A Discrete Crack Dynamics Model of Toughening in Brittle Polycrystalline Material by Crack Deflection

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Abstract

This paper focuses on the study of the effect of the interfacial strength of grain boundaries and elliptical inclusions on crack path deflection. The method is developed to channel a crack into a toughening configuration (arrays of elliptical holes and inclusions are considered) in order to obtain the optimised microstructure required to enhance fracture toughness through different mechanisms. The proposed technique is shown to reproduce experimental crack propagation paths in various configurations and is capable of capturing the effect of that variation of the GB and the inclusion interfacial strength; it provides a powerful tool to understand the interplay between microstructural features and improve materials performance.

\textit{Keywords:} Interfacial energy, Grain boundary, Discrete Crack Dynamics

Nomenclature

\begin{equation*}
\begin{align*}
\epsilon_{ij} & \quad \text{Kronecker delta} \\
\Gamma & \quad \text{Fracture energy} \\
\Gamma_0 & \quad \text{Fracture energy of the matrix material}
\end{align*}
\end{equation*}

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\[ \Gamma_{GB} \quad \text{Fracture energy of the grain boundary} \]
\[ \gamma_{GB} \quad \text{Energy per unit area of the grain boundary} \]
\[ \Gamma_{inc} \quad \text{Fracture energy of the inclusion} \]
\[ \Gamma_{int} \quad \text{Fracture energy of the interface} \]
\[ \gamma_s \quad \text{Surface energy per unit area} \]
\[ \kappa \quad \text{Kolosov’s constant} \]
\[ \mu \quad \text{Shear Modulus} \]
\[ \mu_0 \quad \text{Shear Modulus of the matrix material} \]
\[ \mu_{inc} \quad \text{Shear Modulus of the inclusion} \]
\[ \nu \quad \text{Poisson’s ratio} \]
\[ \sigma^{\infty} \quad \text{Far-field load} \]
\[ E \quad \text{Young’s modulus} \]
\[ G \quad \text{Energy release rate} \]
\[ G_C \quad \text{Critical energy release rate} \]
\[ G_d \quad \text{Maximum energy release rate of the deflecting crack} \]
\[ G_p \quad \text{Maximum energy release rate of the penetrating crack} \]
\[ K_C \quad \text{Critical stress intensity factor} \]
\[ K_{IC} \quad \text{Mode I critical stress intensity factor} \]
\[ K_{mode} \quad \text{Stress intensity factors} \]
\[ 2D \quad \text{Two-dimension} \]
\[ 3D \quad \text{Three-dimension} \]
\[ \text{DCD} \quad \text{Discrete Crack Dynamic} \]
\[ \text{GB} \quad \text{Grain Boundary} \]
\[ \text{SIF} \quad \text{Stress Intensity Factor} \]
1. Introduction

In polycrystalline material, crack propagation paths depend on micro-structures (impurities, micro-cracks, defects, etc.), and the strength of the grain boundaries (GBs) and micro-structural features. The important research questions that come to the mind is: can the interactions between micro-cracks, grain boundaries, and micro-structures be used to manipulate the evolution of a crack propagation path to improve the material toughness? Studies show that interactions between a crack and inclusions, small voids, and grain boundaries (GBs) can deflect and channel the crack along a predefined path (1–5). Also, the ability to deflect and channel a crack is an attractive means to enhance the toughness of brittle polycrystalline materials (6–8). The objective of this paper is to develop a method to study the interfacial effects on crack propagation path and then to apply the method to investigate material toughness variations and structural optimisation associated with the crack deflection at the interfaces.

In an earlier paper, we addressed several techniques that have been developed to predict crack paths such as the finite element method (FEM) (9–11), the extended finite element method (XFEM) (12–14), the boundary element method (BEM) (15–18), and the phase-field approach based on energy minimization principles (19). Although the simulation of crack growth including interactions with inclusions is possible, these methods become computationally expensive when the number of localised features is significantly increased. Thus, we introduced Discrete Crack Dynamics (DCD), a method to predict the quasi-static growth of a micro-crack and its interaction with other cracks and inclusions in two-dimensional, finite systems (20). In this method, crack growth is an incremental process modelled by introducing a small crack ahead of the existing crack tip in the predetermined propagation direction. Crack growth is modelled as a process comprising sequential micro-crack initiation events ahead of the main crack tip followed by merging of the crack ensemble. In DCD the interactions between elements of a system are accurately computed using the multipole method (21–26). Here, we develop the DCD method further to study fracture of polycrystalline materials, which incorporates the influence of interfacial strength on the crack trajectory. Figure 1a is a schematic representation of a polycrystalline material where the crack propagates through several grains while it interacts with inclusions, other cracks, voids and grain boundaries. In Section 2 first a method to study the influences of interfaces on the crack trajectory is introduced, which is applied to grain boundaries (Figure 1b), inclusions (Figure 1c), and inclusions present at grain boundaries (Figure 1d). Our results are compared with experimental and other computational results in the literature. In Section 3 the model
is used to study the crack energy variation, while it is propagating through a toughening configuration (array of elliptical holes and soft inclusions), in order to obtain the relevance between the material toughness and the microstructure distribution.

