Quasicontinuum simulation of single crystal nano-plate with a mixed-mode crack

Tao Zhou, Xinhua Yang*, Chuanyao Chen

Department of Mechanics, Huazhong University of Science and Technology, Hongshan District, Wuhan, Hubei Province 430074, China

1. Introduction

Computer simulation is a valuable tool for understanding the fundamental physical processes in which a material responds to external loads. At present, there are two classes of approaches that have proven particularly useful: atomistic and continuum simulations. Compared with phenomenological descriptions from continuum simulations, atomistic approaches provide more detailed information about microscopic processes in accordance with high-quality efficient energy functionals, so that mechanisms that control deformation and fracture in materials can be carefully investigated.

Atomistic simulation of fracture has been pursued by a number of researchers. For examples, Zhou et al. (1994) used atomistic calculations to simulate dislocation emission from cracks in a hexagonal lattice model in order to correctly estimate the critical stress intensity factors. Yang et al. (2007) employed molecular dynamics method to simulate unilateral extension processes of a single crystal nano-plate with a void, and investigated influences of structural parameters of a void and its neighboring atom distribution on the effective elastic modulus and atomic stress concentration.

The challenges in atomistic simulation come both from the huge computational power and storage required, as well as from the need to make sense of the vast quantities of information. Although advances in computer design and algorithms have made possible the simulation of ever larger systems, even the most ambitious atomic simulations using empirical potentials can only deal with systems of sizes of about 10^9 atoms. Due to limitations on the length and time scales, it is very difficult to use atomistic calculations for large-scale calculation, such as mechanical behaviors of materials with various kinds of defects like dislocation, fracture and impurity. The multi-scale method combining atomistic and continuum simulations can largely reduce the number of degrees of freedom in systems, and has recently received much attention. Gumbsch and Beltz (1995) analyzed fracture or dislocation nucleation for several crack orientations in a nickel crystal using a hybrid atomistic-finite-element model which divided the problem into two distinct zones, one which is fully atomistic and the other which is modeled using conventional finite element method. Kadowaki and Liu (2004) proposed a bridging multi-scale method for the analysis of a class of localization problems in which the micropolar-continuum model is used to describe the localized deformation and the dynamic failure occurs only in a small number of localized regions, and applied it to one-dimensional and two-dimensional dynamic shear localization problems. Guo and Gao (2006) studied the size-dependent behavior of atomistic simulation for brittle fracture in bcc-iron by the combined continuum-atomistic method, and gave displacement distribution at the crack tip.

The quasicontinuum (QC) method is a mixed continuum and atomistic method which significantly reduces the number of atoms whose degrees of freedom must be explicitly considered. It was originally introduced by Tadmor et al. (1996) to study single crystal mechanics and later extended by Shenoy et al. (1999) to treat polycrystals and polyphase materials. The representative atoms are used as the computational points in regions in which deformations changed slowly. Finite element mesh is formed based on these atoms, while positions of other atoms are obtained from the displacements of representative atoms by interpolation functions. Meanwhile, the atom-scale method is adopted around the defects where the deformation gradient is great. This adaptive method reduces degrees of freedom greatly, simplifies the calculation of atomistic potential energy, and appropriately describes...
material defects at the atomic scale. Miller et al. (1998) used this method to study the deformation at the tip of a mode I crack in a single crystal nickel, and computed the critical stress intensity factors and J-integral for Griffith fracture, which is consistent with Griffith theory. Hai and Tadmor (2003) used it to carry out simulations of deformation twinning occurring at aluminum crack tips under a variety of loading modes, and found that deformation twinning is in agreement with experimental observation for certain combinations of loading mode and orientation. Park et al. (2006) presented a coarse-graining computation for deformations of carbon nanotubes via QC, particularly targeting analysis of carbon nanotubes. Their computing scheme enables one to differentiate the fully atomistic zone from the coarse-grained zone in the framework of the multi-scale computation.

