Application of Multiscale Cohesive Zone Model to Simulate Fracture in Polycrystalline Solids

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Abstract

In this work, we apply the multiscale cohesive method (Zeng and Li [2010]) to simulate fracture and crack propagations in polycrystalline solids. The multiscale cohesive method uses fundamental principles of colloidal physics and micro-mechanics homogenization techniques to link the atomistic binding potential with the mesoscale material properties of the cohesive zone, and hence the method can provide an effective means to describe heterogeneous material properties at small scale by taking into account the effect of inhomogeneities such as grain boundaries, bi-material interfaces, slip lines, and inclusions, etc. In particular, the depletion potential of the cohesive interface is made consistent with the atomistic potential inside the bulk material, and it provides microstructure-based interface potentials in both normal and tangential directions with respect to finite element boundary separations. Voronoi tessellations have been utilized to generate different randomly shaped microstructure in studying the effect of polycrystalline grain morphology. Numerical simulations on crack propagation for various cohesive strengths are presented, and it demonstrates the ability to capture the transition from the inter-granular fracture to the trans-granular fracture. A convergence test is conducted to study the possible size-effect of the method. Finally, a high speed impact example is reported. The example demonstrates the advantages of multiscale cohesive method in simulating the spall fracture under high-speed impact loads.

Key Words: Cohesive zone model, Crack, polycrystalline solid, Fracture, Multiscale analysis

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Submitted to ASME Journal of Engineering Materials and Technology 20 April 2010
1 Introduction

Due to the exponential growth in microelectronic devices and extensive application of ceramics and ceramic composites, the reliability of polycrystalline materials has become a major concern because most of ceramics and metals are in polycrystalline form in which each grain may have different crystallographic orientation, shape, and size. The discrete nature of crystallographic, which refers the distribution of the grain orientations (Bunge [1982]), slip along certain lattice directions on preferred crystallographic planes entails an anisotropic plastic response (Hosford [1996]; Kocks [1997]; Zhou [1998]; Bhattacharyya [2001]). Many theories have been developed at various size scales form homogenized solids to grain level, and even atomistic modeling. There are mainly two classes of models have been developed in past decade (Espinosa [2003a]). The first class of models belongs to continuum damage model (Bazant [1985]; Addessio [1999]; Curran [1990]; Espinosa [1995]), which are based on homogenization of material properties. Although, it is well known that microstructure characteristics such as grain shape, spatial arrangement of grains, and local crystallographic orientation can obviously influence the materials response, most existing macroscopic nonlocal constitutive models lack of rigorous description of the role of lattice orientations of constituent grains, and the effects of crystal morphology on failure process (Clayton [2005]; Lawn [1993]).

An alternative approach is to combine the so-called cohesive finite element method and polycrystalline constitutive modeling. In the past decade, the cohesive finite element method has gained much popularity, e.g. (Xu and Needleman [1994]; Ortiz and Pandolfi [1999]; Wells and Shuys [2001]; Moes and Belytschko [2002]; Espinosa [2003a]; Liu et al. [2008]). Such methods employ a so-called cohesive zone that is embedded along the edge of finite elements, which may mimic surface decohesion by a prescribed empirical traction-displacement relation. By doing so, stress singularity can be avoided. Moreover, the crack initiation or propagation does not rely on any artificial criterion but a natural outcome of simulations.

In most of the cohesive interface element method, the traction-displacement relations are such that with increasing interfacial separation, the traction across the interface reaches a maximum, then decreases and eventually vanishes, permitting a complete decohesion. In principle, an ideal paradigm of cohesive zone model should be the one that is built on an exact mesoscale cohesive potential in the sense that this exact mesoscale cohesive potential is derived from the atomistic potential based on first-principle calculation, if it is all possible. So far, most of these applications are macro-scale material failure analysis, and the traction cohesive laws adopted are empirical traction-displacement relation. However, the empirical cohesive law may reach to its limit of sub-micron scale because small scale plasticity is highly size-dependent.