2. Capturing the influence of interfaces on crack propagation

A crack approaching an interface may be deflected along the interface, or penetrate the interface along a modified path. Deflection of the crack along the interface may be expected when the interface is relatively weak. The concomitant increase in the crack length provides a toughening mechanism. But weak interfaces can reduce the overall load the material can sustain. Consequently, there is an optimum strength for interfaces in a composite brittle material, which is determined by an appropriate balance between toughness and load-bearing capacity.

2.1. A criterion for crack propagation at an interface

Various scenarios for brittle crack propagation at an interface have been considered to study the competition between penetration and deflection of the crack, where the media on either side of the interface are treated as elastic and isotropic \((27-35)\). In this paper the energy dissipation at the crack-tip is used to determine whether the crack propagates across or within the interface. The energy dissipation is determined by maximising the ratio of the elastic energy released \(G\), when the crack proceeds in a particular direction, to the ideal work of fracture \(\Gamma\) associated with creating free surfaces and the possible simultaneous elimination of interfacial energy. According to the Griffith criterion fracture occurs when \(G/\Gamma \geq 1\). Values of \(G/\Gamma > 1\) imply that when fractures occurs some of the stored elastic energy is dissipated as heat. Therefore, maximising \(G/\Gamma > 1\) is equivalent to maximising the production of entropy. Figure 2 illustrates the crack propagation mechanism at the interface that is implemented into the existing DCD scheme. In DCD crack growth is modelled by the nucleation of small cracks ahead of it, which are then merged with the main crack in an incremental process. At each step of the calculation a variety of possible directions of a small crack is considered, and for each small crack the ratio of \(G/\Gamma\) is calculated. The crack for which \(G/\Gamma\) is maximised is selected and it is then merged with the main crack.

Cracks are modelled in DCD (as narrow elliptical voids) with an extremely small finite tip radius. We have carefully investigated the sensitivity of the calculations for cracks at interfaces to the thickness and tip radius of the elliptical
Figure 1: Schematic illustration of crack problems considered in this paper. Crack propagation in a polycrystalline material: (a) overview of the main crack interacting with smaller cracks, inclusions, voids and grain boundaries; (b) the crack impinging on a GB, (c) the crack meeting an inclusion in the grain and (d) a crack meeting inclusions along a GB.
voids. We have found that elliptical holes with aspect ratios of 0.01 or less can be used to approximate the stress fields of singular cracks extremely accurately. Please see Appendix A for further details.

2.2. Simulations of cracks impinging on interfaces

In this section we use DCD to consider first a crack meeting a grain boundary in isotropic elasticity. The boundary is characterised as a plane with an energy per unit area, and no associated elastic field of its own. We then consider a crack interacting with an elliptical inclusion, where the inclusion is considered to be incoherent with no misfit strain, and it has different elastic constants as the matrix, but its interface has a finite energy per unit area which is assumed to be independent of the interface normal. Finally we consider a crack interacting with a grain boundary containing inclusions. In all these calculations continuity of tractions and elastic displacements is maintained across the interfaces.

2.3. Crack interacting with a grain boundary

It has been reported (36, 37) that the orientation of the boundary plane with respect to an impinging crack, and the relative fracture energies of the matrix and the GB, can influence the path followed by a brittle crack. In this section we consider the influences of the ratio $\Gamma_{GB}/\Gamma_0$ and the angle $\phi$ between the crack plane and the boundary plane on the crack path. Here $\Gamma_{GB} = \Gamma_0 - \gamma_{GB}$ and $\Gamma_0 = 2\gamma_S$, where $\gamma_{GB}$ is the energy per unit area of the GB and $\gamma_S$ is the surface energy per unit area. It follows that $\Gamma_{GB}/\Gamma_0 = 1 - \gamma_{GB}/(2\gamma_S)$, and $0 < \Gamma_{GB}/\Gamma_0 < 1$. Figure 3 depicts a crack in a finite bicrystal loaded in tension by a stress $\sigma^a$ along the vertical direction. The width and height of the bicrystal were $W = 80 \mu m$ and $L = 20 \mu m$ respectively. The surfaces of the bicrystal in the horizontal direction are free. The elastic constants of the isotropic media on either side of
the GB were as follows: Young’s modulus $E = 120$ GPa and Poisson’s ratio $\nu = 0.3$. Numerical results obtained using the DCD method are compared with those obtained with the finite volume method (FVM) \(38\) in Figs. 4a and 4b for cases where $\Gamma_{GB}/\Gamma_0 = 0.1$ and 0.3 with $\varphi = 90^\circ$. It is seen that the two methods agree qualitatively.

A further set of simulations was performed to investigate the influence of the inclination angle $\varphi$ between the GB and the impinging crack on the propagation path. In these simulations the crack approaches the GB in the horizontal plane from the left. The calculations of Hutchinson \textit{et al.} \((27, 28)\), Cook \textit{et al.} \((29)\)
and Ebrahimi (39) found that the stored elastic energy required to deflect a crack along a GB at $\varphi = 90^\circ$ under mode-I loading is at least four times that needed for the crack to propagate without deflection across the GB. This implies that for the same stored elastic energy $\Gamma_{GB}/\Gamma_0$ must be reduced to less than 0.24 to deflect a crack along the GB when it is incident normally at the GB. In these simulations the ratio of fracture energies $\Gamma_{int}/\Gamma_0 = 0.24$ was fixed to ensure that the $90^\circ$ deflection at the interface can take place.