Up to now, however, no simulation using the mixed atomistic and continuum method for fracture problems of mixed-mode cracks is found in the published literatures. In this paper, the QC method will be used to simulate a nickel single crystal plate with a mixed-mode crack. Our interest is twofold. First, it is to observe the atomic scale deformation mechanisms which occur at the mixed-mode crack tip. Second, it is to evaluate critical quantities associated with the deformation and fracture process of the material on the atomic scale. The atomic stress fields ahead of the crack tip will be analyzed and compared with the predictions of linear elastic solutions at first, the critical condition for crack-opening or slipping subsequently discussed, and finally the slip direction determined by comparing the shear stresses in four possible slip directions.

2. Basic method

The QC method used here is a mixed continuum and atomistic method. Its basic idea is that in a crystal undergoing mechanical deformation, the majority of the lattice experiences a slowly varying deformation on the atomic scale which is well characterized by the continuum approximation, but in the vicinity of defects discrete atomic effects generally become important. In general, the QC method includes the following four main procedures (Tadmor et al., 1996; Shenoy et al., 1999).

2.1. Atomic description

As a reference configuration, a purely crystallographic description is adopted here. The body is assumed to be made up of a great number of atoms. The reference position of each atom can be determined by the representative atom and Bravais lattice vectors as

\[ \mathbf{X}_i(l) = \sum_{j=1}^{3} l_j \mathbf{B}_j^i + \mathbf{R}_i \]  

where \( l_j = (l_1, l_2, l_3) \), \( \mathbf{B}_j^i \) is the \( j \)th Bravais lattice vector associated with the \( i \)th grain, and \( \mathbf{R}_i \) is the position vector of a reference atom, which is taken to be the origin for the atoms in the \( i \)th grain.

Coincident with the nodes of a finite-element mesh, the deformed position of the \( i \)th atom may be obtained by interpolation from

\[ \mathbf{x}_i = \sum_{z=1}^{R} N_z(\mathbf{X}_i) \mathbf{x}_z \]  

where \( R \) is the number of the representative atoms, and \( N_z \) and \( \mathbf{x}_z \) are the finite-element shape function and the position of the representative atom \( z \), respectively.

Once all the atomic positions are obtained, the total energy of the body can be given in terms of the interpolated atomic sites from the standpoint of a strictly atomistic perspective. The assumption is made that the total energy of the collection of atoms can be expressed as a sum of the energies associated with each atom, namely

\[ E_{\text{tot}} = \sum_{i=1}^{N} E_i \]  

where \( N \) is the total number of atoms, \( E_i \) is the well-defined atomic site energy of the \( i \)th atom and calculated from the embedded atom potential (Daw and Baskes, 1983) as the following:

\[ E_i = \frac{1}{2} \sum_{j} \phi(r_{ij}) + F(r_i) \]

in which \( \phi(r_{ij}) \) is a pairwise potential, \( r_{ij} = |\mathbf{x}_i - \mathbf{x}_j| \) is the distance between atoms \( i \) and \( j \), \( F(r_i) \) is the embedding energy, and \( \rho_i = \sum_j \phi(r_{ij}) \) is the electron cloud density at the site of atom \( i \). The details of the potential function and the energy function can be found in Daw and Baskes (1984) and Foiles et al. (1986).

The potential function of the system under consideration is defined as

\[ \Pi = E_{\text{tot}} - \sum_{i=1}^{N} \mathbf{f}_i \cdot \mathbf{u}_i \]

where \( \mathbf{u}_i \) is the displacement of the \( i \)th atom, and \( \mathbf{f}_i \) is the external force acting on the \( i \)th atom.