On the other hand, the multiscale approach has been viewed as the most promising candidate that may ultimately replace the empirical cohesive potential approach. In a recent work (Zeng and Li [2010]), Zeng and Li have proposed and implemented a multiscale
cohesive zone model. They have successfully built a multiscale cohesive zone model to relate the mesoscale interface properties to the atomistic potential, which naturally takes into account material microstructures such as interface lattice orientation and rotation. In this method, there are two coarse graining models: one for the bulk medium and another for the material interfaces, or defects. By constructing a finite width cohesive zone and extending the Cauchy-Born rule to coarse scale deformation field, the multiscale cohesive zone model can simulate the overall behaviors of a non-uniform deformation caused by defects. With the aid of multiscale cohesive zone method, it is much easier and more efficient to study polycrystalline materials in grain level with fully consideration of microstructure characteristics.

2 A Multiscale Cohesive Zone Method

In multiscale cohesive zone method, the global non-uniform deformation field may be represented by a macroscale piece-wise uniform deformation field that consists of the bulk element of uniformed deformation, which are connected together by finite-width cohesive zones with highly non-uniform deformations. Meanwhile, Cauchy-Born rule was proposed to model the effective constitutive properties of the cohesive zone as well as in bulk elements as show in Fig. 1(a). The beauty of such coarse-grain procedure is that the effective deformation field inside the cohesive zone can be uniquely determined by the bulk finite element nodal displacements, and there is no finite element interpolation inside the cohesive zone. The coarse grain model for the cohesive zone is properly connected with the kinematics of bulk elements. Another advantage of the multiscale cohesive zone approach is that it eliminates the discontinuous jump operator approach in description of the displacement field that has been employed in the conventional cohesive finite element method.

![Multiscale cohesive zone model](image)

(a) Triangular bulk element and cohesive zone; (b) Hexagonal lattice used in this paper.

First, the cohesive zone region is assumed to be a quasi-crystalline layer with finite volume or finite thickness $R_0$ although there is no definite lattice structure with atomistic resolution. Indeed, the thickness, $R_0$, can be thought as a physical parameter that is
related to the characteristic length scale of specific defects in consideration. Usually, \( S_0 \times 10^{-3} \leq R_0 \leq S_0 \times 10^{-1} \), and \( S_0 \) is the characteristic length of adjacent bulk elements. By assuming that the cohesive zone is a relatively “soft” interface zone, a so-called *depletion potential* was derived in the interface zone for highly inhomogeneous deformation field inside the cohesive zone. The atomistic potential of the cohesive zone can be obtained by integrating the bulk potential over the rigid bulk medium half space with several assumptions, which the cohesive zone is a compliance interface, and it is much weaker than the adjacent bulk elements, and the intermolecular interaction inside the cohesive zone is a type of the Van der Waals interaction between non-covalent bonds or quasi-covalent bonds. For instance, if the Lennard-Jones potential is chosen as the bulk potential

\[
\phi_{\text{bulk}} = 4\epsilon \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6},
\]

the depletion potential of coarse graining interface can be obtained by analytical integration (Israelachvili [1992]),

\[
\phi_{\text{depl}}(r) = \int_{\text{Half Space}} \beta \phi_{\text{bulk}}(r - r')dV' = \frac{\pi \epsilon}{\sqrt{2}} \left( \frac{1}{45} \left( \frac{r_0}{r} \right)^9 - \frac{1}{3} \left( \frac{r_0}{r} \right)^3 \right),
\]

where \( \epsilon \) is the depth of the potential well, \( \sigma \) is the finite distance at which the bulk atomistic potential is zero, \( r_0 = \sigma^{2/6} \) is the equilibrium bond distance in the bulk material and \( \beta \) is the atomic density. Therefore, the interface depletion potential has close form expressions.