The grain boundary has to be given a width no more than the size of the radius of curvature of the elliptical crack tip to ensure that cracking of the grain boundary involves $\Gamma_{GB}$ only. Grain boundaries have structural widths of several nm in pure materials (40). An aspect ratio of 0.01 for the elliptical void representation of a crack in DCD enables micro-cracks of length up to 10 $\mu$m to interact with a GB represented by a thin slab of thickness 1 nm. Isotropic elasticity was again assumed for both grains with $\nu = 0.07$, $\mu = 570$ GPa and $\Gamma_0 = 10.18$ Jm$^{-2}$; these values are appropriate for diamond materials. The applied tensile stress in the vertical directions was sufficient to propagate a horizontal crack of length 10 $\mu$m towards an inclined GB. The right and left surfaces of the bicrystal were free of tractions.

For $70^\circ \le \varphi \le 90^\circ$ the crack was deflected along the GB and it was then arrested in the GB. When the load was increased further the crack left the GB and entered the grain on the right, eventually becoming normal to the axis of the applied stress. For $\varphi \le 60^\circ$ once the crack reached the GB it continued to propagate along it.

2.4. Crack interacting with an inclusion

Let us now consider a crack in an infinite isotropic elastic medium approaching an inclusion of elliptical cross-section under the influence of a remote applied normal stress $\sigma^\infty$, as depicted schematically in Fig.6. The inclusion is assumed to have no misfit and it generates no elastic field of its own. However, its isotropic elastic constants differ from those of the surrounding isotropic medium.

Before addressing the crack propagation at the inclusion interface problem, we draw your attention to the calculation process in the DCD method. In DCD method, interactions between cracks and inclusions of a system are obtained using the series based multipole method and solving an infinite set of linear equations with the truncation method. Depending on the spacing between elements and the desired accuracy of the calculation, different components of the series can be chosen; the better is the accuracy required, the greater is the number of components required. Thus, for closely spaced inclusions, the higher order terms
Figure 5: Paths followed by a crack in a bicrystal with different angles of inclination between the crack (black) and the GB (red). The crack is initially horizontal in the left grain and advances to the right to meet the inclined GB under the influence of a tensile stress applied in the vertical direction to the upper and lower surfaces of the bicrystal.

Figure 6: Schematic of a crack propagating horizontally towards an elliptical inclusion in an infinite solid. The major and minor axes of the ellipse are $l_1$ and $l_2$. There is a remote applied tensile load in the vertical direction $\sigma^\infty$. 

\[ \begin{array}{c}
\sigma^\infty \\
\sigma^\infty
\end{array} \]
in the series are needed to increase the level of precision used to represent interactions. However, in this case, the matrix of coefficient, representing the system of linear equations, becomes badly conditioned. Thus, to avoid computational cost attributed to the larger number of terms in the series and to avoid badly conditioned matrix, we assumed a finite thickness interface layer, which is substantially greater than what was assumed for a GB in the previous section; this is done to restrict the distance between the interacting crack and inclusion and has been verified to produce no change in the crack propagation path when the chosen thickness is reduced and higher order components of the series expansion have been included for verification; the thickness has been chosen according to Dini et al. study (41).

Figure 7a shows an enlarged picture of a crack approaching an inclusion. Three regions are identified labelled 1, 2 and 3, corresponding to the medium outside the inclusion, the interfacial layer and the medium inside the intrusion. The ideal work of fracture in each of these regions is $\Gamma_0$, $\Gamma_{int}$, and $\Gamma_{inc}$ respectively.

The interface layer depth is an important parameter because once the crack-tip reaches the interface it has to “decide” in which direction it will continue i.e., it will either penetrate through the inclusion or deflect and follow the path through the interface layer (Figure 7b). Therefore, the interface layer has to have an optimum depth in which the crack-tip is close enough to the inclusion to predict correct interactions with the inclusion, while it is far enough away to avoid computational difficulties.
Two factors are considered here to determine the interface layer ($\delta$). First, the interface layer depth must be selected smaller than the crack increment ($\Delta l$) at each simulation step. This fixes the maximum distance between the crack and the inclusion to predict crack penetration correctly. Second, the interface layer depth $\delta$ has to be chosen according to the graph that has been derived in our previous contribution (reported in Fig. 6 of (20)) to determine the distance between pseudo-cracks at each simulation step; this distance was determined in such a way that calculated average stress fields and SIFs for neighbouring cracks and inclusions is reliably captured and is optimised as a function of the other relevant length scales.

Numerical simulations are carried out for the system depicted in Figure 6, where the specimen containing the crack is subjected to a uniform uniaxial tensile loading in the $x_2$ direction. Crack propagating towards an inclusion can either deflect and propagate along the inclusion’s interface (Figure 8a) or penetrate through the inclusion (Figure 8b). If the crack propagate through the inclusion, the DCD method is unable to predict its path reliably as the crack-tip approaches branch points inside the inclusion. However, if we assume the crack follows the path of least energy cost, i.e. the path along which $\Gamma$ is minimised. Assuming that all the inclusion’s atoms have the same bonding energy, crack propagation paths within the inclusion must be such that the crack propagates straight through the material and coincide with the paths seen in Fig. 8b. Furthermore, crack path at boundaries and even crack propagation across the inclusion (Figure 8a) can be predicted.

