The role of cohesive zone properties on intergranular to transgranular fracture transition in polycrystalline solids

Liqiang Lin¹, Xianqiao Wang² and Xiaowei Zeng¹

Abstract
A cohesive zone model is employed to simulate the fracture evolution and crack propagation in polycrystalline solids. Numerical simulations of fracture growth with various cohesive zone properties are presented and the simulation results capture the fracture transition from intergranular to transgranular mode. Three different random Voronoi grain cell tessellations are presented to study the grain size effects. The simulation results show that the intergranular to transgranular fracture transition in the polycrystalline solid is sensitive to key cohesive law parameters such as fracture energy and cohesive strength along grain boundaries and in grain cells. This study also provides evidence that tensile strength of polycrystalline solid increases as grain cell size decreases.

Keywords
Numerical simulation, cohesive zone model, crack propagation, intergranular fracture, transgranular fracture, polycrystalline solid

Introduction
Intergranular and transgranular fractures are two mechanisms in polycrystalline materials. From the experimental perspective, the phenomenon of intergranular/transgranular fracture has been widely investigated in polycrystalline solids (Swab and Quinn, 1998; Yang et al., 1991). Meanwhile, a variety of numerical methods have been developed to study the fracture of polycrystalline solids. For example, to uncover the mechanical behaviors of polycrystalline materials, Curran et al. (1993) and Espinosa et al. (1998) modeled fracture initiation and propagation in polycrystalline materials by micromechanical simulation and captured the failure mechanisms. Cohesive zone method is widely used to simulate fracture in polycrystalline materials as well. For instance, the role of cohesive properties on intergranular crack propagation and the relation between crack path and cohesive

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law parameters was investigated in Al₂O₃ (Shabir et al., 2011). Failure initiation and evolution of polycrystalline brittle materials was studied under quasi-static and dynamic loading (Espinosa and Zavattieri, 2003a, 2003b). The grain boundary sliding and separation in nanocrystalline metals was investigated by so-called rate-independent interface constitutive model (Wei and Anand, 2004). A constitutive framework for modeling the dynamic response of polycrystalline microstructures was presented and crack generation at interfaces between grains of the same or different phases was simulated (Clayton, 2005; Zavattieri et al., 2001). Qian and Li (2011) investigated the intergranular and transgranular crack propagation by using the multiscale cohesive zone model proposed by Zeng and Li (2010). Lin and Zeng (2015) studied the spall fracture in polycrystalline solids by an atomistic-based interfacial zone model. Musienko and Cailletaud (2009) simulated the intergranular and transgranular crack propagation by inserting finite elements in the grain boundary areas for Zircaloy tubes. Quasi-static brittle fracture in polycrystalline materials was also modeled using the extended finite element method (X-FEM) and the transition from intergranular to transgranular mode of crack growth under the various toughness ratios was studied as well (Sukumar et al., 2003). Other numerical methods being utilized were the body force method, in which the crack growth behavior of intergranular stress corrosion cracking was studied by Kamaya (2004) while Kim et al. (1995) investigated the path of a crack impinging on crack propagation. There is a boundary element method (BEM) which is an alternative numerical method to simulate the intergranular microfracture in polycrystalline brittle materials (Sfantos and Aliabadi, 2007).

During the last few years, although the mechanical behavior of polycrystalline solids has been studied quite extensively, such as the penetration of a crack impinging on an interface (Foulk et al., 2008; Parmigiani and Thouless, 2006), these models are statics and without the consideration of the dynamic crack propagation process. The relationship between distributions of stress and crack propagation in polycrystalline materials hasn’t been carefully examined yet. In fact, Zavattieri et al. (2001) presented that the distributions of stress in modeled polycrystalline structure could help us understand the different mechanisms that control macroscopic response. To further advance the research on fracture mechanisms in polycrystalline solids, we conducted an extensive investigation of crack propagation via transition from intergranular fracture to transgranular fracture by cohesive zone model. The interfacial traction-separation law employed here is the exponential law developed by Xu and Needleman (1994). In present work, the distributions of stress contour during crack propagation in polycrystals are obtained to better illustrate the intergranular and transgranular fracture. The relationship between fracture mode transition and cohesive law parameters is discussed. It is shown that cohesive law parameters such as fracture energy and cohesive strength will affect the fracture pattern, and different cohesive zone parameters will result in intergranular or transgranular fracture in polycrystalline solid Al₂O₃.

