Microstructural modeling of transgranular and intergranular fracture in crystalline materials with coincident site lattice grain-boundaries: $\Sigma 3$ and $\Sigma 17b$ bicrystals

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Abstract

The competing microstructural failure mechanisms of transgranular (TG) and intergranular (IG) fracture, in martensitic steel bicrystals with coincident site lattice (CSL) boundaries of $\Sigma 3$ and $\Sigma 17b$, have been investigated, using a dislocation-density-based crystalline plasticity formulation and a recently developed overlapping fracture method. A dislocation-density grain boundary (GB) interaction scheme was coupled within a dislocation-density based crystal plasticity formulation to investigate how different types of CSL GBs affect dislocation-density evolution, plastic deformation, dislocation pile-up formation, TG and IG fracture, and fracture toughness. The computational predictions indicate that the bicrystal, with a $\Sigma 3$ boundary, transitioned from IG to TG fracture, with large dislocation density generation and plastic deformation on the TG fracture planes. Bicrystals with the $\Sigma 17b$ boundary failed due to intergranular fracture and rupture, with much lower, in comparison with the $\Sigma 3$ boundary case, dislocation density generation and plastic deformation. These predictions, which are consistent with experimental observations, indicate that $\Sigma 3$ boundary is resistant to IG fracture with a higher fracture toughness than the $\Sigma 17b$ boundary case. More significantly, the computational

framework can potentially be used as a guideline for GB engineering for failure-resistant materials.

Keywords: Coincident Site Lattice, Grain Boundary, Dislocation-density, Transgranular, Intergranular, Fracture

1. Introduction

Fracture in polycrystalline metals and alloys can be characterized in terms of either TG or IG fracture modes or a combination of both fracture modes [1–5]. TG fracture occurs on microstructural cleavage planes, while IG fracture propagates along GB planes [6–9]. Experimental observations have clearly indicated that GB structures significantly affect TG and IG fracture modes [10–13]. High angle or high CSL boundaries can impede dislocation transmission, lead to dislocation pile-up and accumulation, result in high local stress at GBs, and induce IG fracture [14–17]. Low angle or low CSL boundaries can result in the transmission of dislocations, which can relieve stress at GBs and inhibit IG fracture [10, 11, 18]. Therefore, increasing the fraction of low CSL boundaries in polycrystalline metals and alloys can significantly improve fracture resistance [19, 20].

Experimental observations of bicrystals have further indicated that low CSL GBs are characterized by TG fracture due to dislocation transmission, while high CSL GBs are characterized by IG fracture due to dislocation pile-ups [21, 22]. TG fracture in bicrystals is generally accompanied with large plastic deformation, while IG fracture has relatively, in comparison with low CSL GBs, low plastic deformation [23]. These experimental

investigations indicate that GB characteristics, such as GB structure and orientation, have a significant effect on dislocation-GB interaction, TG and IG fracture, plastic deformation, and fracture toughness.

We developed an integrated framework that can account for the competing failure mechanisms of TG and IG fracture, to investigate how different types of CSL GBs affect the TG and IG fracture modes. A dislocation-density GB interaction scheme was incorporated within the dislocation-density based crystalline plasticity formulation [24–26], and this interaction scheme can account for dislocation transmission and impedance across GB. A recently developed fracture method based on the overlapping element method of Wu and Zikry [27] and Hansbo and Hansbo [28], which can represent the physically-based fracture planes, such as cleavage planes for TG fracture and GB planes for IG fracture in martensitic steels [6, 29], has been used to generate failure surfaces. This formulation is then used to investigate the microstructural competition between TG and IG fracture in b.c.c. bicrystals.

This paper is organized as follows: the dislocation-density based crystalline plasticity formulation, the derivation of the dislocation-density GB interaction, are presented in Section 2, the microstructurally-based TG and IG failure criterion, and the numerical implementation of overlapping element method for fracture are outlined in Section 3, the results are presented and discussed in Section 4, and a summary of the results and conclusions are given in Section 5.

