Grain–boundary interactions and orientation effects on crack behavior in polycrystalline aggregates

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A dislocation-density grain–boundary interaction scheme has been developed to account for the interrelated dislocation-density interactions of emission, absorption and transmission in GB regions. The GB scheme is based on slip-system compatibility, local resolved shear stresses, and immobile and mobile dislocation-density accumulation at critical GB locations. To accurately represent dislocation-density evolution, a conservation law for dislocation-densities is used to balance dislocation-density absorption, transmission and emission from the GB. The behavior of f.c.c. polycrystalline copper, with different random low and high angle GBs, are investigated for different crack lengths. For aggregates with random low angle GBs, dislocation-density transmission dominates at the GBs, which can indicate that the low angle GB will not significantly change crack growth directions. For aggregates with random high angle GBs, extensive dislocation-density absorption and pile-ups occur. The high stresses associated with this behavior, along the GBs, can result in intergranular crack growth due to potential crack nucleation sites in the GB.

1. Introduction

Local behavior at grain–boundary (GB) interfaces is critical in predicting the failure behavior of crystalline aggregates. Complex interactions between dislocations and GBs, such as partial dislocation dissociations, dislocation absorption and transmission, pile-ups, and slip-system incompatibilities can arise due to GB misorientations and the local interactions within GB interfacial regions (Gemperle et al., 2002). These interactions and the initial GB misorientation of crystalline aggregates can lead to different GB behavior that can have a significant effect on the nucleation and propagation of transgranular and intergranular cracks (Kim et al., 2003; Zhang et al., 2003).

The initial GB misorientation of crystalline aggregates has a critical effect on local dislocation behavior and overall response. For random low angle GBs, where misorientations are generally less than 15°, GB dislocation (GBD) networks are usually well organized with periodic patterns, and the GB energy is basically linearly proportional to the misorientation angle (Read and Shockley, 1950). Slip systems on each side of the GB are nearly coplanar, which provide an easy path for dislocation transmission between grains. For random high angle GBs, where misorientations are generally greater than 15°, the GBD networks are usually thick and irregular, and the GB energy is usually much higher than random low angle GBs, and behavior is unpredictable due to the complexity of GBD networks (Amouyal et al., 2005; Read and Shockley, 1950; Watanabe et al., 1999). For these orientations, there are usually no coplanar slip-systems between two neighboring grains, and these high misorientations also are high energy barriers to dislocation transmission. Random low angle GBs sometimes can be treated as single crystals in absence of solutes or other impurities in that dislocations can transmit between neighboring grains without difficulty. Furthermore, SEM and TEM observations have shown that when a random low angle GBs are ahead of a growing crack, the dislocations emitted from the crack transmit in the GB region and then transmit to the neighboring grain, and the crack can easily penetrate the GB region without significant changes in the original crack orientation (Zhang and Wang, 2008; Zhong et al., 2006).

In contrast, random high angle GBs are highly disordered usually with high misorientation and interfacial energies (Amouyal et al., 2005; Shih and Li, 1975; Watanabe et al., 1999). The high misorientation and complex GBD networks in high angle GBs result in dislocation absorption and pile-ups in the GB region. These random high angle GBs act as strong barriers of dislocation movement, and consequently change the original crack directions, and even render transgranular cracks into intergranular cracks (Qiao and Argon, 2003; Robertson et al., 1992; Zhang and Wang, 2008; Zhang et al., 2003; Zhong et al., 2006).

Experimental observations have also clearly indicated that dislocations can interact with GBs in different ways through direct transfer, absorption, or transmission across the GB with residual GB dislocations and pile-ups that can result in dislocation emission...
or the nucleation of intergranular cracks. From these observations, several criteria on dislocation transmission have been proposed for these complex processes Clark et al., 1992; Lagow et al., 2001; Lee et al., 1990a,b; Livingston and Chalmers, 1957; Shen et al., 1986). For example, Lee et al. have proposed three criteria for dislocation transmission: (i) that the angle between the lines of intersection between the GB and each slip plane must be a minimum, (ii) that the magnitude of the Burgers vectors of the dislocations that remains in the GB must be a minimum; (iii) that the resolved shear stress on the outgoing slip-system must be a maximum. These three criteria have been used to understand single dislocation transmissions and to rationalize multiple dislocation activities (Gemperle et al., 2002; Gemperlova et al., 2004; Lee et al., 1990a,b).