### 2.1 Effective deformation gradient in cohesive zone

To quantitatively deal with the non-uniform deformation inside the finite-width cohesive zone, the non-uniform deformation is assumed to be multiscale in character, i.e. the displacement field inside the cohesive zone may be written as

\[
u = \bar{u} + u',
\]

where \( \bar{u} \) is the coarse scale displacement field, whereas \( u' \) is the fine scale displacement fluctuation field. With homogenization technique, the general deformation field can be represented as

\[
x = \bar{F}X + u',
\]

where \( \bar{F} \) may be viewed as the coarse scale deformation gradient. By using the idea of the Hill-Mandel homogenization (Hill [1972]), it can be proved that the average deformation gradient \( \langle F \rangle_{\Omega_0} \) in a cohesive zone is exactly same as \( \bar{F} \), i.e.

\[
\langle F \rangle_{\Omega_0} = \bar{F}.
\]

In particular, if the coarse scale deformation field inside the cohesive zone is compatible with the uniform deformation field inside the bulk elements, the coarse scale deformation
field can then be represented by an affine function of coordinates. Hence,

$$F^c = \langle F \rangle_{\Omega_0} = \bar{F} := \frac{\partial \bar{x}}{\partial X} |_{X \in \Omega},$$

where the computation of effective deformation gradient $F^c$ inside the cohesive zone can be given as (see Fig. 2):

$$
\begin{bmatrix}
F^c_{11} \\
F^c_{12} \\
F^c_{21} \\
F^c_{22}
\end{bmatrix}
= \frac{1}{(ad - cb)} \begin{bmatrix}
d & 0 & -b & 0 \\
- c & a & 0 & 0 \\
0 & d & 0 & -b \\
0 & -c & a & 0
\end{bmatrix} \begin{bmatrix}
x^+_{\ell+1} - x^-_{\ell} \\
y^+_{\ell+1} - y^-_{\ell} \\
x^+_{\ell} - x^-_{\ell+1} \\
y^+_{\ell} - y^-_{\ell+1}
\end{bmatrix},
$$

where

$$a = X^+_{\ell+1} - X^-_{\ell}, b = Y^+_{\ell+1} - Y^-_{\ell}, c = X^+_{\ell} - X^-_{\ell+1}, d = Y^+_{\ell} - Y^-_{\ell+1}.$$}

2.2 Cauchy-Born rule in effective field

To reduce the computational cost and complexity, the potential energy for a crystalline solid is calculated through the employed lattice model. Taking the hexagonal unit for example (see Fig. 1(b)), and bond vector $R_i$ is the distance vector between the center atom and one of the atoms $i$ located at a vertex of the unit cell. When bulk element deformation is considered as uniform, the deformed bond length is a function of deformation gradient $F_e$ of the element, i.e. $r_i = |r_i| = |F_e \cdot R_i| = r_i(F_e)$. Hence, the strain energy density
inside each bulk element is the function of the deformation gradient as

$$W_e = \frac{1}{\Omega_b^0} \sum_{i=1}^{n_b} \phi(r_i(\mathbf{F}_e)) = W_e(\mathbf{F}_e),$$

(9)

where superscript $b$ indicates bulk element, $\Omega_b^0$ is the volume of the unit cell in the referential configuration, $\phi(r_i)$ is the atomistic potential, $r_i, i = 1, 2, \cdots, n_b$ are the current bond lengths in a unit cell. Consequently, the constitutive relations for the bulk medium can be established. For instance, the second Piola-Kirchhoff stress can be written in the following form:

$$\mathbf{P} = \frac{1}{\Omega_b^0} \sum_{i=1}^{n_b} \partial \phi \frac{\partial \mathbf{r}_i}{\partial r_i} \otimes \mathbf{R}_i,$$

(10)

Although it can be argued to directly apply the Cauchy-Born rule in the cohesive zone because of the highly non-uniform deformation inside it, the average deformation gradient provides a means to apply the Cauchy-Born rule to the mean field of interfacial cohesive zone for simplification. It should be noticed that the using of average deformation gradient in cohesive zone is a comprised but simplified way. For more accurate calculation of non-uniform deformation, high order element such as six-node or nine-node triangle element can be employed. Similar to bulk element, the average of deformed lattice bond vector in each cohesive zone may be calculated as follows:

$$\bar{\mathbf{r}}_i = \mathbf{F}_c \cdot \mathbf{R}_i, \quad i = 1, 2, \cdots, n_c.$$

(11)