2. Constitutive Formulation

In this section, only a brief outline of the multiple-slip crystal plasticity rate-dependent constitutive formulation and the evolution equations for the mobile and immobile dislocation-densities, which are coupled to the constitutive formulation, are presented. A detailed presentation is given by Shanthraj and Zikry [24].

2.1. Multiple-slip dislocation-density based crystal plasticity formulation

The dislocation-density based crystal plasticity constitutive framework used in this study is based on a formulation developed by Wu et al. [25], Zikry [30], and Ziaei et al. [31], and a brief outline will be presented here. It is assumed that the velocity gradient is decomposed into a symmetric deformation rate tensor D_{ij} and an anti-symmetric spin tensor W_{ij} [32]. The tensors D_{ij} and W_{ij} are then additively decomposed into elastic and inelastic components as

$$D_{ij} = D_{ij}^* + D_{ij}^p, \quad W_{ij} = W_{ij}^* + W_{ij}^p, \quad (1)$$

The superscript $*$ denotes the elastic part, and the superscript p denotes the plastic part.

W_{ij}^* includes the rigid body spin. The inelastic parts are defined in terms of the crystallographic slip-rates as

$$D_{ij}^p = \sum_a \dot{\gamma}^{(a)} P_{ij}^{(a)}, \quad \text{and} \quad W_{ij}^p = \sum_a \dot{\gamma}^{(a)} \omega_{ij}^{(a)}, \quad (2)$$

where α is summed over all slip-systems, and $P_{ij}^{(\alpha)}$ and $\omega_{ij}^{(\alpha)}$ are the symmetric and anti-symmetric parts of the Schmid tensor in the current configuration respectively.

A power law relation can characterize the rate-dependent constitutive description on each slip system as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_{ref}^{(\alpha)} \left(\frac{t^{(\alpha)}}{t_{ref}^{(\alpha)}} \right)^{\frac{1}{m}-1}, \quad (3)$$

where $\dot{\gamma}_{ref}^{(\alpha)}$ is the reference shear strain-rate which corresponds to a reference shear stress $t_{ref}^{(\alpha)}$, and m is the rate sensitivity parameter. $t^{(\alpha)}$ is the resolved shear stress on slip system α . The reference stress used is a modification of widely used classical forms [33] that relate reference stress to immobile dislocation-density r_{im} as

$$t_{ref}^{(\alpha)} = t_y^{(\alpha)} + G \sum_{b=1}^{nss} \frac{b^{(b)}}{a_{ab}} \sqrt{r_{im}^{(b)}} \left(\frac{T}{T_0} \right)^{-\xi}, \quad (4)$$

where $t_y^{(\alpha)}$ is the static yield stress on slip system α , G is the shear modulus, nss is the number of slip systems, $b^{(b)}$ is the magnitude of the Burgers vector, and a_{ab} are Taylor coefficients which are related to the strength of interactions between slip-systems [34–36]. T is the temperature, T_0 is the reference temperature, and ξ is the thermal softening exponent.

2.2. Mobile and immobile dislocation density evolution equations

Following the approach of Zikry and Kao [37], it is assumed that, for a given deformed state of the material, the total dislocation-density, $r^{(\alpha)}$, can be additively decomposed into a mobile $r_m^{(\alpha)}$ and an immobile dislocation-density, $r_{im}^{(\alpha)}$. Furthermore, the mobile and immobile dislocation-density rates can be coupled through the formation and destruction of junctions as the stored immobile dislocations act as obstacles for

evolving mobile dislocations. This is the basis for taking the evolution of mobile and immobile dislocation densities as

$$\frac{dr_m^a}{dt} = \left[g_{sour}^a \frac{r_{im}^a}{b^2} - g_{mnter-}^a r_m^a - \frac{g_{immob-}^a}{b} \sqrt{r_{im}^a} \right] \quad (5)$$

