduli differences is the proposal that τ_{crit} scales with the self-energy of the residual dislocation left in the interface after transmission (Lim and Raj, 1985; Misra and Gibala, 1999; Ma et al., 2006; Roters et al., 2010). In these studies, $G |\mathbf{b}^r|^2$ is usually used as a measure of self-energy of the residual dislocation. Here, a few issues arise. First, for this model, the intuitively best choice for G would be that for the interface, where the residual dislocation resides. However the shear modulus of an interface is not readily available or easily measured. Second, given the same G , the donor-recipient asymmetry in τ_{crit} would not be captured by $G |\mathbf{b}^r|^2$ since $|\mathbf{b}^r|$ is the same for both the (1)-(2) and (2)-(1) transmission pathways. We can test the $G |\mathbf{b}^r|^2$ scaling for the τ_{crit} values associated with the easier transmission direction, arguably the more likely event of the two pathways. Here, we denote it as τ_{crit}^{easy} . In this analysis, we elect to use the G_{point} , which is the shear modulus of the material into which the Burgers vector of the residual dislocation points for the edge transmission. Figure 8 plots τ_{crit}^{easy} for each composite material system against $G_{point} |\mathbf{b}^r|^2$. As shown, τ_{crit}^{easy} tends to increase with $G_{point} |\mathbf{b}^r|^2$ for both transmission of the edge and screw oriented dislocations. However, we see that this proposed scaling law does not fully agree with the PFDD model results, Al-Pt in particular, which has the largest residual self-energy but not the largest τ_{crit} . Figure 8 reveals that it is not wrong that τ_{crit} is proportional to $|\mathbf{b}^r|$ and that the PFDD results are consistent with this general notion. It confirms that the resistance to transmission is generally higher when the lattice mismatch is higher. However, the aforementioned issues still remain.

At this stage, we have seen that the PFDD calculations for τ_{crit} qualitatively follow many of the trends proposed in the literature. While an important outcome for confirming the PFDD results, we still find that the relationship between

τ_{crit} and key variables, such as lattice and moduli mismatch, have not yet been fully clarified. To see why, we recapitulate the findings thus far. First there are the ideas that interactions between the strain fields of the gliding dislocation and the interface affect τ_{crit} . The misfit strain, arising from the lattice mismatch, and the image forces, arising from the moduli mismatch, across the interface certainly affect the stresses on the dislocation as it approaches the interface from one side and leaves the interface from the other side. The misfit stresses, in particular, more intensively affect the approaching dislocation than the Koehler image forces. It is found that the misfit stress resists (or helps) the gliding dislocation as it approaches the interface from the material with the smaller (or larger) lattice parameter. Notably, this trend is consistent with the donor-recipient asymmetry in τ_{crit} predicted by the PFDD simulations. However, at the same time, we note that these models are based on interaction energies between dislocations and interfaces, and thus have more to do with the stress required for the dislocation *to impinge on* the interface and less so the stress required for it *to cross* the interface. Second, the concept of dislocation self-energy changes governing τ_{crit} is not consistent with the current PFDD results. This idea does not account for dislocation-interface interactions and the interfacial residual dislocation that forms as a consequence of the dislocation crossing the interface. Last, the model that identifies a positive relationship between τ_{crit} and $G|\mathbf{b}^r|^2$ directly accounts for the energy of the residual dislocation only *after* the gliding dislocation has crossed. The residual dislocation self-energy (e.g., $G|\mathbf{b}^r|^2$), is not the energetic barrier associated with forming the residual dislocation as the gliding dislocation *is crossing* the interface. Because it does not account for how the residual dislocation formed it misses the donor-recipient asymmetry.

4. An analytical model for the critical transmission stress

4.1. Formulation

Based on the PFDD results and foregoing analysis, we put forward that the hypothesis that τ_{crit} is governed by the energy to form the residual dislocation. The energy barrier would be related to the pathway taken by the dislocation to cross the interface. More specifically, it would not only depend on the absolute value of the lattice and moduli mismatch, but whether the dislocation transmits from the softer to stiffer material and/or the material with the smaller to larger lattice parameter.

