Multiscale modeling of dynamic crack propagation

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1. Introduction

Multiscale modeling provides an approach to study local physical phenomena in a large structure with microstructural features. It is worthwhile to mention several different multiscale methods: variational multiscale methods [1], homogenized Dirichlet projection method [2] and domain decomposition methods [3], especially the most recent works by Loehnert and Belytschko [4] and Zhou et al. [5].

In Loehnert and Belytschko’s work, their approach is based on a two-scale decomposition of the displacements and a projection to the coarse scale by using coarse scale test functions which integrates the extended finite element method (XFEM). This method is based on exploiting the separation of scales typical of microscale/macrostructure problems. In their recent work [4], they separate the problem in two parts: a macrostructure model which embodies the overall effects of the microcracks and a microstructure model which models detailed interaction of cracks.

Zhou et al. [5] follow the work of Miller et al. in 1998 [6]. Quasicontinuum (QC) is utilized to simulate a nickel single crystal nano-plate with a mixed-mode crack and the atomic stress field at the crack tip is fitted to the elastoplastic fracture mechanics equations. The QC method is a mixed continuum and atomistic method to significantly reduce the numbers of atoms of which the DOF must be explicitly considered. It was originally developed by Tadmor et al. to study single crystal mechanics in 1996 [7] and later extended by Shenoy et al. to treat polycrystals and poly phase material in 1999 [8]. The complete computation domain is divided by several representative atoms. Those representative atoms will be sorted as two kinds of atoms. One is nonlocal atoms, whose energies are computed by an explicit consideration of all its neighbors and another one is local atoms, which are computed from the local deformation gradient using Cauchy-Born rule [9]. After that, the total energy will be the sum of the energy of local atoms and nonlocal atoms. However due to the atoms in the transient
zone, the total energy should be corrected by a ghost force function. To state the system in equilibrium, it demands the gradient of the potential energy is zero, which implies only static cases are concerned.

In the Quasicontinuum model of Miller et al. in 1998 [6], the fracture toughness is calculated when the remotely applied displacement is strong enough to induce the occurrences of dislocation emission or crack advance. All the boundaries except the crack faces are fixed to the crack tip displacement field of LEFM and thus the mesh is embedded in an infinite plate containing a semi-infinite crack.

Sih and Zuo propose an energy density criterion to model the multiscale behavior of crack initiation and growth in piezoelectric ceramics [10]. The energy density criterion is defined on the length scale. A threshold in energy release quantified by energy density intensity factor can be referred to the fracture toughness in fracture mechanics. The critical ligament at the crack tip should be sufficiently large such that homogeneity could be invoked to smear out the discreteness of the material microstructure while sufficiently large amount of energy packed in the ligament could trigger global instability. It is this global instability that defines the fracture toughness.

In our work, the center-cracked specimen is decomposed into three parts: (1) far field, modeled by linear elastic fracture mechanics (LEFM), (2) near field (cf. Fig. 1), modeled by a multiscale field theory developed by Chen and Lee [11] and analyzed by a generalized finite element method (GFEM) [12], (3) crack tip region, modeled by molecular dynamics. The exact and analytical solution of the far field from LEFM is utilized to specify boundary conditions at the interface between the near field and the far field. Full-blown interatomic forces are employed between the near field and the crack tip region. The detailed discussion is presented in Section 2.

In Section 3, a center-crack problem is solved with the purpose to redefine atomistic fracture toughness and to simulate crack propagation in different fracture modes. Microstructural phenomena such as crack closure and crack propagation from atoms to continuum are witnessed.

2. Approaches in regions of different length scales

We consider the center-cracked specimen can be decomposed into three parts. The first one is the far field governed by the linear elastic fracture mechanics (LEFM). At the crack tip, it is modeled by MD simulation. In between, named as the near field, it is simulated by GFEM [12].