Simulations were performed for various ratios of shear moduli in the matrix and inclusion ($\mu_0/\mu_{inc}$), and ratios of fracture energies ($\Gamma_0/\Gamma_{inc}$, $\Gamma_{int}/\Gamma_0$, and $\Gamma_{int}/\Gamma_{inc}$). The relative values of the Poisson’s ratios were kept constant at $\nu_0/\nu_{inc} = 1/3$. Subscripts 0, inc, and int refer to matrix, inclusion, and interface layer re-
spectively. Initially there is a stationary crack of length 5 \( \mu m \) the tip of which is at 12 \( \mu m \) to the left of an inclusion with aspect ratio \( l_2/l_1 = 3/5 \). Under the influence of the applied normal stress the crack propagates towards the intrusion. Li et al. (42) showed that whether a crack is deflected around an intrusion or propagates through it depends on the local curvature of the inclusion interface met by the crack-tip, as well as the external load. Therefore, in each set of simulations the external load and the inclusion dimensions are constant.

A crack propagating toward a hard inclusion is shown in Figure 9. Not surprisingly the crack does not penetrate the inclusion but its path is still sensitive to the relative strength of the interface compared to the matrix, \( \Gamma_{inc}/\Gamma_0 \). Cracks approaching increasingly softer inclusions are shown in Fig. 10. It is seen that as long a \( \Gamma_{inc}/\Gamma_{int} \) becomes smaller than certain value (depending on the material properties and associated Dundur’s parameter (31, 33)), the crack propagates through the inclusion along the same trajectory as in the matrix. Otherwise, the crack is deflected and propagates around the interface.

There have not been many experimental studies of crack-inclusion interactions. The influences of inclusion stiffness and interfacial strength on the crack propagation path was studied experimentally by Tippur et al. (43, 44). It was shown that the crack path does vary with the interfacial strength and the initial location of the crack relative to the inclusion. Experimental results of the crack paths reported in these contributions are in agreement with the paths predicted in Figures 9, and 10.

Buyukozturk et al. studied the crack penetration versus deflection in the interface of a circular hard inclusion subjected to wedge-type loading (45). Figure 11(a) shows the crack propagation path and the specimen configuration. Properties of the matrix material and inclusion are summarised in Table 1. We simulated this experiment as shown in Figure 11(b) using horizontal tensile loads at the top of the specimen to simulate the wedge loading of a vertical crack. It is seen that the simulated crack path is in remarkable agreement with the experiment. However, the agreement between the experiment and simulated crack path depends on different factors such as incremental length in crack propagation at each simulation step. Effects of the incremental crack length on the crack propagation path are shown in Figure 11(a); the DCD crack trajectories using various incremental lengths of 1.2 and 1.4 micro-meter at each simulation step are depicted in red and blue. Comparing simulation results with experimental results shows the better agreement when the incremental crack length 1.2 \( \mu m \) was used.

A study (46) has been made of the toughening by soft Nb-inclusions at ambient temperature of a hard MoSi\(_2\) matrix. The properties of the materials are
Figure 9: Crack trajectory computed for $\mu_{inc}/\mu_0 = 10$, $\Gamma_{inc}/\Gamma_0 = 10$ and values of a) $\Gamma_{int}/\Gamma_0 = 1$, b) $\Gamma_{int}/\Gamma_0 = 0.9$, and c) $\Gamma_{int}/\Gamma_0 = 0.5$

Figure 10: Crack trajectory computed for $\mu_{inc}/\mu_0 = 0.5$, $\Gamma_{inc}/\Gamma_0 = 0.5$ and values of a) $\Gamma_{int}/\Gamma_0 = 1$, b) $\Gamma_{int}/\Gamma_0 = 0.5$, and c) $\Gamma_{int}/\Gamma_0 = 0.12$

Table 1: Properties of the materials used in the experiments of (45, 46) at room temperature.

<table>
<thead>
<tr>
<th>Material</th>
<th>$E$ (GPa)</th>
<th>$\nu$</th>
<th>$\Gamma$ ($J/m^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$MoSi_2$ (matrix)</td>
<td>380</td>
<td>0.17</td>
<td>50-60</td>
</tr>
<tr>
<td>$Nb$ (inclusions)</td>
<td>103</td>
<td>0.38</td>
<td>200-500</td>
</tr>
<tr>
<td>Mortar (Matrix)</td>
<td>28</td>
<td>0.22</td>
<td>7.5</td>
</tr>
<tr>
<td>Granite (inclusion)</td>
<td>55</td>
<td>0.16</td>
<td>17.5</td>
</tr>
</tbody>
</table>

summarised in Table 1. Crack deflection in the vicinity of the Nb-inclusions is seen in Figure 12 and is attributed to the formation of a weak reaction layer at inclusion interfaces and elastic compatibility stresses at the crack tip between the $Nb$ inclusions and matrix material. Although the simulated crack path deviates from the experimental result in Figure 12 the crack is seen to circumvent the first inclusion and pass through its interface, but after that the simulated crack path deviates from the experimental result. This is uncertainty on the boundary conditions issues and the possibility that specimens deformation and rotation affect the path once the crack has left the inclusion. Also, deviation is small and this is not a big issue.
Figure 11: Comparison between trajectories of a crack interacting with an inclusion in (a) experiment [45] and (b) DCD simulation. The experimental crack trajectory is shown in black and the DCD crack trajectories are shown in red and blue. In (a) the DCD trajectory is superimposed on the experimental trajectory to highlight the agreement between experiment and simulation. Red and blue lines are crack trajectories using the incremental crack length 1.2 and 1.4 µm.