The PFDD model not only accounts for the formation energy for the residual dislocation, but for many other effects, such as the line energies of the participating dislocations, and interactions of the residual dislocation with the other dislocations, the misfit stress, and the image forces. In an effort to isolate the effects of the residual dislocation formation energy, we use the PFDD formation to develop a simple, analytical model for the energetic barrier required to form the residual dislocation and the critical resolved shear stress τ_{loc} for slip transmission associated with it. As we will show, comparisons between τ_{loc} and the calculated τ_{crit} indicate that the contribution of the residual dislocation formation energy dominates the slip transmission stress for bimaterial systems with relatively large lattice mismatch. More importantly, the model reveals that less energy is required to form the residual dislocation when the gliding lattice dislocation transmits from the material with the smaller to larger shear modulus G and larger to smaller lattice parameter a . Consequently, τ_{crit} is lower for this pathway than the other way around.

In describing the analytical model below, we maintain the situation in which a perfect dislocation is being transmitted across an fcc/fcc coherent interface with a cube-on-cube orientation relationship, although in principle, this model could apply to any interface character. We begin by considering the evolution of E^{res} as the dislocation transverses the interface region, starting at the interface plane of the donor $x^{(I1)}$ and moving to that of the recipient $x^{(I2)}$. As a simplification, we set the value of the phase field variable at $x^{(I1)}$ equal to 1 to indicate that the dislocation has slipped in material 1 and impinged on the interface. Equation 19 for E^{res} then reduces to the following function of $\xi^{(2)}$ only:

$$E^{res} = \left| (D_{21} + D_{12}) \xi^{(2)} - D_{11} - D_{22}(\xi^{(2)})^2 \right|, \quad (24)$$

where $D_{pq} = C_{ijkl}^{(p)} s_i^{(q)} n_j s_k^{(p)} m_l^{(p)} a^{(q)}$, $p, q = 1$ or 2 . These factors depend on moduli, and the relative orientation of the slip system on which the dislocation glides and the interface normal.

As the dislocation glides from $x^{(I1)}$ to $x^{(I2)}$, the phase field variable $\xi^{(2)}$ at $x^{(I2)}$ will increase from zero to a peak value greater than one. During this process, E^{res} will reach a peak value, denoted as $E_{barrier}^{res}$. Setting the derivative of

E^{res} with respect to $\xi^{(2)}$ equal to zero finds that the peak value is reached when $\xi^{(2)} = \left| \frac{D_{12} + D_{21}}{2D_{22}} \right|$. Substituting this value of $\xi^{(2)}$ into Equation 24 gives the following expression for $E_{barrier}^{res}$:

$$E_{barrier}^{res} = \left| \frac{\Delta}{4D_{22}} \right|, \text{ where } \Delta = (D_{12} + D_{21})^2 - 4D_{11}D_{22}. \quad (25)$$

The threshold resolved shear stress τ_{loc} acting on the dislocation associated with $E_{barrier}^{res}$ can be given by

$$\tau_{loc}d_w \geq E_{barrier}^{res} = \left| \frac{\Delta}{4D_{22}} \right|, \quad (26)$$

where d_w is the distance over which τ_{loc} does work to overcome the energetic barrier. A reasonable estimate for d_w is half the span of the interface region w . In the present work, the span of the interface region is the sum of the width of the two (001) atomic layers of the donor and recipient crystals. Hence, $d_w = \frac{a^{(1)} + a^{(2)}}{2}$. Using this definition for d_w and assuming elastic isotropy, we finally obtain for $E_{barrier}^{res}$ and τ_{loc} the following:

$$E_{barrier}^{res} = \frac{\sqrt{3}a^{(2)}G^{(2)}}{12} \left(\frac{a^{(1)}}{a^{(2)}} - \frac{G^{(1)}}{G^{(2)}} \right)^2, \quad (27)$$

and

$$\tau_{loc} = \frac{\sqrt{3}a^{(2)}G^{(2)}}{12d_w} \left(\frac{a^{(1)}}{a^{(2)}} - \frac{G^{(1)}}{G^{(2)}} \right)^2. \quad (28)$$

Figure 9 compares the calculated τ_{crit} with the analytical τ_{loc} . We find that for the Cu-Ni and Pt-Al composite systems, τ_{crit} and τ_{loc} are nearly equal. This result suggests that for composite systems in which the misfit stresses produced at the interface are large, the resistance to slip transmission is governed by the local energy to form the residual dislocation. For the remaining systems, τ_{loc} underestimates the calculated transmission resistance. This difference can be expected since for composite systems with much lower misfit, the actual barrier to slip transmission across the interface involves contributions of the elastic interactions and line energies of the residual and transmitting dislocation.