$$\frac{dr_{im}^a}{dt} = \left[g_{mnter+}^a r_m^a + \frac{g_{immob+}^a}{b} \sqrt{r_{im}^a} - g_{recov}^a r_{im}^a \right] \quad (6)$$

where g_{sour} is a coefficient pertaining to an increase in the mobile dislocation-density due to dislocation sources, g_{mnter} are coefficients related to the trapping of mobile dislocations due to forest intersections, cross-slip around obstacles, or dislocation interactions, g_{recov} is a coefficient related to the rearrangement and annihilation of immobile dislocations, and g_{immob} are coefficients related to the immobilization of mobile dislocations. These non-dimensional coefficients were determined as functions of the crystallography and deformation mode of the material, by considering the generation, interaction and recovery of dislocation densities as discussed in Shanthraj and Zikry [24].

2.3. Dislocation-density GB interaction scheme

In this section, a dislocation-density GB interaction scheme is presented. For dislocation-density transmission through the boundary, an incoming slip system usually does not completely coincide with an outgoing slip system, and residual dislocations can remain within the boundary due to the conservation of lattice defect vector [10, 38–40]. The energy required to produce the residual dislocation at the boundary is considered as the energy barrier for thermally activated dislocation transmission [41, 42]. The slip-rate

relation (Eq. (3)) has been modified at the boundary through the introduction of a GB transmission factor (GBTF) based on the energy barrier as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_{ref}^{(\alpha)} \frac{\exp\left(-\frac{U_{GB}^{(\alpha)}}{kT}\right)}{\exp\left(-\frac{U_{GB}^{(\alpha)}}{kT}\right)} \left(\frac{\dot{\gamma}^{(\alpha)}}{\dot{\gamma}_{ref}^{(\alpha)}}\right)^{\frac{1}{m}-1} GBTF^{(\alpha)}, \quad (7)$$

where $GBTF^{(\alpha)} = \exp\left(-\frac{U_{GB}^{(\alpha)}}{kT}\right)$. It can range from 0 to 1, where 0 corresponds to full blockage and 1 corresponds to full transmission. $U_{GB}^{(\alpha)}$ is the internal energy for slip system α due to the activation of a Frank-Read source in the presence of a GB, k is the Boltzmann constant, and T is the absolute temperature. Based on a line tension model developed by Koning et al. (2002), this energy barrier due to GB residual dislocations, for incoming and outgoing slip systems α and β , can be postulated as

$$U_{GB}^{(\alpha\beta)} = \kappa G D b_{eff}^2 D_2, \quad (8)$$

where κ is approximately equal to 0.5, G is the shear modulus, $D b_{eff}$ is the magnitude of the effective residual Burger's vector, which is a function of the misorientation of the slip planes and the magnitude of the true residual Burger's vector. D_2 is the length of residual dislocation, and it is a function of the resolved shear stress for the outgoing slip system β . Details for calculation of $D b_{eff}$ and D_2 are given in Shanthraj and Zikry [38] and Koning et al. [43]. Dislocation-density transmission is considered on the most energetically favorable outgoing slip system by using the lowest value of the energy, on all active outgoing slip systems, as

$$U_{GB}^{(\alpha)} = \min_b U_{GB}^{(\alpha b)}, \quad (9)$$

3. Microstructural failure criterion and numerical implementation of overlapping element method

3.1. Microstructural TG failure criterion

The inherent TG fracture mode in b.c.c. materials, such as martensitic steel, is cleavage on $\{100\}_{\alpha'}$ planes [44]. To account for this as a microstructural failure criterion, the orientation of the cleavage planes in the global coordinate system is obtained by

$$n_{cleave} = [T]n_{cleave,\alpha'}, \quad (10)$$

where T relates the orientation of each grain (represented by a set of Euler angles) to the global coordinates. Due to lattice rotations, the global orientation of the cleavage planes in the current configuration is updated at every time-step as $\dot{n}_{cleave} = W^* n_{cleave}$.

