Interface Dislocation Core-Spreading Simulation and Corresponding Response

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Abstract. Dislocation can spread its core at an interface especially at a weak shear interface associated with shearing the interface. Such core-spread dislocation can significantly reduce stress/strain concentration compared with the compact dislocation and thus trap the dislocation in the interface, correspondingly strengthening materials. Employing the Green’s function for a compact dislocation, we derived analytical expressions for the elastic fields of a dislocation with core spreading in anisotropic bimaterials. We proposed a conic model to mimic the spreading core of a dislocation at an interface. The accuracy and efficiency of the conic model are validated by the boundary conditions of both traction and displacement across the interface. Numerical simulation is calculated in the Cu/Nb biomaterial. The results of displacement and stress fields show that: (1) core-spread dislocation can greatly reduce the stress intensity near the dislocation compared with the dislocation with a condensed core; (2) dislocation core spreading has a great influence on the elastic fields near the core region, while the influence can be negligible when the distance of a field point from the center of the dislocation core is greater than 1.51 times the width of the spreading core; (3) near the core region, Peach-Koehler force induced by the core spreading dislocation is larger than that of the compact dislocation.

Introduction

On the one hand, interface acting as sources, may nucleate and emit dislocations, which facilitates the propagation of plastic deformation from one grain to the adjacent grain [1]. On the other hand, interface acting as barriers, can postpone or block dislocation transmission from one crystal to the other, which strengthens the material [2]. The concept of the weak-interface strengthening mechanism has been proposed and demonstrated in metallic multilayer [3-5].

When an interface has a weak shear resistance, such as Cu/Nb metallic multilayers [6] and metal/amorphous interfaces [7], interface dislocations may spread their cores at the interface. Wang et al. demonstrated the existence of the dislocation core spreading in Cu/Nb bimaterial interface with molecular dynamics simulations [8-9] and the influence of the core-spread on slip transmission[10].

In this paper, we derived the elastic fields associated with a dislocation with a spreading core at the interface of anisotropic bimaterials. Conic model was used to mimic the distribution of the Burgers vector in the dislocation core spreading and the corresponding analytical expressions for elastic fields are obtained based on Stroh formula. This paper is organized as follows. In the second section, we briefly review the elastic fields for a compact dislocation and obtain the elastic fields for a dislocation with a spreading core in an anisotropic bimaterial. Numerical examples are shown in section 3. Conclusions and discussions are drawn in the section 4.
Modeling the Core Spreading of Interface Dislocation

Figure 1 is the dislocation core-spreading model in an anisotropic bimaterial. The upper half space ($z>0$) is denoted by material 1 and the lower half space ($z<0$) by material 2. The dislocation spreads at the interface of the bimaterial.

![Figure 1. Dislocation spreads at the interface in an anisotropic bimaterial.](image)

The dislocation array is in a region with the width $w$. The summation of the Burgers vectors of the infinitesimal dislocation array is denoted by $b_0$. The distributed Burgers vector of an infinitesimal dislocation in the spreading region is denoted by $b$. When the spread-out dislocation is located at the interface ($Z=0$) with the line sense along the $y$-axis, the dislocation spreads its core at the interface. For simplicity, the spreading region is assumed from $(-nb_0, 0)$ to $(nb_0, 0)$ in the $x$-$z$ coordinates. The relation between $b$ and $b_0$ can be expressed as

$$b_0 = \int_{-nb_0}^{nb_0} b \, dX$$

(1)

This paper chooses a conic model to mimic the actual distribution of the dislocation core. This conic model can capture the fundamental characteristics and illustrated in Figure 2(a). Figure 2(b) is the corresponding disregistry plot.

![Figure 2. (a) Distribution of Burgers vector in conic model (b) The corresponding disregistry plot.](image)

For the conic model, the distribution of the Burgers vector can be expressed as:

$$b = k \left( X^2 - n^2 b_0^2 \right) b_0.$$  

(2)

According to Eq. (1), the constant $k$ is

$$k = -\frac{3}{4n^2b_0^2}.$$  

(3)

Elastic Fields Due to Dislocation Core Spreading

On the basis of Stroh formalism and the Green’s functions for a single dislocation, the displacements of dislocation core spreading at interface can be derived as follows.
\[ u^i = \frac{1}{\pi} \sum_{\mu=1}^{3} k A_i \left( 16n b_0 - 6n b_0 z^{(1)}_i - 6n b_0 z^{(1)}_i + 3z^{(1)}_i - 9n b_0 z^{(1)}_i \right) \ln \frac{-n b_0 - z^{(1)}_i}{-n b_0 + z^{(1)}_i} \ln \left[ \left( -n b_0 + z^{(1)}_i \right) \left( n b_0 + z^{(1)}_i \right) \right] q_i^{(1)} \]  
\[ + \frac{1}{\pi} \sum_{\mu=1}^{3} k A_i \left( 16n b_0 - 6n b_0 z^{(2)}_i - 6n b_0 z^{(2)}_i + 3z^{(2)}_i - 9n b_0 z^{(2)}_i \right) \ln \frac{-n b_0 - z^{(2)}_i}{-n b_0 + z^{(2)}_i} \ln \left[ \left( -n b_0 + z^{(2)}_i \right) \left( n b_0 + z^{(2)}_i \right) \right] q_i^{(2)} \]  
\[ \left( 4 \right) \]  
\[ u^i = \frac{1}{\pi} \sum_{\mu=1}^{3} k A_i \left( 16n b_0 - 6n b_0 z^{(1)}_i - 6n b_0 z^{(1)}_i + 3z^{(1)}_i - 9n b_0 z^{(1)}_i \right) \ln \frac{-n b_0 - z^{(1)}_i}{-n b_0 + z^{(1)}_i} \ln \left[ \left( -n b_0 + z^{(1)}_i \right) \left( n b_0 + z^{(1)}_i \right) \right] q_i^{(1)} \]  
\[ + \frac{1}{\pi} \sum_{\mu=1}^{3} k A_i \left( 16n b_0 - 6n b_0 z^{(2)}_i - 6n b_0 z^{(2)}_i + 3z^{(2)}_i - 9n b_0 z^{(2)}_i \right) \ln \frac{-n b_0 - z^{(2)}_i}{-n b_0 + z^{(2)}_i} \ln \left[ \left( -n b_0 + z^{(2)}_i \right) \left( n b_0 + z^{(2)}_i \right) \right] q_i^{(2)} \]  
\[ \left( 5 \right) \]  