Subsequently, the effective 1st Piola-Kirchhoff stress tensor in each cohesive zone can be calculated as

$$\bar{\mathbf{P}} = \frac{\partial W}{\partial \mathbf{F}_c} = \frac{1}{\Omega_c^0} \sum_{i=1}^{n_c} \partial \phi_{\text{depl}} \frac{\partial \mathbf{r}_i}{\partial \bar{r}_i} \otimes \bar{\mathbf{r}}_i,$$

(12)

### 3 Polycrystalline microstructure

Voronoi tessellations have been widely utilized to generate different randomly shaped microstructure in studying the effect of polycrystalline grain morphology (Ghosh [1995]; Bolander [1998]; Liu et. al. [1998]; Espinosa [2003a,b]). In this paper, the test samples are generated by Voronoi diagram too as shown in Fig. 3(a). Therefore, each Voronoi cell represents a grain. Consequently, all edges of cells are considered as the grain boundaries. Then, triangular elements or bulk element are generated over all grains. It can be seen from Fig. 3(b) that the meshes are conforming between grains. For the implementation of cohesive zone method, cohesive zones are constructed on all interfaces among bulk elements.

Meanwhile, to characterize the varying grain morphology, each grain is assigned an individual set of material properties such as lattice orientation and parameters of potential.
In those models used in this paper, each grain is randomly assigned a lattice orientation $\alpha^g$. That means all the bulk elements in one grain have same lattice orientation. And, so do those cohesive zones among them. Here, the superscript $g$ indices granular region, whereas, the superscript $gb$ denotes the zones on grain boundaries. Simultaneously, the lattice orientation of grain boundary zones $\alpha^{gb}$ may be assigned according to various principles and assumptions. For simplicity and demonstration purpose, the lattice orientation of grain boundary zone as shown in Fig. 4 is taken as the average of orientations from the two adjacent grains, i.e. $\alpha^{gb} = \frac{1}{2}(\alpha_A + \alpha_B)$.

The other factor affected by granular structure is the depletion potentials of cohesive zones. Since it is not necessary that the interface zone on grain boundary is always softer than cohesive zones in grain, two hypotheses will be considered in simulations. First, both types of the cohesive zones have same potential well depth, $\epsilon^{\text{depl}}_g = \epsilon^{\text{depl}}_{gb}$. Second, the cohesive strength inside grains are stronger than that of the grain boundary, e.g. $\epsilon^{\text{depl}}_g > \epsilon^{\text{depl}}_{gb}$.
The Galerkin weak formulation of the multiscale cohesive zone model may be expressed as follows,

\[
\sum_{e=1}^{n_{b\text{elem}}} \left\{ \int_{B_0^e} \rho_0 \dot{\varphi}^h : \delta \varphi^h dV + \int_{B_0^e} P(\varphi) : \delta F^h dV \right\} + \sum_{i=1}^{n_{c\text{elem}}} \int_{B_i^c} P : \delta F^c dV \nabla \frac{\partial t}{B_0^e} T_c : \delta \varphi^h dS \right\} + \sum_{i=1}^{n_{c\text{elem}}} \int_{\partial B_i^c} T_{\text{cohe}} : \delta \varphi dS ,
\]

(13)

where \( B \) is the body force, \( B_0^e \) is the e-th element domain, \( \partial_t B_0^e \) is the traction boundary of the element, and \( S_c^e \) is the cohesive boundary of the element.

Integration by parts or divergence theorem yields

\[
\int_{B_c^e} P : \delta F^c dV = \int_{\partial B_c^e / \partial B_0^e} T_c : \delta \varphi dS + \int_{\partial B_i^c} T_{\text{cohe}} : \delta \varphi dS ,
\]

(14)

for each cohesive element. Considering the fact that the boundary of the cohesive element is also the part of the boundary of the bulk element with the opposite out-normal and the fact

\[
\Gamma_t = \bigcup_{e=1}^{n_{b\text{elem}}} \partial_t B_0^e \cup \bigcup_{i=1}^{n_{c\text{elem}}} \partial_t B_i^c.
\]

The final Galerkin weak formulation of the multiscale cohesive zone model becomes

\[
\sum_{e=1}^{n_{b\text{elem}}} \left\{ \int_{B_0^e} \rho_0 \dot{\varphi}^h : \delta \varphi^h dV + \int_{B_0^e} P(\varphi) : \delta F^h dV - \int_{S_c^e} T_{\text{cohe}} : \delta \varphi^h dS \right\} + \sum_{i=1}^{n_{c\text{elem}}} \int_{\partial B_i^c} T_{\text{cohe}} : \delta \varphi dS ,
\]

(15)

where \( S_c^e := \partial B_0^e / \partial_t B_0^e \).