The normal component of the traction acting on each cleavage plane has a direct influence on fracture along that plane [8, 9]. The maximum normal component of the traction, over all the $\{100\}_{\alpha'}$ cleavage planes, is monitored and compared with a critical fracture stress σ_{frac} to determine TG failure. The TG failure criterion is then given by

$$t_{cleave} > S_{frac}, \quad (11)$$

where $t_{cleave} = \max_{\{100\}_{\alpha'} \text{ planes}} \langle n_{cleave}^T [S] n_{cleave} \rangle$.

3.2. Microstructural IG failure criterion

IG cracks propagate along GBs, and experimental observations have indicated that IG crack nucleation and growth occur at those GBs, where the normal component of traction on GB planes has a higher value [8, 45]. Therefore, the normal component of traction on GB plane is monitored and compared with a critical GB fracture stress S_{GB} to determine IG fracture. The failure criterion for IG fracture can be given by

$$t_{GB} > S_{GB}, \quad (12)$$

where $t_{GB} = n_{GB}^T [S] n_{GB}$, n_{GB} is the normal vector of GB plane.

3.3. Computational implementation of overlapping element method

We follow the approach of Wu and Zikry [27] and Hansbo and Hansbo [28], and consider one element with a crack defined implicitly by $f(X)=0$. This divides the element domain into two subdomains with areas A_{e1} and A_{e2} . The direction of crack propagation would be along the most favorable cleavage plane or GB plane [6–9]. Adding phantom nodes on top of the existing nodes, the original cracked element is replaced by two overlapping elements. The two overlapping elements do not share nodes, and therefore can have independent displacement fields. For each overlapping element, only the subdomain with area A_{e1} or A_{e2} , corresponding to one of the two subdomains for the original cracked element, is considered as active. Details for implementation of overlapping element method are given in Wu and Zikry [27].

3.4. Computational techniques for dislocation-density-based crystal plasticity

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 the one developed by Zikry [30] and Shanthraj and Zikry [24] for rate-dependent crystalline plasticity formulations, and only a brief outline will be presented here. For quasi-static deformations, an implicit FE method with BFGS iteration is used to obtain the total deformation rate tensor, D_{ij} . To overcome numerical instabilities associated with stiffness, a hybrid explicit-implicit method is used to obtain the plastic deformation rate tensor, D_{ij}^p . This hybrid numerical scheme is also used to update the evolutionary equations for the mobile and immobile dislocation densities.

4. Results and discussion

The competing failure mechanisms of TG and IG fracture, and the underlying microstructural mechanisms in bicrystal martensitic steels have been investigated in this section. The $\Sigma 3$ CSL GB with a misorientation of $[111]/60^\circ$ and $\Sigma 17b$ CSL GB with a misorientation of $[110]/86.63^\circ$ [14], were chosen to represent low and high CSL GBs and investigate how different types of CSL GBs affect TG and IG fracture. The material properties (Table 1) that are used are representative of b.c.c. low-carbon martensitic steel [46–48] with potentially 24 unique slip systems.

Table 1 Material Properties

Properties	Martensite
Young's modulus, E	228 GPa
Static yield stress, τ_y	517 MPa
Poisson's ratio, ν	0.3
Rate sensitivity parameters, m	0.01
Reference strain rate, $\dot{g}_{ref}$	0.001s^{-1}
Critical strain rate, $\dot{g}_{critical}$	10^4s^{-1}
Burger vector, b	$3.0 \times 10^{-10}\text{m}$
Initial immobile dislocation density r_{im}^0	$1.0 \times 10^{10}\text{m}^{-2}$
Initial mobile dislocation density r_m^0	$1.0 \times 10^7\text{m}^{-2}$
Saturation dislocation density, ρ_s	$1.0 \times 10^{16}\text{m}^{-2}$
Fracture stress, σ_{frac}	$5\tau_{y_martensite}$
Fracture stress on GB planes, σ_{gb}	$6.5\tau_{y_martensite}$

A model size of 0.5 mm×1.0 mm was used with a convergent plane strain FE mesh of 5000 elements, and a displacement load was applied for a quasi-static nominal strain rate on top surface with symmetric boundary condition (Fig. 1). A pre-existing crack at the GB, with the normalized initial crack length of a_0/w of 0.1, was used, where a_0 is the initial crack length, and w is the specimen width.