Computer simulations also provide understanding on different scales. It was observed in the molecular dynamics (MD) simulations that the GB may act as sink and source of dislocation (Schiøtz, 2004; van Swygenhoven et al., 2006), dislocations may be absorbed in the GB and then cause pile-ups (Schiøtz, 2004; Yamakov et al., 2003) and cross-slip (Yamakov et al., 2003). Transgranular cracks have been predicted to change its direction, and even become intergranular cracks in the presence of high angle GBs (Farkas et al., 2002). These MD methods provide insights that may not be possible with TEM in-situ observations on the nano scale. But, severe limitations on time and length scales may render these simulations ineffective on the micro-structural physical scale that pertains to the inelastic behavior of crystalline aggregates (Meyers et al., 2006; Schiøtz, 2001).

Finite element methods (FEM) and crystal plasticity formulations have provided further understanding on GB and crack behavior. Ashmawi and Zikry (2003) have introduced interfacial GB regions to track slip and dislocation-density transmissions and intersections for a formulation based on dislocation-density based crystalline plasticity for analyses of voids and cracks. Cohesive zone method is the one that has been widely used to study intergranular crack. A traction–displacement relation is defined in the cohesive element to simulate the crack opening (Wells and Sluys, 2001; Yamakov et al., 2006). Other FE method that has been used is the extended finite element method (XFEM). The biggest advantages of XFEM are that it does not predefine the crack path, and it totally avoids remeshing. However, the drawbacks are also significant: in each element, more degrees of freedom are needed to represent the crack behavior; also a fine mesh must be used in the high stress gradient region in order to accurately predict the crack propagation direction, and if the crack propagation direction is unknown in advance, fine meshes through the whole model are needed (Karihaloo and Xiao, 2003; Yang and Deeks, 2007). Furthermore, none of these methods consider the dislocation activities in the GB region and their effect on crack propagation behavior, and hence they are not able to distinguish different GBs and predict intergranular and transgranular crack on a micro-structural scale.

Therefore, it is essential to understand and to predict how different random orientations affect behavior in aggregates with a pre-existing cracks of different lengths. In this paper, a methodology based on a multiple slip dislocation-density crystalline formulation and specialized finite-element approaches is introduced to predict how local GB behavior can affect crack behavior and overall response. As part of this framework, a dislocation-density grainboundary interaction (DDGBI) scheme between GBs and adjacent grain interiors has been developed. This scheme is based on accounting for three interrelated processes: dislocation-density absorption, emission and transmission. A conservation law for dislocation-density is used to balance dislocation activities within GB regions. This detailed representation of local dislocation-density activities for random low and high angle GBs can provide detailed understanding and predictive capabilities of how local microstructural interactions can affect intergranular and transgranular crack growth.

This paper is organized as follows: the constitutive formulations are presented in Section 2, which include the computational approach and the proposed dislocation-density grain–boundary interaction scheme; the results and discussions are presented in Section 3, which include the behavior of a polycrystalline aggregate with a pre-existing crack; a summary of the significant results is given in Section 4.

2. Constitutive formulation

2.1. Multiple-slip dislocation-density based crystalline formulation

In this section, a constitutive formulation for the finite deformation of rate dependent multiple-slip crystal plasticity is outlined. The detailed presentation of this constitutive formulation is given by Zikry and Kao (1996a,b).

It is assumed that the deformation gradient can be decomposed into elastic and plastic components, starting from the decomposition of the velocity gradient $V_{ij}$, into symmetric and anti-symmetric parts as

$$
V_{ij} = D_{ij} + W_{ij},
$$

where $W_{ij}$ is the anti-symmetric part, representing the spin tensor, and $D_{ij}$ is symmetric part, representing the deformation rate tensor. It is assumed that the spin tensor $W_{ij}$ and deformation rate tensor $D_{ij}$ can be further decomposed into elastic and plastic parts as

$$
D_{ij} = D_{ij}^e + D_{ij}^p,
$$

$$
W_{ij} = W_{ij}^p + W_{ij}^e.
$$

The superscript * means that the elastic part and the superscripts $p$ denote the plastic part. $W_{ij}^p$ represents the rigid body spin. The elastic components of the velocity gradient $D_{ij}^e$ correspond to the elastic lattice distortion and the inelastic parts are defined in terms of the crystallographic slip-rates as

$$
D_{ij}^e = p^{(x)}_{ij}(x^{(x)}),
$$

$$
W_{ij}^p = \alpha^{(x)}_{ij}(x^{(x)}),
$$

where $x$ is summed over all slip-systems and the tensors $p^{(x)}_{ij}$ and $\alpha^{(x)}_{ij}$ are defined in terms of the unit normals and the unit slip vectors as

$$
p^{(x)}_{ij} = \frac{1}{2} \left( s^{(x)}_i n^{(x)}_j + s^{(x)}_j n^{(x)}_i \right),
$$

$$
\alpha^{(x)}_{ij} = \frac{1}{2} \left( s^{(x)}_i n^{(x)}_j - s^{(x)}_j n^{(x)}_i \right).
$$