Consider following linear FEM interpolation in each bulk element,

\[
u^h(X) = \sum_{I=1}^{n_{\text{node}}} N_I(X) d_I ,
\]

Following the standard FE discretization procedure, e.g. Hughes [1987], we have the following discrete equations of motion

\[
M \ddot{d} + f^{\text{int}}(d) - f_{\text{cohe}}(d) = f^{\text{ext}} ,
\]

(16)
where

\[ M = \sum_{e=1}^{n_{elem}} \int_{B_e^0} \rho_0 \mathbf{N}^e \mathbf{N}^e dV \]

\[ \mathbf{f}^{int} = \sum_{e=1}^{n_{elem}} \int_{B_e^0} \mathbf{B}^e \mathbf{P}(\mathbf{d}) dV \]

\[ \mathbf{f}^{cohe} = \sum_{e=1}^{n_{elem}} \int_{S_e} \mathbf{N}^e \mathbf{T}^e_{cohe} dS \]

\[ \mathbf{f}^{ext} = \sum_{e=1}^{n_{elem}} \left\{ \int_{B_e^0} \mathbf{N}^e \mathbf{B}^e dV + \int_{\partial B_e^0} \mathbf{N}^e \mathbf{T}^e_{cohe} dS \right\} , \]

where \( A \) is the element assemble operator, \( \mathbf{N}^e \) is the element shape function matrix, \( \mathbf{B}^e \) is the element B-matrix.

The explicit time integration based Newmark-\( \beta \) method with \( \beta = 0 \) (Belytschko [1983]) is used in displacement update,

\[ d_{n+1} = d_n + v_n \Delta t_n + \frac{1}{2} a_n (\Delta t_n)^2 \]

\[ a_{n+1} = M^{-1} (\mathbf{f}^{ext} - \mathbf{f}^{int} + \mathbf{f}^{cohe}) \]

\[ v_{n+1} = v_n + \frac{1}{2} (a_n + a_{n+1}) \Delta t_n , \]

where \( d_n \) is the displacement field at the time step at time step \( n \), \( v_n \) is the velocity field at the time step \( n \), and \( a_n \) is the acceleration field at the time step \( n \). The subscript \( n \) and \( n + 1 \) denote to quantities evaluated at time \( t_n \) and \( t_{n+1} \). After the displacement field is updated, the deformation gradient in each bulk element can be subsequently updated as,

\[ \mathbf{F}^e_n = I + \sum_{i=1}^{n_{node}} \mathbf{B}_i^e \mathbf{d}^e_i \]

and subsequently the stress measures can then be updated too.

Similarly, the effective deformation gradient in each cohesive element can be also updated. For the case of plane strain, it is updated based on the following equations

\[
\begin{bmatrix}
F_{11}^e(t_n) \\
F_{12}^e(t_n) \\
F_{21}^e(t_n) \\
F_{22}^e(t_n)
\end{bmatrix}
= \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} + \frac{1}{LR_0} \begin{bmatrix}
d & -b & 0 & 0 \\
-c & 0 & a & 0 \\
0 & d & 0 & -b \\
0 & -c & 0 & a
\end{bmatrix}
\begin{bmatrix}
u_{I+1}^e(t_n) - u_I^e(t_n) \\
v_{I+1}^e(t_n) - v_I^e(t_n) \\
u_I^e(t_n) - u_{I+1}^e(t_n) \\
v_I^e(t_n) - v_{I+1}^e(t_n)
\end{bmatrix},
\]

where \( (u_I^e(t_n), v_I^e(t_n)) = \mathbf{d}^e_I(t_n) \), and the meaning of the superscripts \( \pm \) is referred to Fig. 2 for their definitions; \( L \) is side length of the adjacent bulk elements, and \( R_0 \) is the thickness of the cohesive element. The constants, \( a, b, c, d \), are defined in Eq. (8) The stress inside the cohesive zone can then be updated by using Eq. (12).
5 Numerical Simulations