The first-order derivatives of the displacements in Eqs. (4) and (5) with respect to the field point \( x \) can be expressed as:

\[ u^i = \frac{1}{\pi} \sum_{\mu=1}^{3} k A_i \left[ -2n b_0 z^{(1)}_i + \left( z^{(1)}_i - n^2 b_0 \right) \ln \frac{-z^{(1)}_i + n b_0}{-z^{(1)} - n b_0} \right] \frac{\partial z^{(1)}_i}{\partial x} q_i^{(1)} \]  
\[ + \frac{1}{\pi} \sum_{\mu=1}^{3} k A_i \left[ -2n b_0 z^{(2)}_i + \left( z^{(2)}_i - n^2 b_0 \right) \ln \frac{-z^{(2)}_i + n b_0}{-z^{(2)} - n b_0} \right] \frac{\partial z^{(2)}_i}{\partial x} q_i^{(2)} \]  
\[ \left( 6 \right) \]  

\[ u^i = \frac{1}{\pi} \sum_{\mu=1}^{3} k A_i \left[ -2n b_0 z^{(1)}_i + \left( z^{(1)}_i - n^2 b_0 \right) \ln \frac{-z^{(1)}_i + n b_0}{-z^{(1)} - n b_0} \right] \frac{\partial z^{(1)}_i}{\partial x} q_i^{(1)} \]  
\[ + \frac{1}{\pi} \sum_{\mu=1}^{3} k A_i \left[ -2n b_0 z^{(2)}_i + \left( z^{(2)}_i - n^2 b_0 \right) \ln \frac{-z^{(2)}_i + n b_0}{-z^{(2)} - n b_0} \right] \frac{\partial z^{(2)}_i}{\partial x} q_i^{(2)} \]  
\[ \left( 7 \right) \]  

The strain fields can be easily obtained on the basis of Eqs. (6)-(7) and the corresponding stress fields can be derived through constitutive relation. In a word, the analytical expressions of the elastic fields due to dislocation core spreading have been acquired.

**The Numerical Simulation for Dislocation Core Spreading at Cu/Nb Interface**

The Cu-Nb interface with the Kurdjumov-Sachs (K-S) orientation has low shear resistance through many atomistic simulations and experimental measurements[6,10]. Dislocations can easily spread their cores in the interface.

The upper half space of the bimaterial is assigned to be copper and the lower half space is niobium. The elastic moduli are: \( C_{11} = 168.4 \) GPa, \( C_{12} = 121.4 \) GPa and \( C_{44} = 75.4 \) GPa for copper, and \( C_{11} = 246.0 \) GPa, \( C_{12} = 134 \) GPa and \( C_{44} = 28.7 \) GPa for niobium. The x-axis is parallel to \([11-2]_{\text{Cu}}\) and \([1-12]_{\text{Nb}}\), the z-axis parallel to \([111]_{\text{Cu}}\) and \([110]_{\text{Nb}}\), and the y-axis pointing into the paper and parallel to \([-110]_{\text{Cu}}\) and \([1-1-1]_{\text{Nb}}\).

The stress component \( \sigma_{13} \) is shown in Figure 3.

![Figure 3. The contour of the stress field \( \sigma_{13} \) (GPa) with respect to different models: (a) the compact model (Model 1), (b) the conic model (Model 2).](image)

The relative error between the two models is shown in Figure 4.
Figure 4. The relative error of the compact model and conic model.

Conclusions

The elastic fields due to dislocation core spreading in an anisotropic bimaterial are derived in this paper. We choose the conic model to mimic the distribution of the Burger’s vector in the core region along the interface. For a dislocation located at a bimaterial, the elastic fields are associated with two. One corresponds to the elastic fields of a dislocation in an infinite plane and the other corresponds to the effect of the interface.

Numerical results for the Cu/Nb bimaterial with the K-S orientation relation demonstrate that the displacement jump condition and the traction continuity on the interface are well satisfied. The results show that dislocation core spreading has a great influence on the elastic fields in the core region. Besides, the stress singularity in the compact model can’t be found in the core-spreading model. When the distance of the field points from the original dislocation is larger than 1.51 times the core width, the relative error of stress fields due to Model 1 and Model 2 is lower than 5%, which means the influence of the core can be ignored when the field point is far from the dislocation. The analysis of the P-K force acting on the approaching dislocation shows that the attraction or repulsion force of the core spreading model within the core region is larger than the compact model.

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References