Figure 12: Experimental image of a crack propagating through a hard MoSi$_2$ matrix with soft Nb-inclusions from [46]. Superimposed in red is the path of a simulated crack obtained with the DCD method.
2.5. Crack propagation at grain boundaries containing elliptical inclusions/voids

In this section we consider the propagation of intergranular cracks where there is an elastic elliptical inclusion in the grain boundary. Inclusions at grain boundaries normally consist of two hemispherical caps, as shown in Fig. 13. The contact angle $\theta/2$ is determined by a balance of surface tensions: $\cos(\theta/2) = \gamma_{GB}/(2\gamma_{int})$. In this expression $\gamma_{GB}$ and $\gamma_{int}$ are the energies per unit area of the grain boundary and the interface of the inclusion respectively. This expression ignores Herring torque terms arising from any dependence of these interfacial energies on the inclination of the interfaces. The angle $\theta$ is determined by lenticular geometry. The geometry of these lenticular inclusions is approximated here as an elliptical cross-section with semi-major and semi-minor axes of $l_1$ and $l_2$ respectively. It follows that $(l_2/l_1)^2 = [2\gamma_{int} - \gamma_{GB}]/[2\gamma_{int} + \gamma_{GB}]$.

The set-up for the simulations is illustrated in Figure 14. The origin of the $x_1 - x_2$ Cartesian coordinate system is at the centre of the inclusion and aligned with its major and minor axes. Under the influence of the load the crack propagates along the grain boundary towards the inclusion and its path is followed.

Simulations were performed with hard and soft inclusions and voids at the
Figure 15: Propagation path and variation of the normalised energy release rate and the normalised Mode-I SIF for a crack at a GB containing an elliptical hard inclusion, with $\mu_{\text{inc}}/\mu_0 = 10$, $\Gamma_{\text{inc}}/\Gamma_0 = 2\gamma_{\text{inc}}/2\gamma_0 = 1.1$, $\Gamma_{\text{inc}}/\Gamma_{\text{int}} = 2\gamma_{\text{inc}}/(\gamma_{\text{inc}} + \gamma_0 - \gamma_{\text{int}}) = 4$. $\mu_{\text{inc}}$ and $\mu_0$ are the shear moduli of the inclusion material and the matrix material respectively. $\gamma_0$ is the energy per unit area of a surface of the matrix material, $\gamma_{\text{inc}}$ is the energy per unit area of a surface of the inclusion material, $\gamma_{\text{int}}$ is the energy per unit area of an interface between the inclusion and the matrix. a) $l_2/l_1 = 0.5 \implies \gamma_{\text{GB}}/\gamma_{\text{int}} = 1.2$. b) $l_2/l_1 = 0.8 \implies \gamma_{\text{GB}}/\gamma_{\text{int}} = 0.44$.

Figure 15 shows that as the crack approaches a hard inclusion in the grain boundary both the SIF and the energy release rate decrease below the corresponding values for a crack at a grain boundary without such an inclusion. This is because the crack is approaching a region where the local strain is reduced by the larger shear modulus of the inclusion, i.e. the crack tip is shielded by the inclusion. With $\Gamma_{\text{inc}}/\Gamma_{\text{int}} = 4$ in both (a) and (b) of Fig. 15 it is energetically favourable for the crack to progress along the inclusion interface rather than through the grain boundary. voids are included as special cases of elliptical inclusion of zero stiffness and as favourable path for crack propagation. For hard inclusions $(l_1, l_2) = (5 \, \mu\text{m}, 2.5 \, \mu\text{m})$ and $(5 \, \mu\text{m}, 4 \, \mu\text{m})$, while for soft inclusions and voids $(l_1, l_2) = (5 \, \mu\text{m}, 2.5 \, \mu\text{m})$ and $(5 \, \mu\text{m}, 1 \, \mu\text{m})$. Figures 15 - 17 show the variations of the energy release rate $G$ and mode-I SIF $K_I$, normalised respectively by the energy release rate $G_0$ and mode-I SIF $K_{I0}$ in the same system without an inclusion.

Figure 15 shows that as the crack approaches a hard inclusion in the grain boundary both the SIF and the energy release rate decrease below the corresponding values for a crack at a grain boundary without such an inclusion. This is because the crack is approaching a region where the local strain is reduced by the larger shear modulus of the inclusion, i.e. the crack tip is shielded by the inclusion. With $\Gamma_{\text{inc}}/\Gamma_{\text{int}} = 4$ in both (a) and (b) of Fig. 15 it is energetically favourable for the crack to progress along the inclusion interface rather
than through the inclusion. (It may be helpful to note that the $\Gamma$ parameters imply $\gamma_{\text{int}} = 1.55\gamma_0$ while $\gamma_{\text{inc}} = 1.1\gamma_0$). The deflection of the crack path produces an increase of both the normalised SIF and the normalised energy release rate above unity. It should be noted that the values obtained when computing the variation of the energy and SIFs depend on the crack incremental size and its angle. When the crack propagates along the inclusion/matrix interface, the system is no longer symmetric and this explains why the energy and SIF profiles are not symmetric and show different trends. Calculated crack energies and SIFs in the present model agree well with other numerical results using the boundary element method of Bush (2), the symmetric-Galerkin boundary element method (SGBEM) of Kitey (3), and the FEM of Boselli (47) and Ayyar (48).

