

# Influence of Grain Size Distribution on Ductile Intergranular Crack Growth Resistance

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The influence of grain size distribution on ductile intergranular crack growth resistance is investigated using full field microstructure-based finite element calculations and a simpler model based on discrete unit events and graph search. The finite element calculations are carried out for a plane strain slice with planar grains subjected to mode I small scale yielding conditions. The finite element formulation accounts for finite deformations and the constitutive relation models the loss of stress carrying capacity due to progressive void nucleation, growth and coalescence. The discrete unit events are characterized by a set of finite element calculations for crack growth at a single grain boundary junction. A directed graph of the connectivity of grain boundary junctions and the distances between them is used to create a directed graph in J-resistance space. For a specified grain boundary distribution, this enables crack growth resistance curves to be calculated for all possible crack paths. Crack growth resistance curves are calculated based on various path choice criteria and compared with the results of full field finite element calculations of the initial boundary value problem. The effect of unimodal and bimodal grain size distributions on intergranular crack growth are considered. It is found that a significant increase in crack growth resistance is obtained if the differ-

ence in grain sizes in the bimodal grain size distribution is sufficiently large.

## 1 Introduction

Several physical processes can be viewed as a problem of path selection, for example, flow of a river stream [1] or crack growth in a complex heterogeneous material microstructure [2–4]. Although the problems of path selection for flow of a river stream and of crack growth in a heterogeneous material involve very different length-scales, their solutions share common features. For example, path selection criteria based on fracture mechanics can be used to predict growth of streams in a diffusion field [1], while a directed graph constructed using microstructure specific discrete unit events can be used to predict crack growth in heterogeneous materials [4]. Intuitively, one expects that the path of a physical process involving path selection can be controlled by engineering the discrete unit events.

It has been shown that it is possible to engineer crack paths by controlling the distribution of second phase particles in a ductile matrix to increase the material's crack growth resistance [3]. In [3], the controlled microstructure was char-

acterized by various sinusoidal distributions of particles with fixed mean particle spacing. The results presented in [3] indicate that the crack path can be engineered to increase the crack growth resistance by appropriately adding or removing particles that guide the crack path.

Although near room temperature ductile fracture in polycrystalline metals and alloys is typically transgranular, several materials of technological interest that have a high specific strength (strength to weight ratio), such as, Al-Li alloys [5] and metastable  $\beta$  Ti alloys [6] undergo intergranular ductile fracture near room temperature. Furthermore, several technologically important multiphase materials, such as multiphase advanced high strength steels undergo ductile fracture along the interface between the hard and the soft phase [7, 8].

Here, we focus on a scenario involving ductile intergranular (or interfacial) crack growth. In particular, we explore the possibility of engineering the crack path to increase the material's crack growth resistance by controlling the grain size distribution. Experiments have shown that the grain size distribution of a variety of materials can be controlled by advanced processing routes [6, 9–13]. Experiments have also shown that a controlled grain size distribution, such as a bimodal grain size distribution, can enhance the crack growth resistance of brittle ceramics [14], the fatigue properties of titanium alloys [15] and the corrosion resistance of steels [16].

Following such experimental observations, we carry out analyses of ductile intergranular crack growth in material microstructures with unimodal and bimodal grain size distributions. The bimodal grain size distributions are characterized by varying grain sizes in layers. Ductile intergranular crack growth is analyzed using both microstructure-based finite element crack growth calculations based on a constitutive framework for a progressively cavitating ductile solid with an isotropic and isotropically hardening matrix material as in [2], and a simple model based on discrete unit events and graph search developed in [4]. In [4], the key unit event associated with intergranular crack propagation was found to be the interaction of a grain boundary crack with a grain boundary segment located at an angle with the initial crack plane. Finite element calculations are also carried out for various orientations of a single grain boundary segment with the initial crack plane to characterize the unit events.

Our calculations show that increasing the overall grain size in microstructures with unimodal and bimodal grain size distributions can result in an increase in the crack growth resistance. However, decreasing the grain size in one layer and increasing the grain size in another layer, such that the overall grain size is fixed, can give an even greater increase in the crack growth resistance. Furthermore, the predictions of the simple model based on discrete unit events and graph search are found to be in general agreement with the results of full field microstructure-based finite element crack growth calculations. This suggests that the computationally efficient unit event based graph search model can provide a tool for designing material microstructures with improved intergranular crack growth resistance.

## 2 Theoretical framework

### 2.1 Initial/boundary value problem formulation

The material model and the numerical implementation are the same as in [2, 4]. Here, for completeness, we briefly describe the formulation. Further details and more complete references are given in [2, 4].

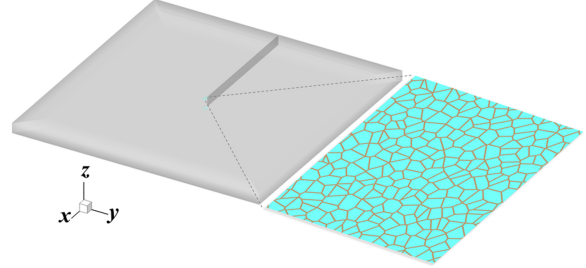


Fig. 1. Sketch of the initially cracked slice of material analyzed, showing the grain boundary distribution in the region in front of the initial crack tip.

The finite element formulation is based on the finite deformation dynamic principle of virtual work written as

$$\int_V \boldsymbol{\tau} : \delta \mathbf{D} dV = \int_S \mathbf{T} \cdot \mathbf{u} dS - \int_V \rho \frac{\partial^2 \mathbf{u}}{\partial t^2} dV \quad (1)$$

where  $\mathbf{u}$  is the displacement vector,  $t$  is time,  $V$  is the volume of the region analyzed in the reference configuration,  $S$  is its surface in the reference configuration,  $\rho$  is the density in the reference configuration,  $\boldsymbol{\tau}$  is the Kirchhoff stress tensor, and  $\mathbf{T} = \boldsymbol{\tau} \cdot \mathbf{n}$  with  $\mathbf{n}$  being normal to  $S$ .