For a rate dependent formulation, the slip-rates are functions of the resolved shear stress and the reference shear stress on each slip-systems in a power law form of

$$
\dot{\gamma}_{ij}^{(x)} = \frac{\dot{\gamma}_{ij}}{\tau_{ij}^{ref}} \left[ \frac{\tau_{ij}^{(x)}}{\tau_{ij}^{ref}} \right]^{(1/m) - 1}.
$$

(5)

where $\dot{\gamma}_{ij}$ is the reference shear strain rate which corresponds to a reference shear stress $\tau_{ij}^{ref}$, and $m$ is the rate sensitivity parameter, and for most of the metals, $m$ is close to 100 at room temperature. The reference shear stress is a modification of widely accepted classical forms that relate the reference shear stress to a square-root dependence on the immobilized dislocation-density as

$$
\tau_{ij}^{(x)} = \tau_{ij}^{ref} + aGb \sum_{n=1}^{12} \sqrt{P_n^{(x)}},
$$

(6)

where $b$ is the magnitude of burgers vector, $G$ is the shear modulus, $\tau_{ij}^{ref}$ is the static yield stress, and $a$ is interaction coefficients, and generally have a magnitude of unity.
The resolved shear stress $\tau^{(x)}$ on the $x$th slip-system is given in terms of the Cauchy stress, $\sigma_{ij}$ as

$$\tau^{(x)} = p^{(x)}_i \sigma_{ij}. \tag{7}$$

For a deformed material, it can be assumed that the dislocation structure of total dislocation-density $\rho^{(x)}$ can be additively decomposed into two components: immobile dislocation-density $\rho^{(x)}_{im}$ and mobile dislocation-density $\rho^{(x)}_{m}$ as

$$\rho^{(x)} = \rho^{(x)}_{im} + \rho^{(x)}_{m}. \tag{8}$$

During an increment of strain, the dislocation-density generates at an intersection, trapping and recovery as:

$$d \rho^{(x)}_{im} = \frac{1}{b^2} \left( \frac{\rho^{(x)}_{m}}{\rho^{(x)}_{im}} \right) \frac{g_{mn}^\text{m,n}}{b^2} \exp \left( - \frac{H}{kT} \right) - \frac{g_{mn}^\text{m,mob}}{b} \sqrt{\rho^{(x)}_{im}}. \tag{9a}$$

$$d \rho^{(x)}_{m} = \frac{1}{b^2} \left( \frac{\rho^{(x)}_{m}}{\rho^{(x)}_{im}} \right) \frac{g_{mn}^\text{m,n}}{b^2} \exp \left( - \frac{H}{kT} \right) - \frac{g_{mn}^\text{m,mob}}{b} \sqrt{\rho^{(x)}_{im}} - \frac{g_{mn}^\text{m,recov}}{b} \exp \left( - \frac{H}{kT} \right) \rho^{(x)}_{m}. \tag{9b}$$

where $g_{mn}^\text{m,n}$ is a coefficient pertaining to an increase in the mobile dislocation-density due to dislocation sources; $g_{mn}^\text{m,mob}$ is a coefficient related to the trapping of mobile dislocation due to forest interactions; $g_{mn}^\text{m,recov}$ is a coefficient related to the rearrangement and annihilation of immobile dislocations; $g_{mn}^\text{m,mob}$ is a coefficient pertaining to the immobilization of mobile dislocations; $H$ is the activation energy; and $k$ is the Boltzmann’s constant. As these evolutionary equations indicate, the dislocation activities related to recovery and trapping are coupled to thermal activation.

2.2. Dislocation-density grain–boundary interaction (DDGBI) scheme

In this section, a dislocation-density grain–boundary interaction (DDGBI) scheme is presented to account for the GB dislocation-density activities. It is assumed that the dislocation-density interactions occur between slip-systems on each side of the GB interface. Based on the single transmission criteria by Clark et al. (1992), a transmission criteria for multiple slip is proposed as follows:

**Criteria 1.** A transmission factor is proposed based on two components. The first one is the angle $\alpha$ (Fig. 1), which is the angle between the intersection lines of the slip planes and GB planes; the second part is the angle $\beta$ between slip directions of these two slip-systems. Hence, the transmission factor $M_{gb}$ can be denoted as

$$M_{gb} = \cos \alpha \cdot \cos \beta, \tag{10}$$

where $\alpha = \arccos(\hat{l}_1 \cdot \hat{\beta})$ in which $\hat{l}_1 = \hat{n}_1 \cdot \hat{n}_{GB}$ and $\hat{l}_2 = \hat{n}_2 \cdot \hat{n}_{GB}$, and $\beta = \arccos(\hat{\beta}_1 \cdot \hat{\beta}_2)$.

