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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 material 2 is not the same as that from material 2 to material 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, the analysis 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.

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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

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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). 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 composites can be attributed to the interaction of dislocations with the bimetal interfaces (Embury and Hirth, 1994; Werner and Stüwe, 1985; Wang et al., 2008; Martinez et al., 2014; Beyerlein et al., 2015b). Unfortunately, gaps still exist in understanding 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, ones that could potentially 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 (Rao and Hazzledine, 2000; Misra et al., 2005; Hoagland et al., 2004). 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 in 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 (~$2b$, where b is the value of the Burgers vector). The interfaces modeled were nearly coherent so that the lattice mismatch and resulting misfit strains were negligible. In two-phase bimaterial systems, the difference in line energy (~Gb^2, where G is the shear modulus) 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 $G^{(1)}(G^{(2)} - G^{(1)})/(G^{(2)} + G^{(1)})$, where the superscript (1) and (2) refer to material 1 and 2 respectively (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-

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