2.2. Representative atoms

The QC method formulates approximation strategies that preserve the essential details of the problem while reducing degrees of freedom. A subset of \( R \) atoms (\( R \ll N \)) are selected from the system of \( N \) atoms as representative atoms. Details about the representative atoms can be found in Shenoy et al. (1999). The displacements of the representative atoms are considered as the relevant degrees of freedom of the system, and the reduced total energy is given by summing only over the representative atoms with weights as

\[ \Pi = \sum_{z=1}^{R} n_z E_z(\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_R) - \sum_{z=1}^{R} n_z f_z \cdot \mathbf{u}_z \]

where \( n_z \) is the number of atoms represented by representative atom \( z \) and satisfies \( N = \sum_{z=1}^{R} n_z \).

In the approximation method, the formulations are not completely compatible, so that non-physical forces, namely so-called the ghost force, arise on atoms in transition zones between different regions. Ghost forces do not come from a potential and as a result they are not symmetrical. In order to avoid the ghost forces, the forces acting on atoms in the transition zones have to be corrected. Because of it, the total energy is modified as

\[ \Pi = \sum_{z=1}^{R} n_z E_z(\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_R) - \sum_{z=1}^{R} n_z f_z \cdot \mathbf{u}_z - \sum_{z=1}^{R} f_z^c \cdot \mathbf{u}_z \]

where \( f_z^c \) is the ghost force acting on atom \( i \).

2.3. Local and nonlocal atoms

It is noticed that there generally are two kind of atoms in the body under consideration, called atoms A and B. Atom A lies near defects, and the deformation fields are changing rapidly in the region around it, so that its neighboring atoms experience completely different environments. Atom B is further away from defects, and the neighbors experience environments nearly identical to that of atom B.
The QC method requires an explicit list of neighboring atoms to compute each of the representative atoms, and proves to be very time-consuming. A more efficient method is to divide the representative atoms into two classes: (a) nonlocal atoms, whose energies are computed by an explicit consideration of all its neighbors, and (b) local atoms, whose energies are computed from the local deformation gradients using Cauchy–Born rule (Ericksen, 1984).

After that, the total energy of the system can be written as

$$\Pi = \sum_{i=1}^{N_L} n_i E_i^{loc} (F_1, F_2, \ldots, F_M) \sim \sum_{i=1}^{N_L} E_i (u_1, u_2, \ldots, u_N) \sim \sum_{j=1}^{N} f_j^{\text{loc}} (u_j)$$

where \(E_i^{loc}\) is the energy of local atom \(i\), and \(M\) and \(F\) are the number of elements and the local deformation gradient of element \(i\) associated with local atom \(x\). \(E_i\) is the energy of the nonlocal atom \(x\). \(N_L\) and \(N_{NL}\) are the total numbers of local and nonlocal atoms, respectively, and \(R = R_L + R_{NL}\).

2.4. Energy minimization

The principle of minimum potential energy states that a system is at equilibrium when its potential energy is minimum. It demands that the gradient of the potential energy is zero, namely

$$\frac{\partial \Pi}{\partial u_j} = 0$$

Displacements of atoms are achieved by iteratively solving a series of nonlinear equations and then other results may be obtained.

3. A single crystal nickel plate with a mixed-mode crack

A schematic of the geometry used in the simulation is shown in Fig. 1. A single crystal nickel plate with dimensions of 244.9 nm \(\times\) 274.36 nm \(\times\) 2489 nm is generated in accordance with the ideal geometrical fcc lattice. An inclined center crack with dimensions 149.3 nm \(\times\) 0.704 nm \(\times\) 2489 nm inside the plate is parallel to the crystal directions of [1 1 0], but has an angle of \(\alpha = 54.74^\circ\) with respect to the length direction. The plate is subjected to uniform tensile displacement loads parallel to the width direction at the two ends and the other sides are free. Due to less thickness, the plate is treated as a plane stress problem in the later analysis.

The rectangular coordinate system is employed, and the elastic constants are calculated by the derivative of the energy density to strain, namely

$$C_{ijkl} = \frac{\partial^2 E_{tot}}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} = 0$$

where \(C_{ijkl}\) is the elastic constant component.