**Criteria 2.** The ratio of resolved shear stress to the reference shear stress of the outgoing slip-system ($\text{stress ratio}$) should be greater than a critical value $c_\alpha$, which is approximately one.

If these transmission criteria are satisfied, a dislocation-density can emit from a higher dislocation-density region to a lower dislocation-density region. It is assumed that the dislocation-densities will be redistributed according to these transmission factors as shown in Fig. 2. Based on this, a balance of dislocation-densities due to these different dislocation-density interactions, $\Delta \rho^{(x)}_{out}$, can be defined as

$$\Delta \rho^{(x)}_{out} = \sum_{m=1}^{n} M_{gb} \left( \frac{\tau^{(x)}_{out}}{\tau^{(x)}_{ref}} \right)^{\beta} \cdot \Delta \rho^{(x)}_{im}, \tag{12}$$

where $\alpha$ is an incoming slip-system, $\beta$ is an outgoing slip-system, $\tau^{(x)}_{out}$ is the corresponding resolved shear stress, and $\tau^{(x)}_{ref}$ is the reference shear stress of the outgoing slip-system $\beta$. $m$ is the number of all possible outgoing slip-systems, and $M_{gb}$ is the transmission factor between the incoming and outgoing slip-systems.

When dislocation-densities emit from one element to the other, a balance for the dislocation-densities can be obtained by considering dislocation-density conservation (Aifantis, 1987).

$$\frac{\partial \rho^{(x)}}{\partial t} = \hat{\tau}^{(x)} - div \hat{j}^{(x)}, \tag{13a}$$

where

$$div \hat{j}^{(x)} = \frac{\partial}{\partial x} \left( \int \frac{\phi_{n}}{\phi_{x}} \hat{\mu} dA \right) + \frac{\partial}{\partial y} \left( \int \frac{\phi_{n}}{\phi_{y}} \hat{\mu} dA \right). \tag{13b}$$

where $\hat{j}^{(x)}$ represents the flux of dislocation-densities in slip-system $x$, $A$ is area of integration, $\hat{\mu}$ is the GB surface normal, $\Delta \rho^{(x)}$ is the summation of the dislocation-densities changes in the domain indicated by Eq. (12), and $\hat{\tau}^{(x)}$ represents the generation, immobilization or annihilation of dislocations densities. $\hat{\tau}^{(x)}$ is given by the statistical distribution of the immobile and mobile dislocation-densities from Eqs. (14a), (14b).

$$\hat{\tau}^{(x)}_{im} = \tau^{(x)}_{im} \left( \frac{g_{mn}^\text{m,n}}{b^2} \exp \left( - \frac{H}{kT} \right) \frac{g_{mn}^\text{m,mob}}{b} \sqrt{\rho^{(x)}_{im}} \right), \tag{14a}$$

$$\hat{\tau}^{(x)}_{m} = \tau^{(x)}_{m} \left( \frac{g_{mn}^\text{m,n}}{b^2} \frac{g_{mn}^\text{m,mob}}{b} \sqrt{\rho^{(x)}_{im}} \right). \tag{14b}$$

So that the evolution of dislocation-densities is updated as

Fig. 1. Intersection angles $\alpha$ between intersections of slip planes and GB planes.

Fig. 2. Dislocation-density redistribution according to transmission factors and resolved shear stress.
2.3. Computational methods

The total deformation rate tensor $D_{ij}$, and the plastic deformation rate tensor $D_{ij}^p$ are needed to update the material stress state. The method used here is one developed by Zikry (1994) for rate dependent crystalline plasticity formulations, and a brief outline will be given here. An implicit finite-element method is used to obtain the total deformation rate tensor $D_{ij}$. To overcome numerical instabilities associated with stiffness, an adaptive explicit–implicit method is used to obtain the plastic deformation rate tensor $D_{ij}^p$. An explicit fifth order Runge–Kutta method is used most of the times, and when numerical stiff occurs, the computation scheme automatically switches to the implicit backward Euler method. This adaptive numerical scheme is also used to update the evolutionary equations for the mobile and immobile dislocation-densities and the resolved shear stress.

$$\frac{d\rho_{im}^{(a)}}{dt} = \frac{\rho_{im}}{b} \exp \left( \frac{H}{kT} \right) - \frac{\rho_{im}}{b} \sqrt{\frac{\rho_{im}}{\rho_{im}^{(a)}}} \exp \left( -\frac{H}{kT} \right) \rho_{im}^{(a)} - div \bar{\rho}_{im}^{(a)}. \tag{15a}$$

$$\frac{d\rho_{im}^{(a)}}{dt} = \frac{\rho_{im}}{b} \exp \left( \frac{H}{kT} \right) - \frac{\rho_{im}}{b} \sqrt{\frac{\rho_{im}}{\rho_{im}^{(a)}}} \exp \left( -\frac{H}{kT} \right) \rho_{im}^{(a)} - div \bar{\rho}_{im}^{(a)}. \tag{15b}$$