It is worthwhile to mention some of the representative works in LEFM, especially the crack-tip stresses and displacements [13–17]. In this work, we utilize the Sneddon’s solution, i.e., the stress and displacement fields of an infinite plate with a center-crack, in the case of 2D plane stress or plane strain, as (cf. Fig. 2) [17,18]:

![Fig. 1. Finite element mesh for near field and atomic region. Only the tip region of the right half plane is modeled. In the center, it is the crack tip region, which is modeled by MD simulation. Outside the center, it is the near field, which is modeled by the Generalized Finite Element Method. The displacement imposed on the boundary of near field is obtained from the Sneddon’s solution.](image-url)
The displacements along the interface between the near field and the far field will be used as the boundary conditions imposed on the near field. The near field solution can be obtained through GFEM based on the multiscale field theory [11,12], which can be reduced to MD simulation if the finite element size is reduced to the lattice constant. On one hand, it provides the accuracy similar to MD simulation but in a much more computationally effective way. The balance law of linear momentum theory and therefore detailed atomic motion can be observed in the continuum region. On the other hand, it provides to MD simulation if the finite element size is reduced to the lattice constant. On one hand, it is an atom-embedded continuum where the superscript $a$ refers to the $a$th atom in the lattice cell; the terms on the RHD are respectively interatomic force density, body force density, and kinetic part of homogeneous and inhomogeneous stresses due to temperature field. It is

$$
\begin{align*}
\rho \frac{d(v + \Delta v^o)}{dt} &= f^s + \phi^s + \nabla_x \cdot \tau^{\text{kinetic}} + \nabla_y \cdot \tau^{\text{kinetic}},
\end{align*}
$$

where the superscript $x$ refers to the $x$th atom in the lattice cell; the terms on the RHD are respectively interatomic force density, body force density, and kinetic part of homogeneous and inhomogeneous stresses due to temperature field. It is
noticed that temperature is an independent variable in this atom-embedded continuum theory, while, in MD simulation, temperature is computed from the velocity field. In this work, only the interatomic force is considered. Therefore the balance law of linear momentum can be re-written as

$$\rho \dddot{\mathbf{r}}(k, x) = \sum_{l=1}^{n} \sum_{\beta=1}^{n} f(k, x; l, \beta) \quad (k = 1, 2, 3, \ldots, n; \quad x = 1, 2, 3, \ldots, \lambda).$$

(5)

where \( f(k, x; l, \beta) \) is the interatomic force acting on the \( x \)th atom of the \( k \)th unit cell due to \( \beta \)th atom of the \( l \)th unit cell. The inner product of Eq. (5) with virtual displacement \( \delta u(k, x) \) leads to

$$\rho \dddot{\mathbf{r}}(k, x) \cdot \delta u(k, x) = \sum_{l=1}^{n} \sum_{\beta=1}^{n} f(k, x; l, \beta) \cdot \delta u(k, x) \quad (k = 1, 2, 3, \ldots, n; \quad x = 1, 2, 3, \ldots, \lambda).$$

(6)

Suppose we have \( N_e \) finite elements, each with eight Gauss points and we have a weak form of GFEM as [20]

$$\frac{1}{N_e} \sum_{i=1}^{N_e} \sum_{j=1}^{8} \left( J \cdot \mathbf{f}(l_e, g, x) \right) - \frac{1}{2} \sum_{l=1}^{n} \sum_{\beta=1}^{n} \left( \delta u(l_e, g, x) - \delta u(l, \beta) \right) = 0,$$

(7)

where \( J(l_e, g) \) is the Jacobian of the \( g \)th Gauss point of the \( l \)th element; \( f(l_e, g, x; l, \beta) \) is the force density acting on the \( x \)th atom in the unit cell located at the \( g \)th Gauss point of the \( l \)th element due to the interaction with the \( \beta \)th atom of the \( l \)th unit cell.