In Figure 10, we compare the calculated τ_{crit} for all systems studied here against the bimaterial-dependent scaling factor $\frac{a^{(2)}G^{(2)}}{a^{(1)} + a^{(2)}} \left(\frac{a^{(1)}}{a^{(2)}} - \frac{G^{(1)}}{G^{(2)}} \right)^2$ that emerges from the analytical formulation. As shown, we find a strong correlation between τ_{crit} and $\frac{a^{(2)}G^{(2)}}{a^{(1)} + a^{(2)}} \left(\frac{a^{(1)}}{a^{(2)}} - \frac{G^{(1)}}{G^{(2)}} \right)^2$. This factor contains the product of two terms. The first one is $G^{(2)}a^{(2)}/a^{(1)} + a^{(2)}$. It shows that transmission is more difficult when the lattice parameter of the recipient material is relatively large compared to that of the donor material. The second is $\left(\frac{a^{(1)}}{a^{(2)}} - \frac{G^{(1)}}{G^{(2)}} \right)^2$. It indicates that the transmission resistance would increase with the degree of disparity between the lattice and elastic moduli of the two materials. In particular, this term is large when $G^{(1)} > G^{(2)}$, when the dislocation transmits from the stiffer to the softer material. To summarize, we reveal a path dependence in the formation energy of the residual dislocation. It can give rise to a donor-recipient asymmetry, where τ_{crit} is harder when the dislocation transmits from a stiffer material with a smaller lattice parameter to a softer material with a larger lattice parameter.

4.2. Connections with MD simulation results

An fcc/fcc system in which slip transmission has been studied with atomistic methods is the Ag-Cu system (Hoagland et al., 2002; Wang et al., 2011). The lattice mismatch for this system is very large (approximately 12.5%, with Ag having the larger lattice parameter). We have not included it in our calculations thus far since the misfit strain cannot be adequately calculated using Equation 14. Hoagland et al. (2002) report that the experimental maximum in-plane misfit stress for Cu-Ag is equal to 1.5 GPa¹. Rather than calculate the misfit stress using Equation 14, we used the experimentally measured misfit stress in the PFDD formulation (directly into Equation 16) and carried out the PFDD simulation for slip transmission of an edge dislocation. We found that $\tau_{crit} = 2.56$ GPa for slip transmission

¹In this interface, misfit dislocations form and relieve the coherency strains. Misfit strains calculated by Equation 14 would overestimate the actual misfit strains and hence the corresponding misfit stresses would be overestimated as well

Figure 9: The critical transmission stress, τ_{crit} as calculated with the PFDD model versus the analytically derived transmission stress, τ_{loc} , which is based on the energetic barrier required to form the residual dislocation. The diagonal dashed line represents $\tau_{crit} = \tau_{loc}$.

from Cu-Ag, and $\tau_{crit} = 1.68$ GPa for transmission from Ag-Cu. These values for τ_{crit} are indicated with a + symbol in Figure 6. As shown, we observe the same relationship between τ_{crit} and the misfit stress as the other fcc/fcc systems; that is, the slip transmission direction experiences a higher resistance when the donor material has a smaller lattice parameter than the recipient material. Although an experimental value of the misfit stress had to be imported into the model, the consistency with the trends in τ_{crit} predicted for the coherent fcc/fcc systems emphasizes the important influence of the misfit stress on τ_{crit} .

In prior work, MD or atomically informed numerical simulations have been carried out for mixed-type and screw-type perfect dislocations transmitting from Cu to Ni across the Cu(001)-Ni(001) cube-on-cube interface (Hoagland et al., 2002, 2004; Rao and Hazzledine, 2000; Anderson et al., 2000). In these simulations, the dislocations in Cu dissociated into leading and trailing Shockley partials. The leading partial transmits first across the interface, followed by transmission of the trailing partial. In the present PFDD model, the dislocations are perfect dislocations, thus, making direct comparison of our results for τ_{crit} with MD calculations is difficult.