As in [2, 4], a mode I small scale yielding boundary value problem is analyzed for a slice of material with an initial crack at  $x = 0$  and  $y = 0$ , as shown in Fig. 1. Initial and boundary displacements and velocities corresponding to the isotropic linear elastic mode I plane strain singular field are applied in such a way as to minimize dynamic effects. The amplitude of the remote displacements are proportional to an imposed stress intensity factor  $K_I$  which is taken to increase monotonically with time with  $\dot{K}_I = 1.2 \times 10^7 \text{ MPa} \sqrt{\text{ms}}^{-1}$ . In presenting the results, the remote loading is characterized by Rice's  $J$ -integral [17] which, for small scale yielding, is related to the imposed stress intensity factor  $K_I$  by

$$J = K_I^2 \frac{(1 - \nu^2)}{E} \quad (2)$$

A uniform  $1000 \times 600$  in-plane (the  $x - y$  plane) mesh is used in a  $0.01 \text{ m} \times 0.006 \text{ m}$  region in front of the initial crack tip. In this region, the in-plane elements are  $10 \mu\text{m}$  by  $10 \mu\text{m}$ . Although, finite element calculations are based on the dynamic principle of virtual work for numerical convenience, the focus is on quasi-static response. Since the constitutive formulation here does not contain a material length scale, in a

quasi-static analysis only relative length scales matter. Thus, we normalize all length scales by a reference length scale,  $e$ , which we choose to be the in-plane element side length in the fine mesh region so that  $e = 10 \mu\text{m}$ . The total number of finite elements and the total number of nodes in the calculations are 760,000 and 5,328,253, respectively.

The microstructure is taken to be constant through the slice thickness with only one element through the thickness so that the deformation field is essentially two dimensional. However, the finite element formulation is three dimensional using twenty-node brick elements with the out of plane displacements constrained to give overall plane strain. The internal force contributions are integrated using eight point Gaussian integration and the explicit Newmark  $\beta$ -method with  $\beta = 0$  [18] is used for time integration and a rate tangent modulus constitutive update is used [19].

The constitutive relation is based on writing the rate of deformation tensor  $\mathbf{d}$  as the sum of an isotropic elastic part,  $\mathbf{d}^e = \mathbf{L}^{-1} : \dot{\boldsymbol{\sigma}}$  characterized by Young's modulus  $E$  and Poisson's ratio  $\nu$ , and a viscoplastic part,  $\mathbf{d}^p$ . The elastic strains are presumed to remain small.

The plastic part of the rate of deformation tensor  $\mathbf{d}^p$  is given by a rate dependent modified Gurson [20] constitutive relation for a progressively cavitating solid with the flow potential given by

$$\Phi = \frac{\sigma_e^2}{\bar{\sigma}^2} + 2q_1 f^* \cosh\left(\frac{3q_2 \sigma_h}{2\bar{\sigma}}\right) - 1 - (q_1 f^*)^2 = 0 \quad (3)$$

where  $q_1 = 1.25$ ,  $q_2 = 1.0$  are parameters introduced in [21, 22],  $f$  is the void volume fraction,  $\bar{\sigma}$  is the matrix flow strength and

$$\sigma_e^2 = \frac{3}{2} \boldsymbol{\sigma}' : \boldsymbol{\sigma}', \quad \sigma_h = \frac{1}{3} \boldsymbol{\sigma} : \mathbf{I}, \quad \boldsymbol{\sigma}' = \boldsymbol{\sigma} - \sigma_h \mathbf{I} \quad (4)$$

with  $f^*$  given by Eq. (5) as introduced in [23]

$$f^* = \begin{cases} f, & f < f_c \\ f_c + (1/q_1 - f_c)(f - f_c)/(f_f - f_c), & f \geq f_c \end{cases} \quad (5)$$

where the values  $f_c = 0.12$  and  $f_f = 0.25$  are used.

The plastic part of the rate of deformation tensor  $\mathbf{d}^p$ , is obtained from the plastic potential, Eq. (3), as

$$\mathbf{d}^p = \left[ \frac{(1-f)\bar{\sigma}\dot{\bar{\epsilon}}}{\boldsymbol{\sigma} : \frac{\partial \Phi}{\partial \boldsymbol{\sigma}}} \right] \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} \quad (6)$$

The matrix plastic strain rate,  $\dot{\bar{\epsilon}}$ , is given by

$$\dot{\bar{\epsilon}} = \dot{\epsilon}_0 \left[ \frac{\bar{\sigma}}{g(\bar{\epsilon})} \right]^{1/m} \quad g(\bar{\epsilon}) = \sigma_0 [1 + \bar{\epsilon}/\epsilon_0]^N \quad (7)$$

with  $\bar{\epsilon} = \int \dot{\bar{\epsilon}} dt$  and  $\epsilon_0 = \sigma_0/E$ .

The material microstructure is taken to consist of hard grains with relatively soft thin layers along the grain boundaries. The elastic constants  $E = 116\text{GPa}$  and  $\nu = 0.3$ , the hardening exponent  $N = 0.1$  and the rate sensitivity parameters  $m = 0.01$  and  $\dot{\epsilon}_0 = 10^3 \text{s}^{-1}$  are all taken to be the same for both the grains and the soft grain boundary layers. The flow strength of the grains,  $\sigma_0$ , is taken to be 1200MPa and for the softer grain boundary layers  $\sigma_0^\ell = 800\text{MPa}$ .

The initial void volume fraction is taken to be zero and the evolution of the void volume fraction is governed by

$$\dot{f} = (1-f)\mathbf{d}^p : \mathbf{I} + \dot{f}_{nucl} \quad (8)$$

where the first term on the right hand side of Eq. (8) accounts for void growth and the second term for void nucleation.

Stress controlled void nucleation is taken to occur in the softer grain boundary layers via

$$\dot{f}_{nucl}^{\text{stress}} = \frac{f_N^{\text{stress}}}{s_N^{\text{stress}} \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\bar{\sigma} + \sigma_h - \sigma_N}{s_N^{\text{stress}}} \right)^2 \right] (\dot{\bar{\sigma}} + \dot{\sigma}_h) \quad (9)$$

if  $(\bar{\sigma} + \sigma_h)$  is at its maximum over the deformation history. Otherwise  $A = 0$ . Here,  $f_N^{\text{stress}} = 0.06$ ,  $\sigma_N = 1.5\sigma_0^\ell$  and  $s_N^{\text{stress}} = 0.3\sigma_0^\ell$ .

Plastic strain controlled void nucleation is taken to occur both in the grains and in the grain boundary layers via

$$\dot{f}_{nucl}^{\text{strain}} = \frac{f_N^{\text{strain}}}{s_N^{\text{strain}} \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\bar{\epsilon} - \epsilon_N}{s_N^{\text{strain}}} \right)^2 \right] \dot{\bar{\epsilon}} \quad (10)$$

with  $f_N^{\text{strain}} = 0.04$ ,  $\epsilon_N = 0.2$  and  $s_N^{\text{strain}} = 0.2$  for both phases.