4.1. Microstructural fracture in bicrystals with $\Sigma 3$ boundary

The crack opening mode stresses on all the microstructural cleavage planes of $\{100\}$ and GB planes were monitored and compared with the critical fracture stresses for failure to investigate the competing mechanism between TG and IG fracture. To elucidate the microstructural mechanisms for the case with $\Sigma 3$ boundary, the normalized (by the static yield stress) normal stress, normalized (by the initial immobile dislocation density) immobile dislocation density and GBTF for the most active slip system $(\bar{1}10)[11\bar{1}]$, at a nominal strain of 1%, are shown in Figs. 2(a-c). The maximum normalized normal stress was 5, and it occurred ahead of crack front (Fig. 2(a)). This high local stress activated slip systems, and led to dislocation densities with a maximum normalized value of 450 for slip system $(\bar{1}10)[11\bar{1}]$ (Fig. 2(b)). For the $\Sigma 3$ boundary, dislocation densities can accumulate at the GB, and then transmit through the GB, which has been experimentally observed in martensitic steels and nickel [10, 11, 15, 49]. In our modeling, the high dislocation density transmission is indicated by large GBTF with a maximum value of 0.55 (Fig. 2(c)). Dislocation density transmission across the GBs can relieve or relax the stresses. Therefore, there was a competing mechanism between stress accumulation due to the crack front and stress relaxation due to dislocation density transmission for the bicrystal with $\Sigma 3$ boundary.

At the low nominal strain of 1%, stress accumulation caused by crack front (Fig. 2(a)) was dominant due to the low dislocation density, which resolved large crack opening mode stresses on the GB plane and resulted in IG fracture at the first stage (Fig. 3(a)). As the nominal strain increased, large dislocation densities were generated (Fig. 4(a)), which can relieve stresses and release strain energy [50–53]. These large dislocation densities can transmit across the $\Sigma 3$ GB, which further relieved stresses at the

GB and inhibited IG crack growth (Fig. 3(a)). Meanwhile, the large lattice rotation with a maximum value of 5° (Fig. 4(c)) rotated microstructural cleavage planes $\{100\}$ onto a favorable orientation, and induced TG fracture on cleavage planes (Figs. 3(b-c)). This resulted in the transition from IG fracture to TG fracture (Figs. 3(a-c)), which is consistent with experimental observations in bicrystals with $\Sigma 3$ boundary [22].

The high strength martensite can impede TG crack growth, as indicated by the large normalized normal stress of 8 ahead of the crack front (Fig. 3(b)). This high local stress activated slip systems and generated dislocation densities, with a maximum normalized total dislocation density generation of 5.0×10^4 (Fig. 4(a)), which occurred on the TG fracture surface. This large dislocation density generation led to large plastic deformations, with a maximum shear slip of 0.2 (Fig. 4(b)), and it impeded TG crack growth (Fig. 8) and improved fracture toughness significantly (Fig. 9). The total dislocation density generation and shear slip on TG fracture surface or cleavage plane, were much higher than those on the IG fracture surface or GB plane, almost by an order of magnitude. These lower values on the IG fracture surface resulted in faster IG crack growth in comparison with the TG crack (Fig. 8).