5.1 Fracture in polycrystalline material

In this example, the test specimen is a 2D plate with dimension (2 mm × 2 mm) that is subjected to unilateral tension in Y-axis (see Fig. 5(a)). As shown in Fig. 5(b), there are 121 grains and 2,376 bulk elements in this model. Also, a pre-crack is set along several grain boundaries on the left side of the plate. During the calculation, the time step is chosen as \( \Delta t = 1 \times 10^{-10} \) Sec. For the first case, the depletion potentials in both the cohesive zones in grains and the grain boundary have same depth, i.e., \( \epsilon_{g}^{depl} = \epsilon_{gb}^{depl} \). From Fig. 6, it can be seen that crack propagation can go through grains. However, if the cohesive strength in the cohesive zones inside grains are set to be much stronger than that of the grain boundary, e.g., \( \epsilon_{g}^{depl} = 5\epsilon_{gb}^{depl} \), the crack path will only follow grain boundaries as shown in Fig. 7. In addition, some minor cracks can be watched around the main crack surface and tip for the reason of crack bifurcation. Although the grain shape looks uniform in current example, there is no any technical difference or difficulty to apply this method to polycrystalline solids with grains in random shape.

![Fig. 5. Example of unilateral tension: (a) Sketch of unilateral tension model; (b) Mesh of the plate.](image)

5.2 Convergence test

Generally, the results of cohesive method are sensitive to its elements size. To test the effects of mesh size in multiscale cohesive zone method, a unilateral tension test is implemented with four different meshes. And, the test specimen is a 2D plate with dimension (0.02 mm × 0.02 mm), which contains 121 grains. Constant velocity boundary condition is applied on both top and bottom edges. Moreover, the ration \( \rho \) between average element size and average grain size is chosen to define mesh density. Hereby, four cases, which are corresponding to \( \rho = 0.5, 0.2, 0.1, 0.05 \), are employed as shown in Fig. 8. Meanwhile,
Fig. 6. Inter-granular crack propagates through grains: (a) $t=1.5$ $\mu$s; (b) $t=2.5$ $\mu$s; (c) $t=3.5$ $\mu$s; (d) $t=4.5$ $\mu$s.

Fig. 7. Trans-granular crack propagates along grain boundaries: (a) $t=1.5$ $\mu$s; (b) $t=2.5$ $\mu$s; (c) $t=3.5$ $\mu$s; (d) $t=4.5$ $\mu$s.
cohesive strength in the cohesive zones inside grains is set to be stronger than that of
the grain boundary. As result, Fig. 9 shows the crack propagation in specimen. It can be
seen clearly that the crack propagates along same grain boundaries although mesh density
varies so much.

![Fig. 8. Different meshes over grains: (a)Case 1: $\rho = 0.5$; (b)Case 2: $\rho = 0.2$; (c)Case 3: $\rho = 0.1$; (d)Case 4: $\rho = 0.05$.](image)

On the hand, the total reaction forces $r_i^j$ on top edge are calculated in each cases for a
further comparison. As illustrated by Fig.10 that the reaction forces becomes closer as
mesh density increases. For a quantitative comparison, the error between two cases is
defined as

$$Err_i = \int_0^t |r_i^j - r_i^{j-1}| dt, \quad i = 2, 3, 4.$$  \hspace{1cm} (20)

And the errors are listed in Table 1. The error decreases as the element size becomes
smaller.