The extent of crack growth,  $\Delta a$ , is defined by the maximum projected length on the  $x$ -axis of the void volume fraction contour,  $f = 0.1$ .

## 2.2 Microstructure generation

For a uniform grain size distribution, the microstructure is generated using Dirichlet tessellation [24] with  $N_g$  random points chosen in the fine mesh region in front of the initial crack tip. The fine mesh region of dimensions  $A = 1000e \times 600e$  is partitioned with the  $N_g$  random points to form  $N_g$  Voronoi cells with one generator inside each cell. Each Voronoi cell corresponds to a grain. The grain boundary layers are generated along each grain with a thickness of  $4e$ . The finite element Gauss integration points in the fine mesh region are assigned the material properties associated with a grain or a grain boundary layer depending on where they are located, Voronoi cell or grain boundary layer. This method generates  $N_g$  grains having an average grain size,  $D_g = \sqrt{A/N_g}$ .

For microstructures with a bimodal grain size distribution, the fine mesh region is divided into five regions of equal area. In terms of  $e$ , the area of each subdivided region is  $A_s = 200e \times 600e$ . Along the  $x$ -axis these regions lie in  $(K-1)200e \leq x \leq K200e$ , where  $K = 1, 3, 5$ , for regions I

and  $K = 2, 4$  for regions II. The regions I and II are partitioned with  $N_g^I$  and  $N_g^{II}$  random points, respectively, and the microstructure is generated following the procedure used to generate uniform grain size distribution. This results in average grain size  $D_g = \sqrt{A_s/N_g^I}$  in regions I and  $D_g = \sqrt{A_s/N_g^{II}}$  in regions II. This forms a layered microstructure with regions I having one average grain size and regions II having a different average grain size. Subsequently, we will refer to these as type I regions and type II regions, respectively.

### 2.3 Unit event modeling

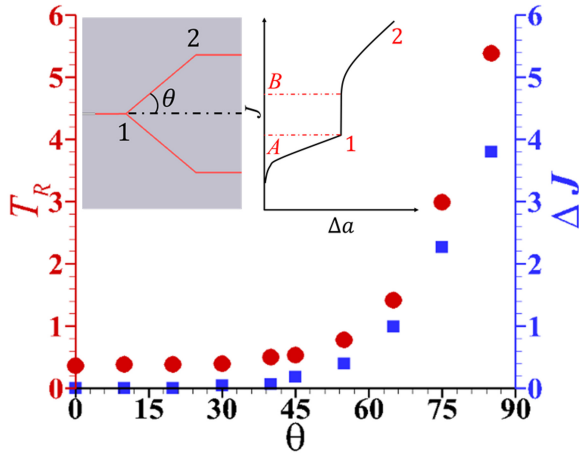


Fig. 2. The tearing modulus,  $T_R$  (circles) of a crack propagating along a grain boundary oriented at angle  $\theta$  with respect to the plane of crack propagation and the increment in  $J/(\sigma_0 e)$ ,  $\Delta J$  (squares) arising from the crack reaching triple junction, as shown in the inset.

As in [2, 4], crack growth is modeled as a series of unit events comprising growth of a crack along a grain boundary connected to the current crack tip placed symmetrically at angle  $\theta$  to the current crack, as illustrated in the inset of Fig. 2.

Small scale yielding calculations are carried out for various angles  $\theta$ . There is an initial increase in  $J$  without any increase in crack length, as sketched in the inset in going from A to B. The value of  $\Delta J$  on the right side axis of Fig. 2 is defined as  $(J_B - J_A)$ . Eventually, crack growth occurs along the grain boundary so that the direction of crack growth changes by  $\theta$  and the crack grows to point 2.

The tearing modulus,  $T_R$ , [25] defined as

$$T_R = \left( \frac{E}{\sigma_0^2} \right) \frac{dJ}{d(\Delta a)} \quad (11)$$

is calculated by identifying  $dJ$  with  $(J_2 - J_1)$  and identifying  $\Delta a$  with  $(\Delta a_2 - \Delta a_1)$  where points 1 and 2 are shown in the inset of Fig. 2. The length of the unit event grain boundary facet is taken to be such that  $\Delta a_2 - \Delta a_1 = 100e/\tan \theta$ .

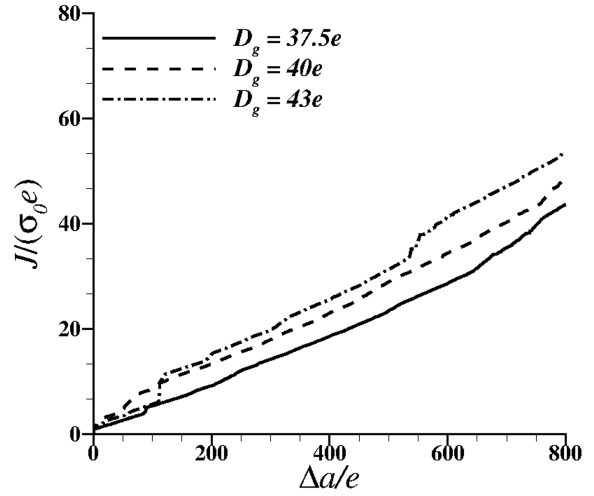


Fig. 3. Comparison of normalized  $J$ ,  $J/(\sigma_0 e)$ , versus normalized crack extension,  $\Delta a/e$ , curves from full field finite element calculations for three unimodal grain size distributions with average grain sizes,  $D_g = 37.5e$ ,  $D_g = 40e$  and  $D_g = 43e$ .

### 2.4 Intergranular fracture prediction as graph search

The aim is to calculate the crack path and crack growth resistance in a microstructure for which the position, orientation and segment length of each grain boundary is known. To this end, the graph search procedure used here is described in more detail in [2, 4]. With each grain boundary junction taken to be a node on a graph, all crack growth trajectories through the microstructure are obtained using a breadth-first search algorithm [26]. The crack growth resistance curve for a given crack path through the grain boundary network is obtained from a similar graph built in  $J$ -resistance space using the unit event crack growth resistance data in Fig. 2. Once constructed, the graph contains information regarding the crack growth resistance for every possible crack path in a given microstructure. The path of least resistance for a specified amount of crack growth can then be found using Dijkstra's algorithm [27]. Dijkstra's algorithm is a graph search algorithm that produces the minimal distance between two nodes. The distances in this case are the increments in  $J$  for a crack traversing between two nodes. The current unit event based graph search model does not account for the crack branching that can sometimes occur.