4.2. Microstructural fracture in bicrystals with $\Sigma 17b$ boundary

In this section, crack propagation in bicrystals with $\Sigma 17b$ boundary was investigated and compared with the case of the bicrystal with a $\Sigma 3$ boundary. Similar to the analysis of the $\Sigma 3$ bicrystal, the crack opening mode stresses on all the microstructural cleavage planes of $\{100\}$ and GB planes were monitored and compared with the critical fracture stresses to determine whether TG and IG fracture would occur. The normalized

normal stress, normalized immobile dislocation density and GBTF for the most active slip system $(\bar{1}01)[1\bar{1}1]$ at a nominal strain of 1%, are shown in Figs. 5(a-c). The maximum normalized normal stress was 5 (Fig. 5(a)), which occurred ahead of the crack front. Even though the maximum normalized normal stress was the same as that for the case with $\Sigma 3$ boundary, distributions of normal stress were significantly different due to the activation of different slip systems. One of the most active slip systems for the current case was $(\bar{1}01)[1\bar{1}1]$, with a maximum normalized dislocation density of 400 (Fig. 5(b)), and it occurred ahead of crack front. For the $\Sigma 17b$ boundary, dislocation-densities would pile up at GBs [14, 15, 54], which is indicated by the low GBTF of 0.2 (Fig. 5(c)). These dislocation density pile ups at the GB further resulted in stress accumulations, in combination with the large normal stresses at the GB, induced IG fracture and rupture (Figs. 6(a-c)), which was significantly different from crack propagation for the case with the $\Sigma 3$ boundary.

To further delineate the microstructural mechanisms for IG fracture, the normalized total dislocation density generation at a nominal strain of 4% is shown in Fig. 7(a). The normalized total dislocation density generation at the IG fracture surface was approximately 3000, and it was only 6% of that on TG fracture surface for the case with $\Sigma 3$ boundary (Fig. 4(a)). This low dislocation density generation resulted in low shear slips at the IG fracture surface, with a value of 0.035 (Fig. 7(b)), which was approximately 18% of that on TG fracture surface for the case with $\Sigma 3$ boundary (Fig. 4(b)). Low dislocation density generation and shear slip for IG fracture have been observed in copper and Ni_3Al bicrystals [21, 23]. This would result in almost brittle fracture, and accelerated IG crack growth (Fig. 8). The lattice rotation (Fig. 7(c)) for the

regions adjacent to IG fracture surface was 0, which further indicates brittle cracking of the $\Sigma 17b$ boundary. This accelerated crack growth also significantly decreased, in comparison with the case with $\Sigma 3$ boundary, fracture toughness (Fig. 9).

Conclusions

A dislocation-density GB interaction scheme was coupled to a dislocation-density based multi-slip crystal plasticity formulation to investigate how different types of CSL GBs affect dislocation-density transmission and impedance, and subsequently TG and IG fracture in bicrystal martensitic steels. Failure criteria based on the stresses on microstructural cleavage planes and GB planes were used to characterize the competition between TG and IG fracture.

For the case with the $\Sigma 3$ CSL boundary, there was a competition between stress accumulation due to crack front and stress relief due to dislocation density generation and transmission at the GB. At low nominal strains, stress accumulation ahead of the crack front was dominant due to low dislocation density, and it resulted in IG fracture at low nominal strains. As the nominal strain was increased, dislocation densities increased on specific slip systems, and stress relief due to dislocation density generation and transmission occurred, which inhibited IG crack growth and led to a transition from IG fracture to TG fracture. The TG crack was blunted by the high dislocation density generation and shear slip, which also significantly increased fracture toughness.

For the case with the $\Sigma 17b$ CSL boundary, there were stress accumulations at the crack front, but also dislocation density pile-ups at the GBs. These pile-ups resulted in opening mode stress accumulations at the GB, which subsequently induced complete IG

fracture. This IG fracture had much lower dislocation density generation and shear slip, which indicates an almost brittle-like cracking of the GB. These predictions, which are consistent with experimental observations, can provide guidelines for the engineering of GBs for failure resistant behavior.

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