Dislocation-density activities can occur in the GB interface and at GB-interior interfaces (Figs. 2 and 3). In the proposed GB representation, we assume that dislocation-density transmission occurs when immobile dislocation-densities transmit through the GB interfaces to compatible slip systems in the neighboring grain. Dislocation-density absorption occurs when mobile dislocation-densities from the grain interior transmit into the GB, but do not transmit out of it. In this case, all of the mobile dislocation-densities are then immobilized to immobile dislocation-densities, and are assumed to be absorbed in the GB. Some of these immobile dislocation-densities in the GB regions may pile-up, but as the deformation evolves can activate neighboring slip systems. This can result in dislocation-density emission, in which the immobile dislocation-densities in the GB become mobile dislocation-densities and emit into the neighboring grain. Hence, all three processes of transmission, absorption, and emission can occur simultaneously on different slip-systems within the GB region and between neighboring grains.

### Table 1a

<table>
<thead>
<tr>
<th>Grain no.</th>
<th>$\phi_1$ (rad)</th>
<th>$\phi_2$ (rad)</th>
<th>$\Phi$ (rad)</th>
<th>Misorientation by Euler angles (°)</th>
<th>Misorientations by axis/angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>22 (crack)</td>
<td>0.164</td>
<td>0.192</td>
<td>0.098</td>
<td>1.031, 1.261, 9.110</td>
<td>(1.000, 0.000, 0.025)/9.1°</td>
</tr>
<tr>
<td>20 (under)</td>
<td>0.182</td>
<td>0.170</td>
<td>0.257</td>
<td>9.282, 6.532, 4.870</td>
<td>(0.296, 0.000, 0.955)/16.6°</td>
</tr>
<tr>
<td>19 (lower left)</td>
<td>0.002</td>
<td>0.078</td>
<td>0.013</td>
<td>1.089, 4.985, 2.636</td>
<td>(1.000, 0.001, 0.017)/2.6°</td>
</tr>
<tr>
<td>21 (ahead)</td>
<td>0.145</td>
<td>0.105</td>
<td>0.052</td>
<td>9.225, 4.698, 5.730</td>
<td>(0.377, 0.000, 0.926)/15.0°</td>
</tr>
<tr>
<td>23 (upper)</td>
<td>0.003</td>
<td>0.110</td>
<td>0.198</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The mechanical properties in the GB region are assumed to be the same as in the grain interior, and the material properties of the f.c.c. crystals are given in Table 1c. The initial immobile dislocation-density, \( \rho_{\text{imm}} \), was chosen as \( 10^{10} \text{ m}^{-2} \), and the initial mobile dislocation-density \( \rho_{\text{mov}} \) was chosen as \( 10^6 \text{ m}^{-2} \). The values of the initial and the saturated dislocation-densities are representative of copper (Mughrabi, 1987). Based on the scheme developed by Zikry and Kao (1996), we have obtained the coefficient values needed for the evolution of the immobile and mobile densities and the specified material properties. These values are 

- \( g_{\text{mter}} = 5.53 \), \( g_{\text{recov}} = 6.67 \), \( g_{\text{immob}} = 0.0127 \), \( g_{\text{crow}} = 2.7 \times 10^{-5} \).

### 3.1. The effects of random low angle and high angle GBs in a crack-free aggregate

Dislocation-densities can interact with GBs due to absorption, transmission and emission, and the GB behavior can be determined by the competition of these interactions, since these local GB interactions can affect overall aggregate behavior. The normalized (normalized by the initial immobile density) immobile dislocation-density behavior of one of the more active slip-systems, for a random high angle aggregate is shown in Fig. 4a and for a random low angle aggregate it is shown in Fig. 5a at a nominal strain of 5%. There are no interactions between dislocation-densities and GBs, since the DDGBI scheme is not used for these predictions. As seen in Fig. 4a, the high angle GB regions approximately have the same dislocation-densities as in the grain interior, which in general is not accurate, since high angle GBs usually have higher dislocation-densities than the grain interior, and dislocation-densities can pile-up (Lee et al., 1990a; Ohmura et al., 2005). In Fig. 5a, the dislocation-densities for the low angle GB region, have accumulated at the GB interface.