For the soft inclusions displayed in Figure 16 the $\Gamma$ parameters imply $\gamma_{\text{int}} = \gamma_0$ and $\gamma_{\text{inc}} = \frac{1}{2}\gamma_0$. Thus the crack passes through the middle of the inclusion because it is the lowest energy path. As the crack approaches the soft inclusions and the voids in Fig.17 both the SIF and the energy release rate increase rapidly because the local stress at the crack tip is amplified. As it was explained earlier (in section 2.4) the crack propagation path inside the inclusion cannot be calculated using the DCD method. Consequently, the energy release rate inside the soft inclusion was not computed. However, Li et al. (49) found both numerically and experimentally that the energy release rate decreases as the crack propagates through the soft inclusion, as one would expect. As the crack exits the inclusion the energy release rate quickly reaches that of a crack at a grain boundary in the absence of a soft inclusion or a void.

In summary, to maximise the degree of crack deflection and thereby maximise the toughness of the material we should have large, hard inclusions at grain boundaries in a soft matrix, and the aspect ratios of the inclusions should be as close as possible to unity. However, hard inclusions may lead to significant elastic compatibility stresses and the formation of stress concentrations. There is therefore a balance to be struck between these two tendencies.

3. Toughening mechanism

In this section, we study a toughening mechanism using inclusions (which in two-dimensional problems can be seen as fibres) reinforcements on the GBs. In general, toughening mechanisms at GBs are associated with deflecting and directing cracks into predetermined propagation tortuous paths (50–54). Effects of an array of hard/soft inclusions and voids on a grain boundary on a crack propagation path, energy and SIF variation are studied. Regardless of the GB
Figure 16: Same as Fig. 15 but for a soft inclusion, with $\mu_{inc}/\mu_0 = 0.10$, $\Gamma_{inc}/\Gamma_0 = 0.5$, $\Gamma_0/\Gamma_{int} = 4$. a) $l_2/l_1 = 0.5 \Rightarrow \gamma_{GB}/\gamma_{int} = 1.2$. b) $l_2/l_1 = 0.2 \Rightarrow \gamma_{GB}/\gamma_{int} = 1.85$.

Figure 17: Same as Fig. 15 but for an elliptical void with $\mu_{inc} = 0.0$, $\Gamma_{inc} = 0.0$, $\Gamma_{int} = \Gamma_0$. a) $l_2/l_1 = 0.5 \Rightarrow \gamma_{GB}/\gamma_0 = 1.2$. b) $l_2/l_1 = 0.2 \Rightarrow \gamma_{GB}/\gamma_0 = 1.85$. 

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Figure 18: Schematic diagram of a crack propagating towards an array of inclusions on the GB in an unbounded solid simulated here as a simplified scenario. Inclusions are assumed to be elliptical in shape and equispaced on a GB.

energy, simulation of this section can be used to study toughening mechanism in the matrix material using a distribution of hard/soft inclusions.

Effects of inclusions on a GB were studied by modelling a system containing an array of equispaced inclusions along the GB. Figure 18 shows an initial configuration of a system schematically. The system is under uniform tension in \( x_2 \) direction, and an initial crack of length 10 \( \mu m \) is introduced along the grain boundary; the original crack-tip is positioned at \((x_1, x_2) = (-20, 0) \mu m\). Preliminarily, the GB and other interfacial energies are fixed; these energies can be obtained from molecular dynamics simulations or experimental results. By preselecting the GB and interface energies, and consequently the size of inclusions, the optimal distance between inclusions can be attained.

**Array of hard inclusions**

A first set of simulations were performed on a system showed in Figure 18. Inclusions with aspect ratio \( e = l_2/l_1 = 4/5 = 0.8 \), and matrix material and inclusions with relative mechanical properties such as \( \mu_{inc}/\mu_0 = 10 \), and \( \nu_{inc}/\nu_0 = 1/3 \), \( \Gamma_{inc}/\Gamma_0 = 2 \), \( \Gamma_{inc}/\Gamma_{int} = 4 \), and \( \Gamma_{GB}/\Gamma_{int} = 1.12 \) were selected to study the toughness enhancement associated with several distributions of the hard inclusions. Figures 19a - 19d show the crack energy shielding for various GB structures where the shielding effect and the distance between two successive inclusions are inversely related. Evidently, the GB toughness is increased by the presence of inclusions, and crack propagates along the structure with almost lower energy compared with the system without inclusions. Furthermore, sudden declines in the crack energy at the vicinity of the hard inclusions show that a propagating crack can be arrested by the hard inclusions.