## 3 Numerical results

Here, results for the crack path and the crack growth resistance predicted using both the microstructure-based finite element calculations and the unit event based graph search model are presented. For the model based on discrete unit events and graph search the crack growth resistances are shown for three crack paths: (i) a path termed 'Local minimum -  $T_R$ ' where at each grain boundary junction the path with the smallest value of  $T_R$  for one of the junction grain boundaries is chosen; (ii) a path termed 'Local minimum -  $\Delta J$ ' where at each grain boundary junction the path with

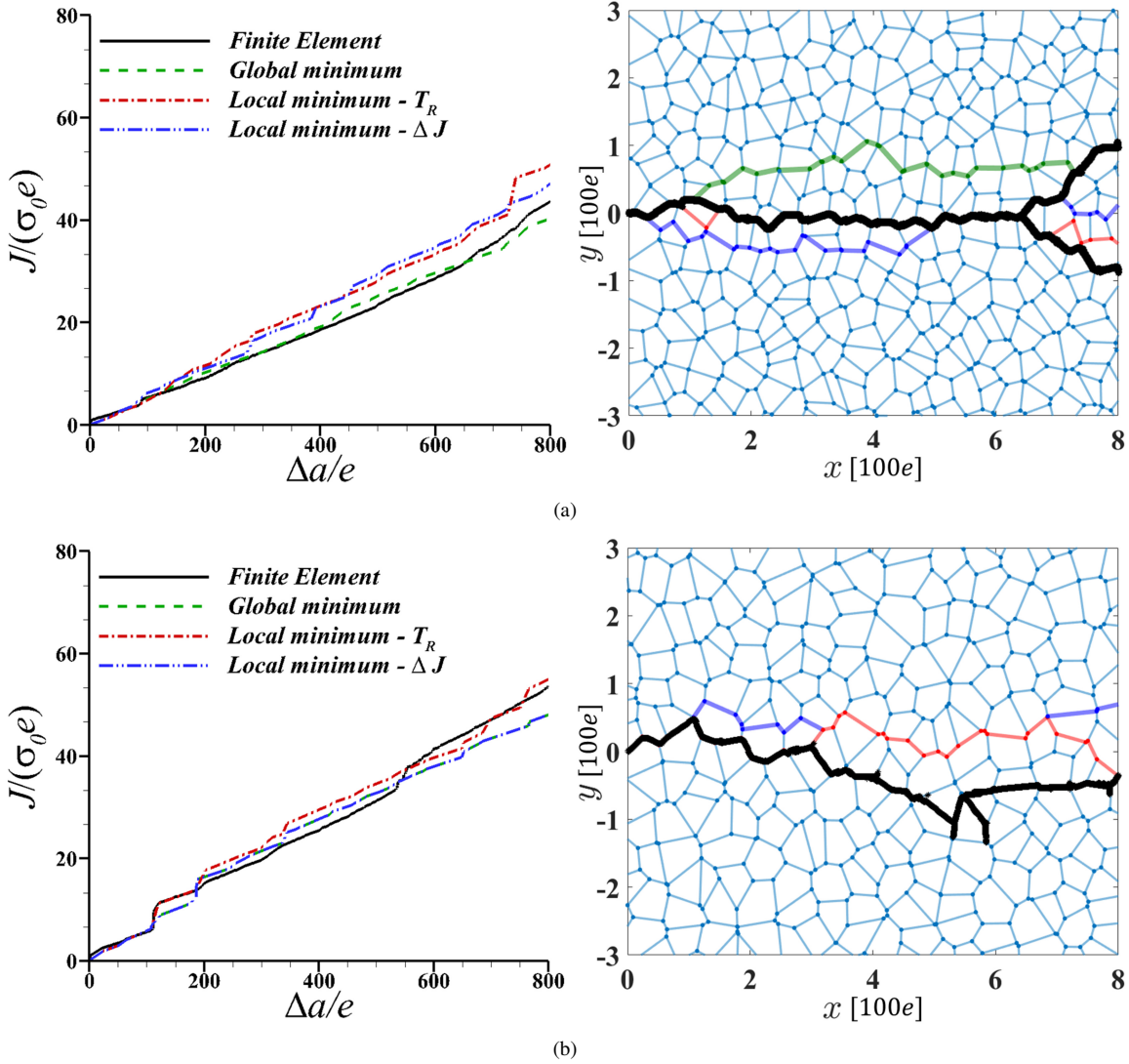


Fig. 4. Comparison of curves of normalized  $J$ ,  $J/(\sigma_0 e)$ , versus normalized crack extension,  $\Delta a/e$  for unimodal grain size distributions. Unit event based graph search model results are shown for the global minimum path; the local minimum path using the  $T_R$  criterion; and the local minimum path using the  $\Delta J$  criterion. Also, the crack path obtained from full field finite element calculations (black) is compared with the crack path obtained using the local minimum- $T_R$  criterion (red), the local minimum- $J$  criterion (blue) and the global crack path (green). Portions of these crack paths overlap. (a)  $D_g = 37.5e$  and (b)  $D_g = 43e$ .

the smallest value of  $\Delta J$  for crack growth over two grain boundary junctions (calculations were also carried out using the ‘Local minimum -  $\Delta J$ ’ criterion for growth over one grain boundary but the resulting crack paths differed little from those obtained using the ‘Local minimum -  $T_R$ ’ criterion so only the results for growth over two grain boundaries are shown); and (iii) a path termed ‘Global minimum’ which is the path with the global minimum crack growth resistance using the ‘Local minimum- $\Delta J$ ’ criterion for all possible crack paths from the initial crack tip location to the end of the fine mesh region. Once the crack path is chosen, the unit event based normalized value of  $\Delta J/\sigma_0 e$  is computed for each increment of normalized crack growth,  $\Delta a/e$ , where  $\Delta a$  is the change in crack length projected onto the  $x$ -axis.

Our modeling aims to isolate the influence of variations

in grain size distribution on the crack growth resistance. We do not account for crystallographic anisotropy or changes in material response that may change with grain size, for example, a layer may have a crystallographic texture and a Hall-Petch effect may lead to different grain sizes having different flow strengths. In our calculations, the grains are isotropic and the flow strength is independent of grain size.

For both the full field finite element calculations and the unit event based graph search model, predicted crack path and crack growth resistance curves are shown for  $\Delta a \leq 800e$  in order to avoid effects arising from the change in element size at the end of the fine mesh region which occurs at  $\Delta a = 1000e$ . In addition, for the calculations here, the main crack path is confined within  $-300e \leq y \leq 300e$  which defines the fine mesh region in the  $y$ -direction.