When the DDGBI scheme is used, the interactions including absorption, emission and transmission can be modeled according to the crystallographic and mechanical behavior of the GBs. As seen in Fig. 4b, the high angle GB region absorbed and piled-up dislocation-densities transmitting from the grain interior, and the immobile dislocation-densities increased by 73% in the GB region. For the random low angle GB, as shown in Fig. 5b, there is significant dislocation transmission through the low angle GB region, which redistributes the immobile dislocation-densities through the GBs, but the immobile dislocation-density in the GB regions increases by approximately 80% due to dislocation absorption in the GB regions.

The dislocation-density activities also affect other GB behavior, such as local normal stresses, accumulated shear slip, and pressure for the random high angle GBs. As seen in Fig. 4c–d, the normal stress in the GB region is approximately 50% higher in comparison for the case when the DDGBI scheme is used, due to dislocation-density absorption in GB regions. As shown in Fig. 4e–f, the shear slip decreases by approximately 20%, in comparison with the case when the DDGBI scheme is not used, because dislocation-density interactions in the GB region impede plastic strain accumulation. For the random low angle GB aggregate, the normal stress (Fig. 5c–d) in the GB regions are approximately 8% higher, and the shear slip is approximately 4% lower in comparison for the case when the DDGBI scheme is not used (Fig. 5e–f). These increases in the normal stress and the pressure, and the decrease in plastic strain is a direct consequence of the interrelated interactions of absorption, transmission, and emission. These results are consistent for predictions related to bicrystal behavior at different length scales (Shi and Zikry, 2009).

### 3.2. Crack behavior and GB interactions

Pre-existing cracks with different crack length are introduced in the 50-grain polycrystal aggregates (Fig. 3b–c). A short crack with a normalized length of \( a/w = 0.05 \) (Fig. 3b) and a longer crack with an \( a/w \) of 0.1 (Fig. 3c) were investigated for the random high and low angle GBs. It should also be noted that the GB misorientation directly ahead of the crack tip is 34.45° for the random high angle GB case, and 2.61° for the random low angle GB case. The mesh was refined until convergent results were obtained for stress gradients in the crack process region. Convergent meshes of 1864 elements for the short crack, and 1830 elements for long crack elements were used for the different GB orientations.

#### 3.2.1. Random low angle GB behavior for the short crack (\( a/w = 0.05 \))

Fig. 6 shows the immobile dislocation-density of the most active slip-system near the crack tip region for the high angle GB model. The GB above the crack tip, which is the GB between grain 22 and grain 23 (GB 22–23), has a misorientation of 15° with respect to grain 22, and the GB ahead of the crack tip (GB 22–21) has a misorientation of 2.61° (Table 1a). There are no interactions between dislocation-densities and GBs when the DDGBI scheme is not used (Fig. 6a). When the DDGBI scheme is used (Fig. 6b), these GBs absorb dislocation-densities from the crack tip regions as shown in Fig. 6a. The maximum dislocation-density is approximately \( 3 \times 10^{15} \text{ m}^{-2} \) in GB 22–23, and \( 1 \times 10^{15} \text{ m}^{-2} \) in GB 22–21. The GB with the higher misorientation angle (15° in GB 22–23) absorbs more dislocation-densities than the GB with the lower misorientation GB (2.61° in GB 22–21). Although there are many factors that control dislocation-density absorption, it is evident that dislocation activities increase as the misorientation angle increases. Fig. 7 shows the consequent normal stress distribution directly ahead of the crack tip. If the DDGBI scheme is not used, the GB has no influence on the stress distribution (Fig. 7a). Since the dislocation-density absorption is insignificant for random low an-
gle GBs, we can see that there is only a minor increase of 29% in normal stress in the GB region (Fig. 7b and Fig. 14a) when the DDGBI scheme is used in comparison for the case when the DDGBI scheme is not used.

3.2.2. Random high angle GB behavior for the short crack \((a/w = 0.05)\)

Fig. 8 shows the immobile dislocation-density of the most active slip-system for a random high angle GB showing dislocation-density absorption: (a) immobile dislocation-density of an active slip-system \([110](111)\) without the DDGBI scheme; (b) immobile dislocation-density of the same slip-system with the DDGBI scheme; (c) normal stress without DDGBI scheme; (d) normal stress with DDGBI scheme; (e) shear slip without DDGBI scheme and (f) shear slip with DDGBI scheme.