**Polycrystalline microstructure**

In the early work, dealing with polycrystalline microstructure is by utilizing simplified grain shapes, such as hexagons of the 2D case (Jivkov et al., 2006) and cubes or truncated octahedrons of the 3D case (Evers et al., 2002; Jivkov et al., 2006). However, Musienko and Cailletaud (2009) presented that this standard hexagons cannot predict local stress-strain fields inside the grains. Thus, Voronoi tessellation has been emerging as a powerful tool to construct different randomly shaped grain structures in polycrystalline materials to study the effect of polycrystalline grain morphology (e.g., Bolander and Saito, 1998; Espinosa and Zavattieri, 2003a, 2003b; Ghosh and Liu, 1995; Liu et al., 1998). Meanwhile, to overcome difficulties in modeling arbitrary microstructures by conventional finite element methods, Ghosh and Liu (1995) and Ghosh et al. (1997) innovated a
material based Voronoi Cell Finite Element Model (VCFEM). The Voronoi domain is considered here as partitioning of a plane with a set of $n$ random distinct points (Du et al. 1999; Lin et al., 2014). The Voronoi tessellation diagram is defined as such convex polygons that each polygon contains exactly one generating kernel point and every point in a given polygon is closer to its generating point than to any other ones. The slope of the line perpendicular to each closest point connection line $L - L_i$, as shown in Figure 1, defines the polygon boundary segment $ab$. For a 2D case, the Voronoi region, or polygon cell assigned to nucleus $P_i$ can be written as:

$$V_i = V(X_{P_i}) = \{X : d(X_{P_i}, X) < d(X_{P_j}, X)\} \quad \text{for} \quad P_i \neq P_j$$

where $X_{P_i}$ represent the coordinates of kernel points $i$; $d(X_{P_i}, X)$ denotes the Euclidean distance between $X_{P_i}$ and $X$; $X$ belonging to Voronoi region $P_i$ is closer to nucleus $P_i$ than other nuclei, as shown in Figure 1.

In this work, the simulation samples are generated by centroidal Voronoi tessellation as shown in Figure 2(a). Each Voronoi cell represents an individual grain cell and the edges of grain cells are considered as grain boundaries. After the generation of grain cell, triangular finite element is used to mesh all grain cells as shown in Figure 2(b). For the application of cohesive zone method, cohesive zones are inserted into all interfaces between bulk elements.

**Cohesive zone model**

The inhomogeneous deformation in the material response is governed by the cohesive law across bulk element interfaces. In this work, the bulk elements are treated as isotropic material as in Xu and Needleman (1994). According to the work of Xu and Needleman, although a finite deformation formulation is employed, finite strain and rotation effects are negligible in the circumstances considered. The current study follows Xu and Needleman’s treatment. In two dimensions, the specific fracture energy $\varphi$ on cohesive zone surfaces employed here is the exponential law of Beltz and Rice (1991) and Sun et al. (1993) derived especially for fracture simulations by Xu and Needleman (1994)

$$\varphi(\Delta) = \varphi_n + \varphi_\Delta \exp\left(-\frac{\Delta_n}{\delta_n}\right) \left\{ 1 - r + \frac{\Delta_n}{\delta_n} \right\}^{1 - q} \left[ q + \left(\frac{r - q}{r - 1}\right) \frac{\Delta_n}{\delta_n} \exp\left(\frac{-\Delta_n^{2}}{\delta_n^{2}}\right) \right\}$$

![Figure 1. Schematics showing Voronoi cell formation.](image-url)
\[ n = \exp(1) / C_{27} \]

where \( \sigma, \delta_n \) represents the work of normal separation and \( \exp(1) = 2.71828 \), \( \sigma_c \) is the cohesive surface normal strength; \( \Delta_n = n \cdot \Delta \) and \( \Delta_t = t \cdot \Delta \). \( n \) and \( t \) are the normal and tangential unit vectors at an appointed element surface in the reference configuration, respectively. The \( \delta_n \) and \( \delta_t \) are normal and tangential characteristic lengths, respectively. Thus, the tractions in the normal and tangential directions on the cohesive surfaces are given as

\[
T_n = \frac{\varphi_n}{\delta_n} \exp\left( -\frac{\Delta_n}{\delta_n} \right) \left\{ \exp\left( -\frac{\Delta_t^2}{\delta_t^2} \right) + 1 - q \left[ 1 - \exp\left( -\frac{\Delta_t^2}{\delta_t^2} \right) \right] \left[ r - \Delta_n \right] \right\} \tag{3}
\]

\[
T_t = \frac{\varphi_t}{\delta_n} \left( \frac{\delta_n}{\delta_t} \right) \Delta_t \left\{ q + \left( \frac{r - q}{r - 1} \right) \frac{\Delta_n}{\delta_n} \right\} \exp\left( -\frac{\Delta_n^2}{\delta_n^2} \right) \exp\left( -\frac{\Delta_t^2}{\Delta_t^2} \right) \tag{4}
\]