The crack tip region is modeled by MD simulation:

$$m^j \dddot{\mathbf{r}}^j = \mathbf{F}^j - \sum_{l} \mathbf{F}^j_l,$$

(8-1)

$$U^j = \frac{Z^j Z^j}{r^j} + A^j e^{\frac{r^j}{c^j}} - C^j (r^j)^6,$$

(8-2)

$$F^j = -\frac{\partial U^j}{\partial \mathbf{r}^j} = \left\{ \frac{Z^j Z^j}{(r^j)^2} + \frac{A^j}{B^j r^j} e^{\frac{r^j}{c^j}} + 6C^j (r^j)^5 \right\} [\mathbf{r}^j - \mathbf{r}^j].$$

(8-3)

Eq. (8-1) is Newton 2nd law, which governs all the detailed atomic motion. It is noticed that the interatomic force is derived from the Coulomb–Buckingham potential. Eq. (8-2). Eq. (8-3) gives the interatomic force derivable from the Coulomb–Buckingham Potential. The coefficients used in this work come from the Ball–Grime Model with formal charges (±2e), and are listed in Table 1 in atomic units [21]. Full-blown interatomic forces connect the near field and the crack tip region.

### 3. Different fracture modes and microstructural phenomena

#### 3.1. Introduction to multiscale linear elastic fracture mechanics

The concept of fracture mechanics that were derived prior to 1960 is applicable only to materials that obey Hooke’s Law. Although corrections for small-scale plasticity were proposed as early as 1948, these analyses are restricted to structures whose global behavior is linear elastic. Since 1960, fracture mechanics theories have been developed to account for various types of nonlinear material behavior as well as dynamic effects. All of these more recent results are extensions of LEFM. A material fractures when sufficient stress and work are applied at the atomic level to break the bonds that holds atoms together. Thus a solid background in multiscale modeling is essential to the understanding of more advanced concepts in fracture mechanics.

The crystal materials considered in the work are Magnesia and Barium Titanate, which are rocksalt-type and perovskite-type crystal lattice respectively. Each convention unit cell of Magnesia has eight atoms: four magnesium and four oxygen. The lattice constant of Magnesia is \( c = 7.93684912 \) Bohr. Each primitive unit cell of Barium Titanate has five atoms: one barium, one titanium, and three oxygen. The lattice constant of Barium Titanate is \( c = 7.54567634 \) Bohr. The specimen occupies the space: \(-50c \leq x \leq 50c, \quad 0 \leq y \leq 2c, \quad -70c \leq z \leq 70c\). In this analysis, we use 62500 time steps, \( \Delta t = 40 \) atomic units.

<p>| Table 1 |
|-----------------|-----------------|-----------------|
| Interatomic potential coefficients of MgO in B–G model [21]. |</p>
<table>
<thead>
<tr>
<th>Mg–Mg</th>
<th>Mg–O</th>
<th>O–O</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A^8 )</td>
<td>0</td>
<td>47.2</td>
</tr>
<tr>
<td>( B^8 )</td>
<td>0</td>
<td>0.56635</td>
</tr>
<tr>
<td>( c^8 )</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
units = 9.6756 × 10⁻¹⁶ s. The system is assumed to be at rest after a period of relaxation time (4000 atomic units in time). In this work, Mode I (Opening mode), Mode II (Sliding Mode) and Mixed Mode (Opening ⊕ Sliding Mode) are investigated and the phenomenon of crack propagation is observed. From simulation result, we can define fracture toughness from atomistic perspective.

The mesh of GFEM for the near field and MD simulation region for crack tip region is shown in Fig. 1. The center square region is a MD simulation region where each point is a unit cell. Outside the center square region, there are four ring regions for GFEM where each point is a representative unit cell. The half crack size of this problem is \( a = 10,000 \) Bohrs. Fig. 1 only shows the region around the crack tip. Figs. 3–6 present the atomic motion in crack tip region (MD simulation region) and part of near field (GFEM region).

3.2. Mode I

Mode I (Opening Mode) means only normal stress \( \sigma \) is applied at infinity (cf. Eqs. (2) and (3)). Fig. 3a is the case for Magnesia and Fig. 3b is the case for Barium Titanate.