Fig. 4. Immobile dislocation-density of the most active slip-system for a random high angle GB showing dislocation-density absorption: (a) immobile dislocation-density of an active slip-system \([110](111)\) without the DDGBI scheme; (b) immobile dislocation-density of the same slip-system with the DDGBI scheme; (c) normal stress without DDGBI scheme; (d) normal stress with DDGBI scheme; (e) shear slip without DDGBI scheme and (f) shear slip with DDGBI scheme.

\[ \frac{110}{111} \]

\[ \frac{111}{222} \]

\[ \frac{111}{111} \]

\[ \frac{111}{111} \]

\[ \frac{111}{111} \]

Similar to the high angle GB case, when the DDGBI scheme is not used, there is no interaction between dislocation-densities and GBs. When the DDGBI scheme is used, the high dislocation-density absorption increases the normal stress in GB 22–21 ahead of the crack tip by 53%, and increases it in GB 22–23 by approximately 40%. The normal stress to the left of GB 22–23 decreases by 29% (Fig. 14b). This is probably because the plastic deformation from the crack tip is impeded by GB 22–23. As these results indicate, the dislocation-density impedance for random high angle GBs is significant.

3.2.3. Random low angle GB behavior for the long crack \((a/w = 0.1)\)

Fig. 10 shows the dislocation-density of an active slip-system \([011](111)\) near the crack tip region for the random low angle GB aggregate when the DDGBI scheme is not used. As we can see, there is significant dislocation-densities accumulation for this slip-system near the crack tip region. When the DDGBI scheme is used, the high dislocation-density absorption increases the normal stress in GB 22–21 ahead of the crack tip by 53%, and increases it in GB 22–23 by approximately 40%. The normal stress to the left of GB 22–23 decreases by 29% (Fig. 14b). This is probably because the plastic deformation from the crack tip is impeded by GB 22–23. As these results indicate, the dislocation-density impedance for random high angle GBs is significant.
not used, the dislocation-densities evolve through the GB as if there is no GB effect (Fig. 10a). When the DDGBI scheme is used, we can see that the low angle (2.61°) GB does slightly absorb dislocation-densities, and the dislocation-density in the GB increases by 60% (Fig. 10b). The higher angle GB (15°) above the crack tip absorbs dislocation-densities, and the density increases by approximately 300%. This result is similar for the predictions associated with the shorter crack, in which the GB with the higher misorientation absorbs more dislocation-densities. Fig. 11 shows the normal stress near the crack tip. When the DDGBI scheme is not used, there are no significant GB effects. The normal stress gradually decreases with a radial increase in distance (Fig. 11a). When the DDGBI scheme is used, due to the GB dislocation-density absorption ahead of the crack tip, the normal stress increases by 42% (Fig. 11b and Fig. 14c). This increase in normal stress along the radial direction of the crack, along with the stress distribution patterns, can indicate that the crack will be probably growing along the initial crack orientation.

3.2.4. Random high angle GB behavior for the long crack (\(a/w = 0.1\))

Fig. 12 shows the dislocation-densities of the most active slip-system [1 1 0](1 1 1) near the crack tip region for the random high angle GB case. When the DDGBI scheme is not used, the dislocation-densities from the crack tip do not have any interaction with the GBs, and the maximum dislocation-density is adjacent to the crack tip region \((3.8 \times 10^{15} \text{ m}^{-2})\). The maximum dislocation-density in the GB 22–21 region is approximately \(\times 10^{14} \text{ m}^{-2}\). When the DDGBI scheme is used, there are extensive dislocation-density accumulations with a maximum of \(7.5 \times 10^{16} \text{ m}^{-2}\) for this slip-system. This is approximately 2000% higher in comparison with the case where the DDGBI scheme is not used. When the DDGBI scheme is not used, the highest normal stress is near the crack tip, and there are no accumulations at the GB regions (Fig. 13a). When the DDGBI scheme is used, the stress increases by 108% due to GB activities. The normal stress behind the high angle GB significantly decreases by 30% (Fig. 13b and Fig. 14d). Compared to the results for the shorter crack (Fig. 8b), we can see that the
longer the crack, the more significant the GB effects will be, since more GBs would interact with the crack. Since the crack can propagate along the direction of the high stress, the stress concentration in the GB region and low stress behind GB can result in crack propagation along these critical GBs, and hence an intergranular crack could propagate for this case. Furthermore, these GB...
regions, with the high stresses and dislocation-density absorption can be micro-crack nucleation sites, which would also be another factor that would affect the intergranular growth of the pre-existing crack.

The normal stress along the direction of crack is shown in Fig. 14 for the above four cases. As we can see from these figures, when the DDGBI scheme is not used, the normal stress decreases as the distance from crack tip increases. When the DDGBI scheme...
is used, there are significant increases of normal stresses in the GB region for both the random low angle and high angle GB. For the random high angle GBs, the stresses are approximately 3–4 times higher in magnitude in comparison with values for the random low angle GB at the same locations. Furthermore, the normal stress on the left side of these critical GB decreases when the normal stress on the right side of the GB region (grain 22) increases, which probably indicates that the GB blocks the transmission of deformation and stress from the crack tip.