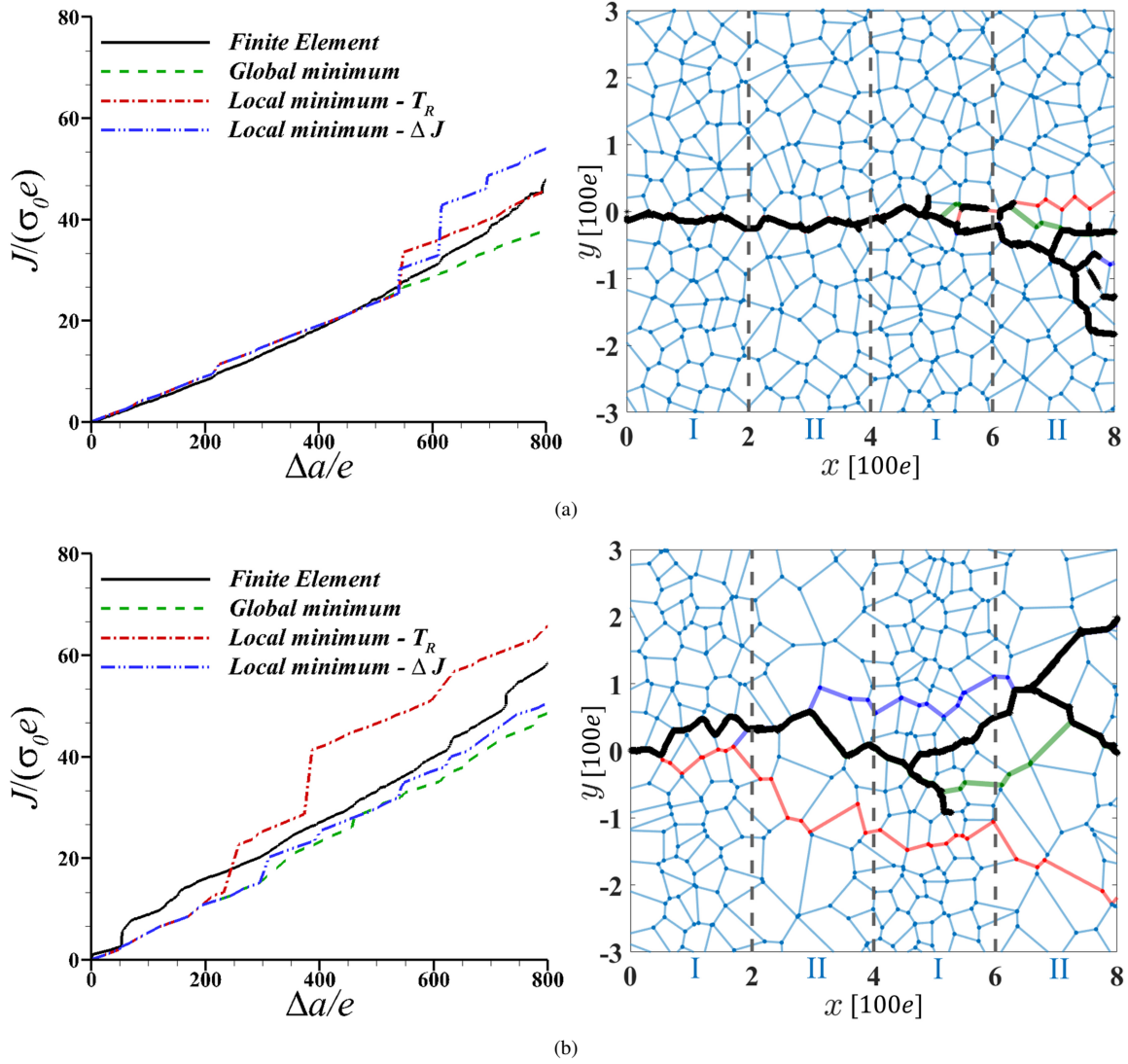


Fig. 6. Comparison of curves of normalized  $J$ ,  $J/(\sigma_0 e)$ , versus normalized crack extension,  $\Delta a/e$  for bimodal grain size distributions with a fixed average grain size in region I and an increased grain size distribution in region II. Unit event based graph search model results are shown for the global minimum path; the local minimum path using the  $T_R$  criterion; and the local minimum path using the  $\Delta J$  criterion. Also, the crack path obtained from full field finite element calculations (black) is compared with the crack path obtained using the local minimum- $T_R$  criterion (red), the local minimum- $J$  criterion (blue) and the global minimum criterion (green). Portions of these crack paths overlap. (a)  $D_g = 37.5e$  in region I and  $D_g = 41.4e$  in region II. (b)  $D_g = 37.5e$  in region I and  $D_g = 58.5e$  in region II.

### 3.1 Effect of grain size

Full field finite element calculations are carried out for three microstructures with unimodal grain size distributions and with values of the average grain size  $D_g = 37.5e$ ,  $D_g = 40e$  and  $D_g = 43e$ . Fig. 3 shows the computed crack growth resistance curves,  $J$  computed from Eq. (2), versus  $\Delta a/e$ . The value of  $J/(\sigma_0 e)$  increases with increasing grain size, varying at  $\Delta a/e = 800$  from 44 for  $D_g = 37.5e$  to 54 for  $D_g = 43e$ , an increase of about 23%.

Fig. 4 compares the full field finite element predictions for crack growth resistance and crack path with those of the simple model based on unit events and graph search. Fig. 4(a) shows the comparisons for  $D_g = 37.5e$  while Fig. 4(b) shows the comparisons for  $D_g = 43e$ . The black

line shows the predictions of the full field finite element analysis. The model predictions of the normalized value of  $J$ ,  $J/(\sigma_0 e)$ , are shown along with three crack paths: (i) the green line is the crack path predicted by the “global minimum” criterion, (ii) the red line is the crack path predicted by the local minimum  $T_R$  criterion and (iii) the blue line is the crack path predicted by the local minimum  $\Delta J$  criterion.