3.3. Mode II

Mode II (Sliding Mode) means only shear stress \( \tau \) is applied at infinity (cf. Eqs. (2) and (3)). Fig. 4a is the case for Magnesia and Fig. 4b is the case for Barium Titanate.

![Fig. 3. Simulation results of Magnesia (left) and Barium Titanate (right) in Mode I.](image)

![Fig. 4. Simulation results of Magnesia (left) and Barium Titanate (right) in Mode II.](image)
Fig. 5. Simulation results of Magnesia (left) and Barium Titanate (right) in mixed mode. (a) Shows crack closure at the crack tip region.

Fig. 6. Simulation results of crack propagation from atomic region to continuum region. The red line is the interface between the MD simulation region (discrete atoms) and the GFEM region (atom-embedded continuum). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
3.4. Mixed mode

Mixed Mode (Opening $\oplus$ Sliding Mode) means both shear and normal stresses are applied at infinity. Fig. 5a is the case for Magnesia and Fig. 5b is the case for Barium Titanate. It is seen that, in the case of Magnesia (cf. Fig. 5a), the crack closes up in the wake of the advancing crack tip, i.e., crack closure; however in the case of barium oxide (cf. Fig. 5b), crack closure doesn’t occur.

3.5. Crack propagation from atomic region to continuum region

From the simulation results, we can easily observe that the crack propagates from the MD region to the continuum region (cf. Fig. 6) simply because the problem is modeled by an atom-embedded continuum theory. The red line is the interface of the near field and the crack tip. In Fig. 6a, the crack starts to propagate at the 6250th step after relaxation. In Fig. 6b, the crack approaches the interface of the MD region (atoms) and the atom-embedded-theory region (continuum) at the 18,750th step. In Fig. 6c, the crack propagates through the interface into the continuum at the 31,250th step. In Fig. 6d, the crack propagates completely into the continuum region but closes up in the wake of the advancing crack at the 62,500th step.

3.6. Fracture toughness at atomic scale

From the onset of instability of MD simulation at crack tip region, we could easily re-define fracture toughness from atomistic point of view. It is the critical value of stress intensity factor at the onset of instability:

\[
\begin{align*}
\text{Mode I : } & K_I = \sigma_{\text{critical}} \sqrt{\pi a} \\
\text{Mode II : } & K_{II} = \sigma_{\text{critical}} \sqrt{\pi a}.
\end{align*}
\]

The numerical values of $K_I$ and $K_{II}$ are shown in Table 2. As a comparison, the fracture toughness from NIST database are: Magnesia: 1.3–2.0 MPa $\sqrt{m}$ and Barium Titanate: 1.05 MPa $\sqrt{m}$. Those numbers in Table 2 are quite close to the above mentioned experimental data from NIST database [22]. Our study also shows the fracture toughness of Magnesia in Mode II is nearly double that in Mode I. It means Magnesia can stand almost twofold better for shear stress than for normal stress.

4. Conclusion

The most interesting physical phenomena always occur at the crack tip. We should use appropriate theories based on length scales. In the critical crack tip region, MD simulation is utilized. Connecting to the crack tip region with full-blown interatomic forces, an atom-embedded continuum theory with GFEM is used to simulate the near field. In the far field, LEFM is accurate enough and it is connected with the near field through boundary conditions.

On the other hand, when simulating hierarchical material, this atom-embedded continuum theory is also a very powerful platform to bridge from classical continuum to discrete atoms. Take bone remodeling as an example, MD simulation can reveal the most important phenomena in critical region while the atom-embedded theory can bridge the gap between classical continuum and discrete atoms and also maintain the similar accuracy as MD simulation.

In this work, results for various fracture modes are discussed. In classical fracture mechanics, the crack initiation and propagation need special treatment in finite element analysis. However, in this atom-embedded continuum theory, each point represents a unit cell which contains several atoms; therefore the crack initiation and propagation are ready to be observed.

References