In equations (2)–(4), the \( q \) and \( r \) is given as

\[
q = \frac{\varphi_t}{\varphi_n}, \quad r = \frac{\Delta_n^*}{\delta_n} \tag{5}
\]

where \( \varphi_t = \sqrt{\frac{\exp(1)}{2}} \tau_c \delta_t \) is the work of tangential separation, \( \tau_c \) is the cohesive surface tangential strength; \( \Delta_n^* \) is the value of \( \Delta_n \) after complete shear separation with \( T_n = 0 \).

**Finite element implementations**

A displacement-based finite element (FE) formulation is derived from the principle of virtual work. During the deformation process, following standard procedures and neglecting the body force, a Galerkin weak formulation of cohesive zone model may be expressed as following

\[
\int_{\Omega} \mathbf{P} : \delta \mathbf{F} \, d\Omega - \int_{S_{int}} \mathbf{T}^{cohe} \cdot \delta \mathbf{A} \, dS = \int_{S_{ext}} \mathbf{T}^\top \cdot \delta \mathbf{u} \, dS - \int_{\Omega} \rho \mathbf{a} \cdot \delta \mathbf{u} \, d\Omega \tag{6}
\]
where $\mathbf{P} : \delta \mathbf{F} = P^{ij} \delta F_{ji}$, $\mathbf{P}$ is the non-symmetric first Piola-Kirchhoff stress tensor; $\Delta$ denotes the interface displacement jump across the cohesive zones; $\Omega$, $S_{\text{int}}$, $S_{\text{ext}}$ are the volume, internal surface and external cohesive surface of solid body in the reference configuration, respectively. $\rho$ is the material density in the reference configuration, $\mathbf{T}$ is the external traction vector and $T_{\text{cohe}}$ is the cohesive surface traction vector. To calculate the nodal displacements, the explicit time integration scheme that is based on the Newmark $\beta$-method (Belytschko et al., 1976), with $\beta=0$ and $\gamma=0.5$.

**Numerical simulations**

**Problem setup**

Numerical simulations have been carried out for specimen with an initial crack. The exact problem statement is shown in Figure 3, in which a 2D plate with dimension ($L_x \times L_y = 0.2$ mm $\times$ 0.2 mm) is under simple tension loading in $Y$-axis. The plane strain conditions are applied and the boundary condition are displacement boundary condition (Lin et al., 2014). In this study, there are 80 grain cells and the average grain size is around 22.5 $\mu$m, which is in the gain size range of Al$_2$O$_3$ (Kraft and Molinari, 2008; Shabir et al., 2011; Zavattieri et al., 2001). A pre-crack is set along several grain boundaries at the central of the right side of the plate as shown in Figure 3, and the pre-crack tip is located at ($l_c = \frac{L_x}{4} = 0.05$ mm).

To ensure the simulation convergence, it is clearly necessary that mesh size $l_m$ must be less than the cohesive zone size $l_c$ (i.e., $l_m < l_c$) for the finite element mesh to provide an accurate solution. Failure to satisfy such requirement has been the source of mesh-sensitivity of cohesive zone model. The cohesive length is approximately set by the elastic properties of the solid, the surface fracture energy $G_{IC}$ for mode-I and the critical cohesive surface strength $\sigma_c$ in normal direction (Falk et al., 2001)

$$l_c = \frac{9\pi}{32} \left( \frac{E}{1-v^2} \right) \frac{2G_{IC}}{\sigma_c^2}$$

(7)

The time step is chosen as $\Delta t = 0.02l_m/V_p \left( V_p = \sqrt{\frac{E(1-v)}{\rho(1-2v)}} \right)$. In equations (2)-(4), we set $q = 1$ as in Xu and Needleman (1994).
Fracture growth in polycrystalline material and mesh convergence test

To study the mechanism of brittle fracture in polycrystalline solids, the polycrystalline alumina (Al₂O₃) is chosen and the grains are assumed to be elastic and isotropic. This assumption is based on the study by Rice (1994) that the elastic anisotropy percentage in Al₂O₃ is low. In addition, simulations conducted by Warner and Molinari (2006) demonstrated that neglecting anisotropy did not have substantial effects on the mesoscopic failure.