As noted earlier, it has been observed and confirmed in numerous experiments that GB behavior can have significant effects on deformation and failure modes. For random low angle GBs, dislocations are commonly observed to transmit through the GBs, and there are very rare cases of dislocation pile-ups (Lee et al., 1990a; Lucadamo and Medlin, 2002). For random high angle GBs, dislocations can be absorbed and piled-up in the GB (Gemperlova et al., 2004; Lee et al., 1990a,b). These predictions are consistent with these experimental observations for the random low and high angle GB cases.

When the DDGBI scheme is not used, for both random low angle and high angle GBs, there are no interactions between dislocation-densities and GBs, such as transmission, absorption and emission. When the DDGBI scheme is used, these complex interactions are accounted for, and hence different behavior between low angle and high angle GBs can be predicted.

For random low angle GBs, it is shown that there are some dislocation-density absorptions in the GB regions, but the absorbed dislocation-densities can transmit through the GBs, and attenuate the dislocation-densities and stresses in the GBs. Hence, crack growth will not be significantly affected by the random low angle GBs. Numerous TEM observations have indicated these crack growth patterns for random low angle GBs (Zhang and Wang, 2008; Zhong et al., 2006). For example, Fig. 15a shows a schematic of the predicted crack growth for a random low angle GB distribution. Dislocation-densities transmit through the GBs, and then attenuate the stresses in the GBs. Hence, the crack may propagate through the GB region without significant directional and orientational changes (Zhong et al., 2006).

For random high angle GBs, the predictions using the DDGBI scheme show severe dislocation-density pile-ups and stress accumulations in the GB regions ahead of the crack tip. The pattern of stress accumulation is within and along the GB regions. The high dislocation-densities and stresses in the GB region can affect the direction of crack propagation along the GB. These GBs, which can be micro-crack nucleation sites, would result in intergranular growth of the pre-existing crack. Several experimental observations have shown that the crack propagation in aggregates with random high angle GBs occurs in this intergranular fashion (Robertson et al., 1991; Zhong et al., 2006). Fig. 15b shows a schematic of crack propagation ahead of high angle GB.
The high dislocation-densities adjacent to the crack tip are absorbed and pile-up along the GBs, and in combination with the high stresses in the GB regions can result in intergranular crack growth.

**Fig. 14.** Normal stress along the direction of crack: (a) short crack with random low angle GBs; (b) short crack with random high angle GBs; (c) long crack low with random high angle GBs and (d) long crack with random high angle GBs. The normal stress increases by 32% for the random low angle GB case, and by 53% for the high angle GB region for the short crack with DDGBI. The normal stress increases by 42% in the low angle GB region, and 108% in the high angle GB region for longer crack with DDGBI.

**Fig. 15.** Schematic on how crack growth can occur: (a) dislocation-densities transmit through low angle GBs; (b) crack penetrates low angle GBs; (c) dislocation-densities piled-up at high angle GB and (d) intergranular crack growth at the pile-up and micro-crack nucleation regions for random high angle GB case.
4. Conclusion

A dislocation-density grain–boundary interaction (DDGBI) scheme has been developed to account for and predict GB interactions with dislocation-densities, such as emission, absorption and transmission in polycrystals with random low and high angle GBs. When the DDGBI scheme is not used, it is not possible to account for dislocation-density–GB interactions, and accurately predict how these GB effects can affect overall behavior. When the DDGBI scheme is used, there are significant predicted differences in behavior. For random low angle GBs, although there is some dislocation-density absorption, the dislocation-densities mainly transmit through the GB. This results in stress attenuation in the GB regions. For the aggregate with the random high angle GBs, the absorbed dislocation-densities dominate, and dislocation-density pile-ups and stress accumulations occur.

For the aggregate with different crack lengths, it was shown that dislocation-densities ahead of the crack tip can transmit through the GBs for an aggregate with random low angle GB. The dislocation-density transmission attenuates the stresses in the GB regions, so that GBs do not significantly change the crack growth directions. However, high dislocation-densities can blunt crack growth. Random high angle GBs ahead of the crack tip had significantly more absorption of dislocation-densities with no transmission from these regions. This can result in extensive severe dislocation-density pile-ups in the GBs. The piled-up dislocation-densities dramatically increase the stresses in the GB, and inhibit plastic deformation transmission to neighboring grains. These GB regions, with the high stresses and dislocation-density absorption can be micro-crack nucleation sites, which would also be another factor that would affect the intergranular growth of the pre-existing crack. The present study underscores that GB activities would significantly affect crack growth behavior. These effects are more significant for longer initial cracks, in which the crack would interact with more GBs.

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