With  $D_g = 37.5e$ , Fig. 4(a), the full field finite element results and the global minimum based unit event model predictions nearly coincide. This is because the full field finite element crack path and that obtained from the global minimum based unit event model nearly coincide except near the end of the region shown,  $\Delta a/e \geq 650$ , where the full field finite element results show crack branching. However, this

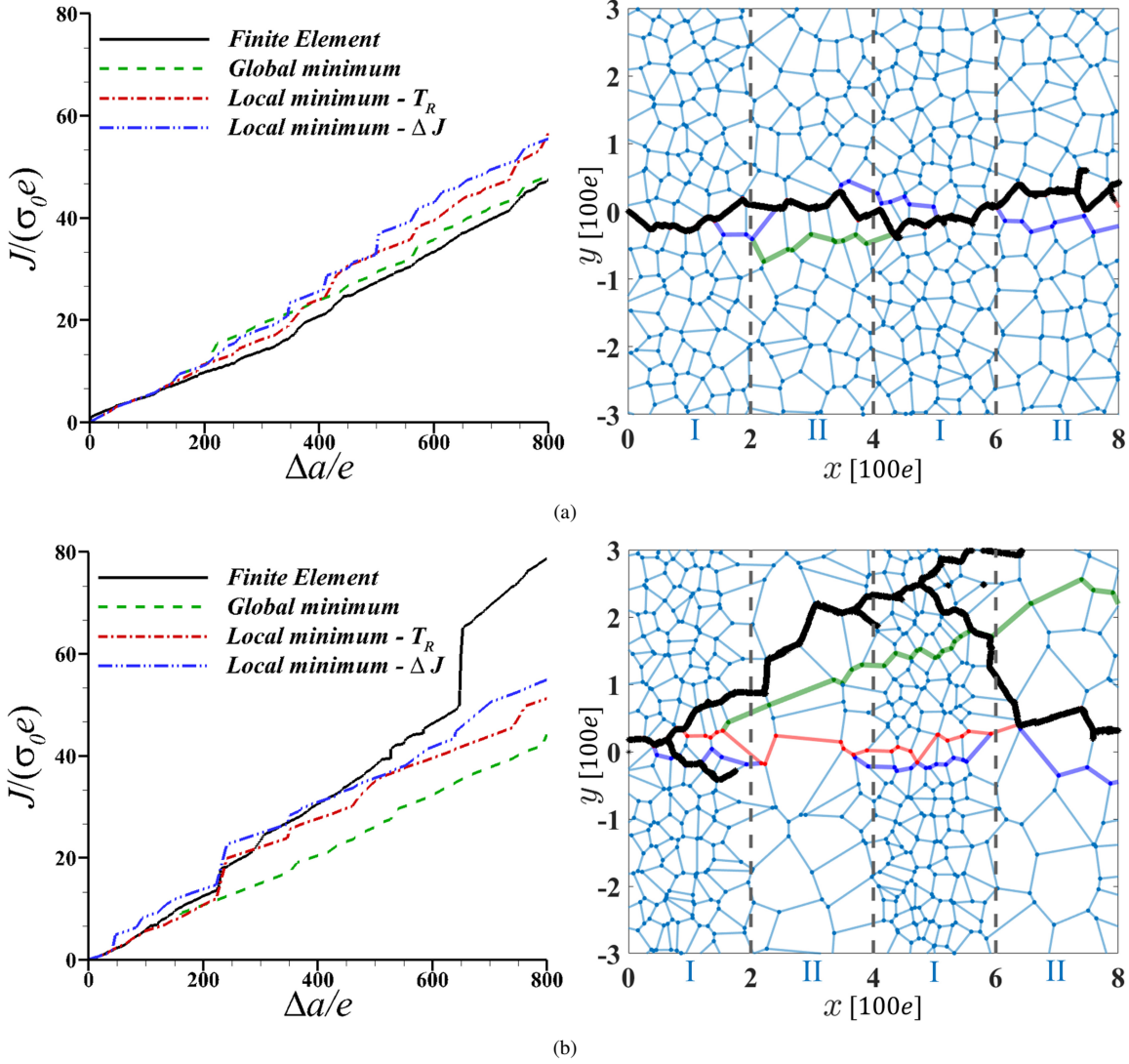


Fig. 8. Comparison of curves of normalized  $J$ ,  $J/(\sigma_0 e)$ , versus normalized crack extension,  $\Delta a/e$ , for bimodal grain size distributions with a decreased grain size in region I and an increased grain size distribution in region II. Unit event based graph search model results are shown for the global minimum path; the local minimum path using the  $T_R$  criterion; and the local minimum path using the  $\Delta J$  criterion. Also, the crack path obtained from full field finite element calculations (black) is compared with the crack path obtained using the local minimum- $T_R$  criterion (red), the local minimum- $J$  criterion (blue) and the global minimum criterion (green). Portions of these crack paths overlap. (a)  $D_g = 34.6e$  in region I and  $D_g = 41.4e$  in region II. (b)  $D_g = 29.8e$  in region I and  $D_g = 58.5e$  in region II.

only leads to a small difference in the crack growth resistance. At  $\Delta a/e = 800$ ,  $J/(\sigma_0 e)$  is 43 for the full field finite element calculation and 40 for the global minimum based unit event model crack path. The crack path obtained using the local minimum  $T_R$  criterion and the crack path obtained using the local minimum  $\Delta J$  criterion give increased values of  $J/(\sigma_0 e)$ . For example, at  $\Delta a/e = 800$ , the local minimum  $\Delta J$  criterion predicts  $J/(\sigma_0 e) = 47$  and that using the local minimum  $T_R$  criterion gives  $J/(\sigma_0 e) = 50$ .

Fig. 4(b) shows corresponding results for  $D_g = 43e$ . In this case, the full field finite element crack path and that obtained from the global minimum based unit event model coincide until  $\Delta a/e \approx 300$  and differ significantly thereafter. The predicted values for the crack growth resistance,

$J/(\sigma_0 e)$ , at  $\Delta a/e = 800$  are 54 for the finite element calculation, 55 for the crack path obtained using the local minimum  $T_R$  criterion and 48 for the crack path obtained using the local minimum  $\Delta J$  criterion.

Fig. 4 shows that which unit event based graph search model gives the best fit to a particular finite element calculation can vary with grain size. Nevertheless, the full field finite element calculations and the unit event based graph search model predictions agree that a change in average grain size from  $D_g = 37.5e$  to  $D_g = 43e$  gives an increase in crack growth resistance. However, it is important to note that the results here are obtained for a single realization of a statistical distribution with a specified mean grain size.