The magnitude of the Burgers vector of the partial dislocations in Cu has a value of 0.147 nm, whereas that of a perfect dislocation is larger, 0.255 nm (based on values in Table 1). The effects of the smaller valued Burgers vector of the leading partial include a lower force on the dislocation and reduced formation energy to form the residual dislocation, making transmission easier. We can mimic this aspect in the present PFDD model by replacing the Burgers vector of the perfect dislocation with its leading partial. We find that $\tau_{crit} = 0.215$ GPa for a dislocation corresponding to a pure edge partial to transmit from Cu to Ni. This value is close to that required for the (pure edge) leading partial to transmit 0.2 GPa, calculated by MD (Hoagland et al., 2002). We also considered transmission of a leading partial associated with a pure screw, which is a 30° mixed dislocation. Experimental measurements for this case range from 0.3402-1.053 GPa (Shen and Anderson, 2007). Using PFDD, we find that $\tau_{crit} = 0.63$ GPa for this leading partial.

While the agreement is promising, it must be kept in mind that these calculations only account for the reduced value of the Burgers vector associated with a partial dislocation and neglect the stacking fault of the extended dislocation, the interaction with the trailing partial, and the elastic anisotropy accounted for in the MD calculations. Recently,

Figure 10: The critical transmission stress, τ_{crit} as calculated with the PFDD model versus the analytically derived bimaterial-dependent scaling factor for edge and screw dislocations in different fcc donor/recipient systems. We see a strong linear correlation. Edge and screw simulations for Ag-Au and Au-Ag have very low threshold stresses and points lie on top of each other.

the PFDD model has been formulated to account for partial dislocations in fcc crystals (Hunter et al., 2011; Hunter and Beyerlein, 2014b; Hunter et al., 2014; Beyerlein et al., 2015a). In these modified versions, E^{core} is defined based on the material γ -surface, calculated from MD or DFT for pure metals and alloys. Advancing the bimaterial interface PFDD model to treat partial dislocations as done in these prior studies is a subject of future work.

5. Conclusions

In this work, we develop a PFDD model for discrete dislocations interacting with a bimetal interface. The model is formulated to treat bimetal systems that form coherent or semi-coherent interfaces. We use the model to simulate the transmission of a single straight dislocation passing from one crystal to another across the bimetal interface and calculate the corresponding critical resolved shear stress, τ_{crit} required for slip transmission to occur. Example calculations are carried out for interfaces created by two dissimilar crystals with an fcc crystal structure, such as Cu-Ni, Ag-Au, Al-Au, and Al-Pt, with a cube-on-cube orientation relationship. The model predicts that the critical resolved shear stress is lower for a screw dislocation than for an edge dislocation of the same Burgers vector. It also suggests an asymmetry in τ_{crit} with respect to the direction of transmission, that is, which material donates the dislocation and which one receives it. τ_{crit} tends to be higher when the dislocation transmits to a material with a lower shear modulus and larger a than the reverse. The degree of this donor-recipient asymmetry increases with the lattice and moduli mismatch. A system with a low lattice mismatch, like Ag-Au, has a small donor-recipient asymmetry, whereas one with a higher lattice mismatch, like Cu-Ni and Al-Pt, exhibits a greater donor-recipient asymmetry. Last, we develop an analytical model for the formation energy of the residual dislocation. It indicates that the energy to form the residual and the resistance to slip transmission exhibits path dependence. It reveals that τ_{crit} scales strongly with a bimaterial-dependent factor $\frac{a^{(2)}G^{(2)}}{a^{(1)}+a^{(2)}} \left(\frac{a^{(1)}}{a^{(2)}} - \frac{G^{(1)}}{G^{(2)}} \right)^2$, where G is the shear modulus, a is the lattice parameter, and the superscripts (1) and (2) refer to the donor and recipient materials, respectively.

Future extensions and simulations using this model include treatment of dislocation loops rather than straight dislocations, incorporation of material γ -surfaces to model partial dislocations rather than full dislocations, and examination of crystal size effects. Such advancements have already been tested in the single-phase version of the PFDD model (Hunter and Beyerlein, 2014b, 2015). More sophisticated modifications would be required, however, to treat incoherent interfaces or interfaces created between crystals with large misorientations.

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