4. Computational results and analyses

4.1. Singularity of atomic stresses near the crack-tip

A single crystal is generally anisotropic. For a finite-thicknessed infinite anisotropic sharp crack loaded in a mixed-mode, stress fields near the crack tip can be expressed from elastoplastic fracture mechanics (Sih and Chen, 1981; Hoenig, 1982) as

$$\sigma_r = \frac{1}{\sqrt{2\pi r}} \text{Re} \left\{ -\frac{1}{\mu_1 - \mu_2} \left[ \frac{\mu_2^2 (\mu_2 K_1 - K_0)}{\cos \theta + \mu_2 \sin \theta} + \frac{\mu_1^2 (\mu_1 K_1 + K_0)}{\cos \theta + \mu_1 \sin \theta} \right] \right\}$$

$$\sigma_\theta = \frac{1}{\sqrt{2\pi r}} \text{Re} \left\{ -\frac{1}{\mu_1 - \mu_2} \left[ -\mu_1 K_1 - K_0 \frac{\cos \theta + \mu_1 \sin \theta}{\cos \theta + \mu_2 \sin \theta} + \mu_2 K_1 + K_0 \frac{\cos \theta + \mu_2 \sin \theta}{\cos \theta + \mu_1 \sin \theta} \right] \right\}$$

$$\tau_{\rho\theta} = -\frac{1}{\sqrt{2\pi r}} \text{Re} \left\{ -\frac{1}{\mu_1 - \mu_2} \left[ \mu_1 (-\mu_2 K_1 - K_0) \frac{\cos \theta + \mu_1 \sin \theta}{\cos \theta + \mu_2 \sin \theta} + \mu_2 (\mu_1 K_1 + K_0) \frac{\cos \theta + \mu_2 \sin \theta}{\cos \theta + \mu_1 \sin \theta} \right] \right\}$$

where \(K_1\) and \(K_0\) are the stress intensity factors for modes I and II, respectively, \(r\) is the distance of the observed point from the crack tip, and the line linking the observed point and the crack-tip point is inclined at angle \(\theta\) with respect to the crack prolongation direction, as shown in Fig. 1, and \(\mu_1\) and \(\mu_2\) are two of the roots of the following eigen-equation:

$$|C_{ijkl} + \mu(C_{ikl2} + C_{jkl1}) + \mu^2 C_{ikl2}| = 0$$

where \(C_{ijkl}\) is the elastic constant component.

Eq. (10) shows that stress fields ahead of the crack tip on the macroscale have singularity of the \(1/\sqrt{r}\) form. A question is if the crack-tip atomic stress fields in the single crystal nano-plate shown in Fig. 1 have also analogous singularity to Eq. (12).

In the region far away from the crack tip, the atomic stresses are computed by multiplying strains and the atomic elastic constants which are calculated by the derivative of the energy density to strain, namely

$$c_{ijkl} = \frac{1}{V_{tot}} \frac{\partial^2 E_{tot}}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

where \(c_{ijkl}\) is the strain and \(V_{tot}\) is the total volume of plate, respectively. But near the crack tip the atomic stresses are directly computed according to the following equation (Yang et al., 2007):

$$\sigma_i^{\text{loc}} = \frac{1}{R_i} \left( -m \varepsilon_i^{\text{loc}} \varepsilon_i^{\text{loc}} + \frac{1}{2} \sum_{j=1}^{N} \left[ \phi_j (\varepsilon_j) + (F (\rho_j) + F (\rho_j) \Phi (\varepsilon_j)) \right] R_i^{\Phi (\varepsilon_j)} \right)$$

Fig. 1. A single crystal nickel plate model with a mixed-mode crack.
where $\sigma_{ij}$ is the component of the atomic stress tensor of atom $i$, $\Omega_i$ is the Voronoi volume at site $i$, $v_i^j$ the $j$th component of the velocity vector of atom $i$, $r_{ij}$ is the $j$th component of the relative position vector between atoms $i$ and $j$, and $r_i$ is its magnitude, respectively. The remaining quantities are as previously defined for the embedded-atom method (Daw and Baskes, 1983).