The values of the material properties for the constituents are chosen as: Young’s modulus $E = 260$ GPa, Poisson’s ratio $\nu = 0.21$, mass density $\rho = 3690$ kg/m$^3$, $\varphi_n = \varphi_t = 34$ J/m$^2$ (Camacho and Ortiz, 1996). According to Klein et al. (2001), the effective modulus of system is defined as

$$E_{\text{eff}} = E \left[ 1 - \frac{1}{1 + (kl_m)/E} \right]$$  \hspace{1cm} (8)

where $k = \frac{\varphi_n}{\varphi_t}$ and $l_m$ is the average mesh size. In fitting the parameters of a cohesive zone model, the $\sigma_c$ has not been certainly determined with experiment methods. Thus, in the study of Klein et al. (2001), the suggested value for $\sigma_c$ is from $E/10$ to $E/600$. In the computational model, there are 4998 bulk elements ($l_m \approx 40 \mu$m) meshed in 80 grain cells. We selected $\sigma_c = E/150 = 1.73$ GPa, it satisfies the cohesive zone condition \( l_m < l_c = \frac{9\pi}{32} \left( \frac{E}{1-E} \right) \frac{2\varphi}{\sigma_c} = 5.6 \mu m \). In addition, as shown in Figure 4, when $\sigma_c = E/150$, the calculated effective modulus is 0.9083$E$.

Buban et al. (2006) illustrated that grain boundaries are generally weaker than grains due to the atomic-scale defects on grain boundaries and the bonds are less in number and weaker than in the grains. To study the effects of cohesive strength $\sigma_c$ or fracture energy $\varphi$ on the intergranular/transgranular fracture, first we considered the cohesive strength inside grains is higher than grain boundaries, for example, $\sigma_c(g) = 3\sigma_c(gb)$, $\sigma_c(g)$ denotes the strength inside the grain and $\sigma_c(gb)$ is the strength along the grain boundary. The simulation shows that the crack propagates only along grain boundaries, as shown in Figure 5.

![Figure 4](image-url)

**Figure 4.** Effective modulus of system versus critical cohesive strength.
Mesh convergence test

Generally speaking, the results of the cohesive zone model are sensitive to its elements size. To study the mesh size dependence, three different meshes are generated in the same specimen. The same displacement boundary condition is applied on the top and bottom edges of the specimen. In this study, the element density $R_p$ in grain cell is defined as

$$R_p = \frac{\text{Average element size}}{\text{Average grain size}}$$

Three cases with three different element densities $R_p = 0.5, 0.25, \text{ and } 0.125$ are employed as shown in Figure 6. The element density $R_p = 0.25$ is the mesh we used in the simulation shown in Figure 5. The cohesive strengths on grain boundaries and in grain cells are the same as in the previous simulation. As shown in Figure 7, the initial crack propagates along the same path although the mesh size varies. That is, the current mesh can accurately capture the crack path.

On the other hand, we plotted the load-displacement curve as shown in Figure 8, and we calculated the errors of boundary reaction force $r^i_b$ between two cases as:

$$Err_f = \int_0^1 |r^i_b - r^{i-1}_b| \, ds, \quad i = 2, 3$$

**Figure 5.** Stress distribution ($\sigma_{22}$) for crack propagation: (a) $t = 0.045 \, \mu s$; (b) $t = 0.06 \, \mu s$; (c) $t = 0.075 \, \mu s$; (d) $t = 0.09 \, \mu s$; (e) $t = 0.099 \, \mu s$; (f) $t = 0.114 \, \mu s$. 
Figure 6. Different mesh densities over grain cells: (a) Case 1 with $R_p = 0.5$; (b) Case 2 with $R_p = 0.25$; (c) Case 3 with $R_p = 0.125$.

Figure 7. Crack propagation for different mesh densities (stress contour for $\sigma_{22}$): (a) Case 1; (b) Case 2; (c) Case 3.

Figure 8. Boundary reaction forces versus displacement for different meshes.
where \( s \) denotes displacement.