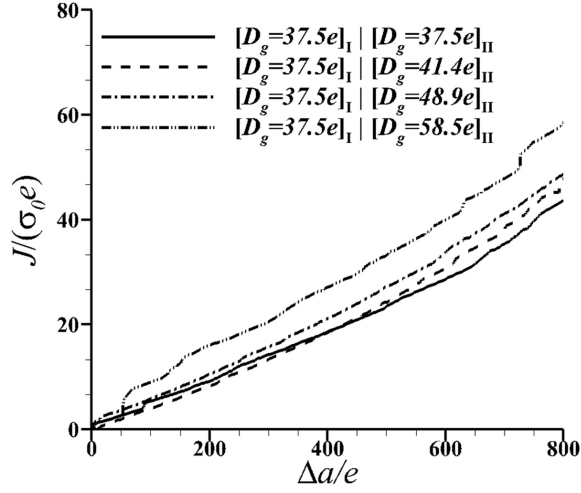


Fig. 5. Comparison of normalized  $J$ ,  $J/(\sigma_0 e)$ , versus normalized crack extension,  $\Delta a/e$ , curves computed from full field finite element calculations for four bimodal grain size distributions with a fixed average grain size in region I and an increased grain size distribution in region II, as shown in Fig.6.

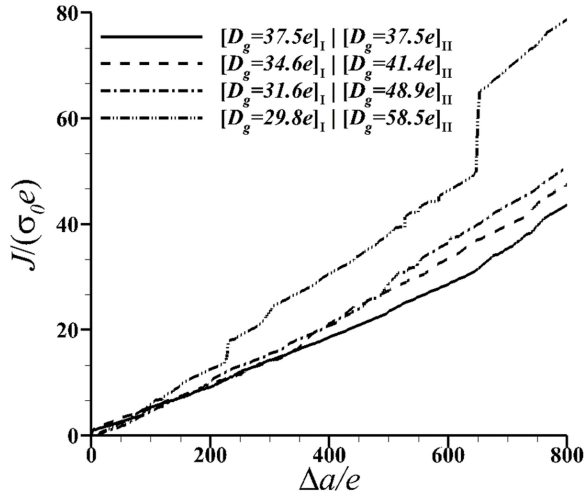


Fig. 7. Comparison of curves of normalized  $J$ ,  $J/(\sigma_0 e)$ , versus normalized crack extension,  $\Delta a/e$ , computed from full field finite element calculations for four bimodal grain size distributions with a decreased grain size in region I and an increased grain size distribution in region II, as shown in Fig.8.

### 3.2 Bimodal grain size distribution - increasing average grain size

Fig. 5 shows full field finite element calculation results for crack growth resistance curves for three bimodal grain size distributions. The grain size in the type I regions have an average grain size of  $37.5e$ . The bimodal grain size distributions have average grain sizes of  $41.4e$ ,  $48.9e$  and  $58.5e$  in the type II regions. For comparison purposes, the results for a uniform grain size of  $37.5e$  are also shown. The crack growth resistance increases with increasing heterogeneity. The value of  $J/(\sigma_0 e)$  at  $\Delta a = 800e$  increases from 44 for the uniform

distribution to 58 for the case where the average grain size in the type II regions is  $58.5e$ , about a 31% increase. By way of contrast, the values  $J/(\sigma_0 e)$  at  $\Delta a = 800e$  show only a relatively small increase for the cases with average grain sizes of  $41.4e$  and  $48.9e$  in the type II regions being  $J/(\sigma_0 e) = 48$  and  $J/(\sigma_0 e) = 49$ , respectively.

The crack growth resistance curves and the crack paths for the cases with an average grain size of  $37.5e$  in the type I regions and average grain sizes of  $41.4e$  and  $58.5e$  in the type II regions are shown in Fig. 6. In Fig. 6(a), where average grain size in the type II regions is  $41.4e$ , the full field finite element predictions and all three predictions obtained from the unit event based graph search models are in close agreement until  $\Delta a/e \approx 600$ , the beginning of the second type II region. The predicted crack growth resistance curves then begin to differ considerably. In this case the finite element predictions most closely agree with the simple model results obtained using local minimum  $T_R$  criterion. At  $\Delta a/e = 800$ , the value of  $J/(\sigma_0 e)$  obtained using the global minimum criterion is about 38 while the local minimum  $\Delta J$  criterion is 54. The full field finite element calculations give  $J/(\sigma_0 e) = 47$  while the simple model based on local minimum  $T_R$  criterion predicts 46.

In Fig. 6(a), the predicted crack path using all the unit event based graph search model are in good agreement with the full field finite element results until  $\Delta a/e \approx 550$  at which point the simple model prediction using local minimum  $T_R$  criterion predicts a rather abrupt increase in  $J/(\sigma_0 e)$ . The associated predicted crack path (red curve) obtained using the local minimum  $T_R$  criterion follows a small grain boundary segment that results in a very small change in  $\Delta a$  whereas the full field finite element calculation leads to short micro-cracks along that path while the main crack follows another path. The value of  $J/(\sigma_0 e)$  predicted using the local minimum  $\Delta J$  criterion gives a smaller increase at this point. This difference is probably associated with the ‘Local minimum -  $T_R$ ’ crack path being based on one grain boundary segment whereas the ‘Local minimum -  $\Delta J$ ’ is based on two grain boundary segments.

Fig. 6(b) shows the results for a case where the average grain size in the type I regions is  $37.5e$ , same as in Fig. 6(a), but the average grain size in type II regions is  $58.5e$ . The  $J/(\sigma_0 e)$  versus  $\Delta a$  curve obtained from the full field finite element calculation shows increases in  $J/(\sigma_0 e)$  associated with crack branching. The simple model prediction using local minimum  $T_R$  criterion also shows fairly abrupt increase in  $J/(\sigma_0 e)$  correlated with the boundaries of the first type II region which are not seen in the full field finite element result. In the finite element results, having a larger grain size in the type II regions leads to more extended branched cracks which increases the crack growth resistance.

In Fig. 6(a) the unit event based graph search model using the local minimum  $\Delta J$  criterion significantly over predicts the crack growth resistance. On the other hand, in Fig. 6(b) the simple model using local minimum  $T_R$  criterion significantly over predicts the crack growth resistance, whereas the unit event model using the local minimum  $\Delta J$  criterion under predicts the crack growth resistance and is

close to the prediction of the global minimum criterion. Also, for certain type I region/type II region interfaces a local minimum criterion predicts a more abrupt increase in  $J/(\sigma_0 e)$  than obtained in the full field finite element calculation.

### 3.3 Bimodal grain size distribution - fixed average grain size

Results of three full field finite element calculations for bimodal grain size distributions where the average grain size is fixed at  $37.5e$  are shown in Fig. 7. In the type I regions, the values of average grain size are  $D_g = 34.6e$ ,  $D_g = 31.6e$  and  $D_g = 29.8e$ . The corresponding grain sizes in the type II regions are  $D_g = 41.4e$ ,  $D_g = 48.9e$  and  $D_g = 58.5e$ , respectively. For comparison purposes, the crack growth resistance curve for a uniform grain size distribution with  $D_g = 37.5e$  is also shown.