<table>
<thead>
<tr>
<th>$\rho$</th>
<th>Element size ($\mu$m)</th>
<th>Bulk elements</th>
<th>$Err$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>1</td>
<td>1428</td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>0.5</td>
<td>6041</td>
<td>3.869E-09</td>
</tr>
<tr>
<td>0.1</td>
<td>0.2</td>
<td>18612</td>
<td>1.652E-09</td>
</tr>
<tr>
<td>0.05</td>
<td>0.1</td>
<td>67182</td>
<td>1.627E-09</td>
</tr>
</tbody>
</table>
5.3 Simulations of high-speed impact and spall fracture

To further demonstrate the versatility of the method, numerical simulations have been carried out to simulate high-speed impact induced spall fractures, which is a very difficult problem that has been elusive to many existing numerical methods Antoun et al [2003] . The exact problem statement is described in Fig. 11. The projectile is a rigid block with impact velocity \( v = 200 \text{ m/s} \), the target is a \((1 \text{ mm} \times 2 \text{ mm})\) block with free boundary. In this example, there are totally 861 grains and 4,838 triangular bulk elements in the
target. The lattice orientation settings for both the bulk element as well as the cohesive zone are exactly the same as in the extension example 5.1.

In time integration, the time step is chosen as $\Delta t = 1 \times 10^{-10}$ Sec. Contact problems are characterized by impenetrability conditions that needs to be enforced during computation. We adopted the exact enforcement of the impenetrability condition in a single time step (Hughes [1976]). The wave propagation from the contact point to the opposite boundary has been observed. The phenomena of spall fracture under impacts has been captured as shown in Fig. 12 and 13.

Fig. 11. Example of high speed impact: (a) Sketch of impact model; (b) Mesh of the plate.

Fig. 12. Inter-granular spall fracture propagates through grains: (a) t=1.0 $\mu$s; (b) t=1.2 $\mu$s; (c) t=1.3 $\mu$s; (d) t=1.5$\mu$s.

6 Conclusions

In this work, we have applied the multiscale cohesive zone model to simulate dynamic fracture in polycrystalline solids. A major advantage of the multiscale cohesive zone model over the conventional cohesive finite element method is that it can accurately formulate
interface depletion potential to represent the mesoscale material properties of the interface. Utilizing this advantage, we have demonstrated that one can use the multiscale cohesive zone finite element analysis to model the grain boundary with accuracy and flexibility to such extent that has not been achieved before.

First, the multiscale cohesive zone model can predict both inter-granular and trans-granular fractures and their transitions by adjusting grain boundary lattice orientation and cohesive strength. Second, the method is applied to simulate spall fracture induced by high-speed impact loads without adding any artificial viscousities. The numerical simulations show excellent qualitatively agreement with the experimental observation. A further study on a quantitative comparison in surface velocity as well as in microstructure evolution during the impact is underway, and it will be reported in elsewhere.

We would like to stress that a main difference between the multiscale cohesive zone model and the conventional cohesive finite element method is how to construct interfacial surface cohesive potential. In the conventional cohesive finite element method, the empirical cohesive traction-separation relation is imposed, and the prescribed cohesive traction-separation relation is fixed in the sense that it does not take into account some most important physical characteristics of interfacial fracture, such as interface orientation, its orientation difference with adjacent bulk elements, interface micro-structures, etc. In fact in the conventional cohesive finite element, one always uses one set of interface cohesive laws to model every cohesive zone. It implicitly views the interface cohesive laws being as a universal constitutive relation as the bulk constitutive relations that are frame-indifference and objective. Therefore in conventional cohesive finite element method there is basically no difference between the mixed mode fracture as well as the mode-specific fracture, because the interface cohesive laws remain same — that is the primary reason why we have so many difficulties in practice to match its results with experimental results. Whereas in the multiscale cohesive zone model, the only objective constitutive relation is again the bulk constitutive relation, and the interface constitutive relation is a derivative of the constitutive relation in the bulk cohesive zone, and they change from interface to interface, from stress state (hence loading conditions) from stress state. It is because of
this difference that the multiscale cohesive zone method provides a better, flexible, and efficient means to simulate fractures in polycrystalline solids.

Last, to probe mesh-dependence and mesh-sensitivity of the method, we have conducted a numerical convergence study based on the Cauchy sequence limit criterion. The numerical results suggest that the method is robust enough to produce convergent results.

Acknowledgements

This work is supported by a grant from NSF (Grant No. CMMI-0800744) and a grant from Army Research Office, which are greatly appreciated.

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