From Table 1, it can be seen that errors of reaction force \( r_i^f \) decrease as the element size decreases.

**Transition from intergranular to transgranular fracture**

**Effect of fracture energy on fracture behavior.** From above simulations, the crack path follows grain boundaries when the cohesive zone strength inside the grains is much stronger than that of the grain boundaries. However, Kraft and Molinari (2008) pointed out the fracture energy ratio between grain boundary and grain cells \( R_{pp} = \frac{\sigma_{gb}}{\sigma_{g}} \) can affect the fracture pattern in polycrystalline solids. Becher (1991) and Evans (1990) also presented that a crack can propagate along grain boundary or pass through grain cells depending on the fracture energy ratio \( R_{pp} \) to some extent. To study the effects of \( R_{pp} \) on polycrystalline crack propagation, \( R_{pp} \) is initially set as 0.1 for the case of very weak grain boundaries, then we increased the value to 0.5 gradually, and keep the cohesive strength constant. It is observed that when \( R_{pp} \) reaches 0.5, the intergranular to transgranular fracture mode transition will be initiated as shown in Figure 9, which is in qualitative agreement with the results obtained by Holm (1998) and Yang et al. (1990). This transition has also been observed by Sukumar et al. (2003) using X-FEM.

To further verify the conclusion, we simulate the case with \( R_{pp} = 1 \). In Figure 10, the conspicuous transition from the intergranular to transgranular fracture is obtained and the transition starts earlier than the simulation with \( R_{pp} = 0.5 \).

**Effect of cohesive strength on fracture behavior.** We believe the fracture energy ratio and strength ratio are two major parameters in determining the intergranular to transgranular fracture mode transition. In the above simulation, the crack propagation path has experienced a transition from intergranular mode to transgranular mode under different fracture energy ratio \( R_{pp} \). In what follows, we intend to investigate how cohesive zone strength along grain boundaries and in grain cells will affect fracture pattern. To better unravel the effects of this parameter, we consider the cohesive strength ratio between grain boundaries and grain cell \( R_{sc} = \frac{\sigma_{c(gb)}}{\sigma_{c(g)}} \) as: 0.4, 0.5, 0.6, 0.7, 0.8, and 0.9 and keep fracture energy the same. From the simulation, it is observed that as \( R_{sc} \) increases to 0.6, the crack propagation starts to pass through grain cells, as shown in Figure 11.

**Effect of grain size.** Since the Voronoi tessellation is used to generate polycrystals, we are able to study the grain grain size effects. In this study, we generate two additional polycrystalline microstructures with 144 and 256 grains. The results are shown in Figure 12 and Figure 13 for fracture energy ratio \( R_{pp} \) study and in Figures 14 and 15 for cohesive strength ratio \( R_{sc} \) study.

Similar to the results obtained in the previous section, the intergranular to transgranular fracture transition takes place in both poly-144 (c.f. Figures 12 and 14) and poly-256 (c.f. Figures 13 and 15). From our fracture energy ratio \( R_{pp} \) study, it can be seen that the grain size has little effect on the

<table>
<thead>
<tr>
<th>( R_p )</th>
<th>Bulk element no.</th>
<th>Force error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.50</td>
<td>1498</td>
<td>–</td>
</tr>
<tr>
<td>0.25</td>
<td>4998</td>
<td>3.12E-9</td>
</tr>
<tr>
<td>0.125</td>
<td>19,966</td>
<td>2.63E-9</td>
</tr>
</tbody>
</table>
fracture mode transition since the transition takes place at energy ratio $R_{ep} = 0.5$ (threshold value) for all three cases. However, from the cohesive strength ratio $R_{es}$ study, we found that grain size has effects on the fracture mode transition because the transition takes place at strength ratio $R_{es} = 0.6$ for 80 grains, increased to $R_{es} = 0.75$ for 144 grains, and $R_{es} = 0.8$ for 256 grains, which means the

Figure 9. The snapshot of stress distribution ($\sigma_{22}$) of fractures in a polycrystalline solid for fracture energy ratio: (a) $R_{ep} = 0.3$ (intergranular); (b) $R_{ep} = 0.4$ (intergranular); (c) $R_{ep} = 0.5$ (transgranular).