Increasing the difference in grain size between the regions can significantly increase the crack growth resistance. With the bimodal distribution  $[D_g = 34.6e]_I$ ,  $[D_g = 41.4e]_{II}$  the value of  $J/(\sigma_0 e)$  at  $\Delta a/e = 800$  is 47. The corresponding value of  $J/(\sigma_0 e)$  with  $[D_g = 31.6e]_I$ ,  $[D_g = 48.9e]_{II}$  is 51 and with  $[D_g = 29.8e]_I$ ,  $[D_g = 58.5e]_{II}$  is 79. For comparison, with a uniform grain size  $D_g = 37.5e$ ,  $J/(\sigma_0 e) = 44$  at  $\Delta a/e = 800$ .

The value of  $J/(\sigma_0 e) = 79$  at  $\Delta a/e = 800$  with  $[D_g = 29.8e]_I$ ,  $[D_g = 58.5e]_{II}$  may be a numerical artifact since (as seen in Fig. 8) the path of one of the crack branches at  $\Delta a/e \approx 600$  reaches the upper,  $y = 300e$ , boundary of the fine mesh region. Nevertheless, even discounting this large jump, the crack growth resistance curve for  $[D_g = 29.8e]_I$ ,  $[D_g = 58.5e]_{II}$  shows that a large grain size difference in a bimodal grain size distribution can significantly increase the crack growth resistance. For example, at  $\Delta a/e = 500$ ,  $J/(\sigma_0 e) = 24$  for a uniform grain size of  $D_g = 37.5e$ , while  $J/(\sigma_0 e) = 38$  for the bimodal distribution with  $[D_g = 29.8e]_I$ ,  $[D_g = 58.5e]_{II}$ , which is about a 58% increase.

Fig. 8 shows comparisons between full field finite element calculations and unit event based graph search model predictions for  $[D_g = 34.6e]_I$ ,  $[D_g = 41.4e]_{II}$ , Fig. 8(a), and for  $[D_g = 29.8e]_I$ ,  $[D_g = 58.5e]_{II}$ , Fig. 8(b). In Fig. 8(a), the full field finite element crack path and the simple model based on global minimum criterion crack path nearly coincide as do the crack growth resistance curves. On the other hand in Fig. 8(b) the full field finite element crack path exhibits branching and associated with each branch is a jump in  $J/(\sigma_0 e)$ . As a consequence, none of the crack path predicted using the unit event based graph search model coincide with the finite element predictions. As noted previously, one of the branches impinges on the fine mesh region boundary  $y = 300e$  at  $\Delta a/e \approx 650$  which probably accounts for the very large jump in  $J/(\sigma_0 e)$  at this value of  $\Delta a/e$ .

The full field finite element results for a bimodal layered microstructure in Figs. 5 and 7 show that if the difference in grain size is sufficiently large, a significant increase in crack growth resistance for materials that fail by grain boundary crack growth can be achieved. Furthermore, the crack paths

in Figs. 6 and 8 show that a bimodal layered grain size distribution enhances the crack growth resistance by altering the crack path near the interfaces and by crack branching. These results indicate that by arranging the grains with different average grain sizes in layers is advantageous for materials that undergo grain boundary fracture, as seen experimentally for other materials and other fracture mechanisms, e.g. [14–16].

## 4 Concluding remarks

We have carried out analyses of ductile intergranular crack growth with the aim of isolating the influence of variations in grain size distribution on crack growth resistance. Analyses were carried out for three grain size distributions; (i) a unimodal distribution; (ii) a bimodal layered distribution consisting of alternate layers with the grain size in one layer type held fixed and with an increased grain size in the other layer type; and (iii) a bimodal layered distribution consisting of alternate layers with a decreased grain size in one layer type and an increased grain size in the other layer type. In (ii) the overall average grain size increases while in (iii) the overall average grain size is fixed.

Our results show that for both unimodal and bimodal grain size distributions, the crack growth resistance increases with increasing overall average grain size. For the bimodal distribution where the overall average grain size is fixed, the crack growth resistance increases with an increasing difference between the average grain size in the two layer types. Hence, a combination of layered smaller grain size regions that have a lower crack growth resistance together with larger grain size regions that have greater crack growth resistance can lead to a material with greater crack growth resistance than a uniform microstructure with large grains. It is worth noting that a wide variety of natural materials rely on a structure consisting of alternating regions of reduced and enhanced crack growth resistance to attain superior overall crack growth resistance [28–31].

In [4], for unimodal grain size distributions, in the absence of crack branching, the unit event based graph search model with a local minimum  $\Delta J$  crack path selection criterion gave good quantitative agreement with the full field finite element predictions. In the calculations here, for the unit event based graph search model, all criteria considered are in qualitative agreement with the full field finite element calculations but none of the criteria used with the unit event based graph search model gave a good quantitative agreement with the full field finite element results for all grain microstructures analyzed. One possible reason for this is that the thickness of the grain boundaries here is greater than that in [4], so that finite deformation effects may play a greater role in the full field finite element calculations, leading, for example, to plastic deformations at some crack tips along the path extending over more grains in some distributions than in others. Nevertheless, the global minimum criterion does provide a lower estimate of the crack growth resistance in all cases analyzed.

A grain size distribution that maximizes the dissipation during crack growth can be realized, at least in principle, by

some sort of iterative optimization method. One way to calculate the crack growth resistance through a grain size distribution is to carry out microstructure-based full field finite element calculations. However, such calculations, especially for three dimensional grain distributions, are extremely time consuming. For an iterative optimization scheme what is needed is a computationally efficient procedure that can correctly rank the crack growth resistance of possible grain size distributions. The computationally efficient simple model based on discrete unit events and graph search developed in [4], and used here, holds promise for this purpose. A more generally predictive crack path selection criterion would enhance the utility of the discrete unit event and graph search model for microstructure optimization purposes.

The results in [4] and here indicate that the unit event based graph search model can at least provide a qualitative prediction of the crack growth resistance when crack branching does not occur. However, our full field finite element results show that crack branching can play a significant role in the increased crack growth resistance of the layered grain size microstructures. Incorporating crack branching into the model will increase its predictive capability so that it can become an engineering tool for optimizing material microstructures to enhance crack growth resistance.

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