**Array of soft inclusions and voids**

Simulations were performed for soft inclusions (with aspect ratio \( e = l_2/l_1 = 2.5/5 = 0.5 \)) and a matrix material with relative mechanical properties \( \mu_{inc}/\mu_0 = 19 \)
Figure 19: Energy evolution of the crack while it is propagating along the GB containing 4 equispaced elliptical hard inclusions with different spacing.
\( \nu_{\text{inc}}/\nu_0 = 3, \Gamma_{\text{inc}}/\Gamma_0 = 0.5, \Gamma_0/\Gamma_{\text{int}} = 4, \) and \( \Gamma_{\text{GB}}/\Gamma_{\text{int}} = 1.6. \)

Figure 20 shows in the cases where the distance between two sequential inclusions is less than the major axis of the inclusions, crack energy amplifications between inclusions are observed. In other words, the crack propagates between inclusions at a higher energy level compared with the system without inclusions. Simulation results predict that increasing spacing between the inclusions can reduce the crack energy and consequently enhance the toughness of the GB. Also, interactions between inclusions with spacing more than 1.5 times of the inclusion size \( (3l_1) \) are negligible. Thus, this structure might not be capable of channelling the crack into a predefined path.

Similar sets of simulations were run for another system, where instead of soft inclusions, elliptical holes of the same size and distance were located on the GB (Figure 21). Maximum energies of the propagating crack in the vicinity of the holes predict that a crack requires less external load to propagate along the array of voids than along the array of soft inclusions. The difference in the average quantities of the maximum energies and maximum SIFs for the crack right at the edge of the elliptical holes and soft inclusions are more than 35% and 20% respectively.

The average quantities of the crack energy and Mode-I SIF of the simulations are calculated and summarised in Table 2. Average relative quantities for the hard inclusions show that increasing the distance between the inclusions does not change the average quantities of the structures illustrated in Figure 19a by more than 1% compared with the one in Figure 19d. In reality, if hard inclusions are situated very close together, the average density of the material will be increased, and the hard inclusion agglomeration is expected to occur. Therefore, increasing the spacing between hard inclusions to the point where the interaction between inclusions becomes negligible, should provide a better toughening mechanism.

Also, comparing the results obtained from simulations for the soft inclusions and voids (Figures 20 and 21) show that crack energy propagating through voids, located on the GB, is higher than the same system containing soft inclusions by more than 10%, and 6% respectively. Calculation of the average quantities is consistent with the earlier prediction that the toughness of the GB containing voids is less than the same GB containing soft inclusions. It should be noted that in the current calculations, toughening due to energy dissipation in the soft inclusions is not considered. Including this energy dissipation in calculations strengthen the previous argument that a system containing soft inclusions is tougher than the same system containing voids. Results of this section can be extended to a more general case where inclusions are distributed evenly in the
Table 2: The average normalised energy and Mode-I SIF at the crack-tip are calculated for different toughening mechanisms where soft inclusions, voids, and hard inclusions were located on the GB. The percentage difference of the results for the soft inclusions and voids are calculated. In the last two columns present the normalised quantities for a GB containing hard inclusions.

<table>
<thead>
<tr>
<th>space/2l₁</th>
<th>soft inclusions</th>
<th>voids</th>
<th>difference (%)</th>
<th>hard inclusions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>G/G₀</td>
<td>K₁/K₁₀</td>
<td>G/G₀</td>
<td>K₁/K₁₀</td>
</tr>
<tr>
<td>0.5</td>
<td>1.16</td>
<td>1.03</td>
<td>1.28</td>
<td>1.10</td>
</tr>
<tr>
<td>0.6</td>
<td>1.08</td>
<td>1.03</td>
<td>1.25</td>
<td>1.09</td>
</tr>
<tr>
<td>1.0</td>
<td>1.13</td>
<td>1.05</td>
<td>1.31</td>
<td>1.12</td>
</tr>
<tr>
<td>1.5</td>
<td>1.12</td>
<td>1.04</td>
<td>1.29</td>
<td>1.11</td>
</tr>
</tbody>
</table>

matrix material; regardless of the aspect ratio limitation that is caused by the $\gamma_{GB}/\gamma_{int} = 2(1 - e^2)/(1 + e^2)$ formula for GBs. Materials containing soft inclusions are tougher than those containing voids. Moreover, the results presented in Table 2 show that the average quantities have a minimum value for the situation in which the spacing between to sequential inclusions is space/2l₁ = 0.6; this is the toughest GB structure among all other calculations. It means that there is an optimal distance between either soft inclusions or voids that can maximise the effect of GB toughening mechanism.

Array of inclusions: General case

In many polycrystalline materials, macroscopic cracks advance along the grain boundaries, where the strength of the GBs is less than the low cleavage energy of the crystal. Inclusions accommodated along the GBs can effectively modify the crack propagation path. Crack propagation depends on various factors such as energy and orientation of GBs, interfacial energies, fracture energies, and size and position of inclusions. Also, these factors are interconnected; for example, strength and energy of the GB and the inclusion’s interface can be modified by adjusting the size and spacing of the inclusions (7). Therefore, it appears that a systematic parametric study of the system, even for a simple problem of inclusions on a GB, is impracticable because many parameters are involved and this is outside of scope of the present contribution. Nevertheless, the proposed method is fast, reliable and accurate and is readily applied to any specific problems with known parameters.
Figure 20: Energy evolution of the crack while it is propagating along the GB containing 4 equispaced soft inclusions with different spacing.

(a) Distance between two sequential inclusions is equal to $l_1$.

(b) Distance between two sequential inclusions is equal to $1.2 l_1$.

(c) Distance between two sequential inclusions is equal to $2 l_1$.