Figure 10. Stress distribution ($\sigma_{22}$) for crack propagation: (a) $t = 0.051 \mu s$; (b) $t = 0.066 \mu s$; (c) $t = 0.075 \mu s$; (d) $t = 0.105 \mu s$; (e) $t = 0.132 \mu s$; (f) $t = 0.147 \mu s$. 

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cohesive strength ratio threshold value for the fracture mode transition is increasing as the grain size decreasing. The possible reason is that the numbers of grain boundaries will increase for the same specimen size when the grain size decreases, in our simulation we assume the grain boundary is weaker than grain, which might allow the crack propagates more easily along grain boundaries as the grain size decreases.

Moreover, the stress-strain relations for the three different polycrystal grain sizes are obtained from the simulations. For each of the polycrystalline grain sizes, four simulation cases with random polycrystalline grain distribution are conducted. As illustrated in Figure 16, the average tensile strength increases from 418.0 to 536.9 MPa, and to 573.6 MPa as grain size decreases for three different grains, which has been observed by Simpson (1973) for polycrystalline crack propagation.

Figure 11. The snapshot of stress distribution (σ_{22}) of fractures in a polycrystalline solid for strength ratio: (a) R_{sa} = 0.5 (intergranular); (b) R_{sa} = 0.6 (transgranular); (c) R_{sa} = 0.7 (transgranular).

Figure 12. The snapshot of stress distribution (σ_{22}) of fractures in a polycrystalline solid (Poly144) for fracture energy ratio: (a) R_{sp} = 0.3 (intergranular); (b) R_{sp} = 0.4 (intergranular); (c) R_{sp} = 0.5 (transgranular).
Figure 13. The snapshot of stress distribution ($\sigma_{22}$) of fractures in a polycrystalline solid (Poly256) for fracture energy ratio: (a) $R_{cp} = 0.3$ (intergranular); (b) $R_{cp} = 0.4$ (intergranular); (c) $R_{cp} = 0.5$ (transgranular).

Figure 14. The snapshot of stress distribution ($\sigma_{22}$) of fractures in a polycrystalline solid (Poly144) for strength ratio: (a) $R_{cs} = 0.6$ (intergranular); (b) $R_{cs} = 0.7$ (intergranular); (c) $R_{cs} = 0.75$ (transgranular).

Figure 15. The snapshot of stress distribution ($\sigma_{22}$) of fractures in a polycrystalline solid (Poly256) for strength ratio: (a) $R_{cs} = 0.6$ (intergranular); (b) $R_{cs} = 0.75$ (intergranular); (c) $R_{cs} = 0.8$ (transgranular).
Discussion and conclusion

In conclusion, we have applied the exponential cohesive zone law developed by Xu and Needleman (1994) to investigate the dynamic crack propagation in polycrystalline solids. In addition, random structures of centroidal Voronoi tessellation have been employed to study how cohesive law parameters influence crack propagation pattern in polycrystalline solids. The phenomenon of intergranular to transgranular fracture mode transition has been captured during the crack propagation. From the simulation of polycrystalline crack propagation, some important findings of current work can be summarized as follows.

First, when the cohesive zone strength along grain boundaries are much weaker than that inside grain cells, that is, $\sigma_{c(g)} = 3\sigma_{c(gb)}$, the crack propagates along the grain boundaries (c.f. Figure 5). The mesh density we used can accurately capture the crack path (c.f. Figure 7).

Second, the intergranular/transgranular fracture mode transition is sensitive to fracture energy ratio $R_{pp}$ and cohesive strength ratio $R_{ps}$. From the fracture energy ratio simulation, the intergranular to transgranular fracture mode transition starts when $R_{pp} \geq 0.5$ (c.f. Figure 9). The conclusion is further verified when we increase $R_{pp} = 1.0$ as shown in Figure 10. From the cohesive strength ratio study, when $R_{ps}$ reaches 0.6 for 80 grains, the crack path transits from intergranular to transgranular fracture mode (c.f. Figure 11).

Last, from the two other sets of polycrystalline microstructures generated by Voronoi tessellations, the simulations captured the fracture transition from intergranular to transgranular for both cases (c.f. Figures 12 and 15). The simulation also shows that the grain size will affect the cohesive strength ratio threshold value for fracture mode transition, but has little effect on fracture energy ratio threshold value. From this study, it is observed that fracture energy ratio and cohesive strength ratio are two major parameters in determining the intergranular to transgranular fracture mode transition. The simulation also provides evidence that the tensile strength increases as grain cell size decreases.

Declaration of Conflicting Interests

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