(d) Distance between two sequential inclusions is equal to $3 l_1$. 
Figure 21: Energy evolution of the crack while it is propagating along the GB containing 4 equispaced elliptical voids with different spacing.
4. Conclusion

This paper explores the possibility to achieve predictive capabilities for the design of advanced engineered materials that rely on GB and inclusions to tune the performance of certain structures. Here it is shown that a crack approaching a weak GB and inclusion’s interface can deflect and release energy. Crack deflection enhances toughness of the materials (27).

Competition between penetration and deflection of crack at interfaces were studied using a crack propagation mechanism based on the energy distribution at the crack-tip and crack coalescence is also taken into account.

The effect of the GB orientation and interfacial strength of the GBs and inclusions on crack propagation path are studied. It is shown that variation of the GB and the inclusion interfacial strength could effectively change the crack propagation trajectory in the quasi-static regime and consequently enhance the fracture toughness of the material under investigation. Also, crack propagation at the interface depends on the relative orientation of the crack and the interface.

Adding and controlling the dispersion of inclusions (or fibers) is a very powerful tool to obtain materials with effective properties in between those of its individual components (matrix material and inclusions) (55). Here, we studied the crack deflection toughening mechanisms in the presence of hard inclusions. The distance between the hard inclusions should be greater than the size of the inclusions themselves to avoid inclusion clustering, which is not beneficial in terms of increased toughness. Also, simulation results show that soft inclusions and voids in brittle materials can improve the material toughness by directing a crack into a predetermined propagation path. Furthermore, considering that additional crack energy dissipation could take place in the presence of soft inclusions which, are often ductile (as is the case for Co used as sintering agent in polycrystalline diamonds (56)), the material toughness could be further enhanced in such configurations.

4.1. Outlook and Suggestions for Further Developments

The method provides an accurate semi-analytical tool to derive full stress and displacement fields, as well as stress intensity factors and energy release rates of cracks, and to predict low-speed crack propagation through complicated defect networks in brittle or quasi-brittle materials in an efficient way, which is in principle much faster than computational methods that rely on mesh discretisation and numerical implementation over grid domains such as the extended finite element method.

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The above method is adequate to deal with individual micro-cracks propagating within a loaded system in the presence of macro-cracks and inclusions at the interfaces and GBs. This can be extended to deal with a network of micro-cracks for example by performing minimisation of the total energy of the mechanical system with respect to the crack extension directions and crack extension lengths to solve for the evolution of the mechanical system over time, as proposed in (57–60).

A straightforward extension of the present work involves incorporating the effect of temperature variation and residual stress. Moreover, the model presented in our previous work (20) and adopted and extended here to tackle important applications was developed for 2D problems in linear elastic solids. The method could be extended to 3D by changing the constituent elements of the system from ellipses to ellipsoids and accordingly changing the basis functions in series expansions of the complex potential fields (21,22). The methodology can also be extended to incorporate different geometry of the inclusions as the solution procedure is identical for different shapes of inclusions, provided that the basis functions are chosen (and potentially derived in case they are not available for specific geometries) according to the inclusions to be studied.

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http://dx.doi.org/10.1016/0020-7683(89)90021-8


Appendix A. Crack-tip curvature and crack singularity

Here, the effect of the crack thickness and curvature on the accuracy of calculations at the interface is investigated. In the case of the collapsed elliptical hole,

\[ G / G_{\text{max}} \]

is maximum energy release rate at the crack-tip. Energy plots are depicted for 3 cracks with different aspect ratios 0.001 (blue), 0.01 (black), and 0.1 (red).

if the singular stress fields dominate the solution at the crack-tip, the crack propagation laws can be reasonably used to predict crack growth. Dini and Hills [41] showed that to approximate a blunt crack (with a finite curvature at the crack tip) to a crack, the applied load on the system should be in a permissible range with a minimum and a maximum load. The former is defined as the load below which the crack radius affects the stress fields, and the latter is the load associated with the concept of “small-scale yielding” in fracture mechanics and depends on the geometry of the problem [61]. Their calculations show for example that for a maximum of 5% to 6% discrepancy between two cases (crack and crack with blunt tip of finite curvature), the relative amount of crack curvature (\( \rho \)) and crack length (\( 2a \)) should be around \( \rho / 2a \leq 0.00005 \). For the case of an elliptical hole, the value of \( \rho / a \) is equal to \( e^2 \), where \( e \) is the ellipse aspect ratio. Therefore, elliptical holes with small aspect ratio \( e \leq 0.01 \) can be used to approximate cracks.

The full stress field distributions and energy at the tip of an elliptical crack with 5 \( \mu \)m length in an infinite plane are calculated using the multipole method. The crack is under uniform tension in the \( x_2 \) direction. Energy varies at the crack-tip as a function of the polar angle \( \theta \). Figure A.22 presents the normalised energy at the crack tip for a range of polar angle \( \theta \). The energy is normalised by the maximum energy at the perimeter of the ellipse. Different colours of
the normalised energy plots express the influence of the crack’s aspect ratio. The normalised energies were evaluated for three different aspect ratios ($e = 0.001, 0.01, 0.1$) and plotted with red, blue and black colours respectively. It is shown that this parameter has no significant effect on the results specifically for the cases with $e < 0.01$, but increasing the aspect ratio further can change the normalised energy distribution. Results of this calculation is compatible with the above discussion.