The calculation of atomic-level stresses according to Eqs. (12) and (13) are performed. For the sake of convenience, the atomic stress components in the observed plane $x_1x_2$ are still denoted by $\sigma_{ij}$ and $\tau_{ij}$ in this paper. Their values at different $\theta$ ahead of the crack tip (namely $\theta = 0$) are plotted in Fig. 2 and their variation curves with respect to $r$ are fitted according to Eq. (10) by replacing the stresses with the atomic stresses. It can be seen that the fitting variation curves are in good agreement with the computational values of the atomic stresses, and $K_I$ and $K_{II}$ are 0.3006 MPa m$^{1/2}$ and 0.3905 MPa m$^{1/2}$, respectively. Accordingly, it can be said that the atomic stress fields around the crack tip are singular and have the same form of $1/\sqrt{r}$ as macrostress fields in linear elastic fracture. Similar to elastoplastic fracture mechanics, $K_I$ and $K_{II}$ can also be regarded as the atomic stress intensity factors controlling the atomic stress fields neighboring the crack tip at nano-scale. Analogous atomic stress curves were also given by Miller et al. (1998), after analyzing semi-infinite mode I cracks in single crystal nickel.

### 4.2. Brittle or ductile fracture

The energy release rates are further computed to predict crack propagation for brittle fracture or dislocation emission for ductile fracture. The energy release rate $G_r$ for brittle fracture is first computed as 1.256 N/m based on the Griffith theory when the crack propagates. And then the critical energy release rate for the ductile fracture is computed by the Rice model (Rice, 1992).

The model supposes that the cracked solid is loaded to induce a general set of intensity factors $K_I$, $K_{II}$ and $K_{III}$ at the crack tip. According to the linear elastic solution, the in-plane shear stress components acting on the slip plane, shown in Fig. 3, are

$$\sigma_{i0} = \frac{|K_{Ii}(\theta) + K_{IIi}(\theta)|}{\sqrt{2 \pi r}}$$

where, for an anisotropic case

$$f_i(\theta) = \text{Re} \left[ \frac{1}{\mu_1 - \mu_2} \left( \frac{\mu_1 \mu_2}{\sqrt{\cos \theta + \mu_1 \sin \theta}} - \frac{\mu_1 \mu_2}{\sqrt{\cos \theta + \mu_2 \sin \theta}} \right) \right]$$

$$f_{IIi}(\theta) = \text{Re} \left[ \frac{1}{\mu_1 - \mu_2} \left( \frac{\mu_1}{\sqrt{\cos \theta + \mu_1 \sin \theta}} - \frac{\mu_2}{\sqrt{\cos \theta + \mu_2 \sin \theta}} \right) \right]$$

The form of the results motivates notion of the effective mode II intensity factor along the slip plane at angle $\theta$, who is defined as

$$K_{IIe}^\text{eff} = K_{Ii}(\theta) + K_{IIi}(\theta)$$

The basic nucleation condition for a complete dislocation becomes, for the anisotropic case, approximately when $\theta \neq 0$

$$K_{IIe}^\text{eff} = K_{Ic}^\text{eff} = \sqrt{\frac{2 \mu}{1 - \nu} \gamma_{\text{us}}}$$

where $K_{IIe}^\text{eff}$ is the critical value of effective mode II intensity factor, $\mu$ is the shear modulus in the slip directions, $\nu$ is the Poisson ratio, and $\gamma_{\text{us}} = 1.139$ N/m is the unstable stacking energy which is calculated by Eq. (73) in Rice (1992). The shear modulus in different directions are calculated from the atomic elastic constants and the Poisson ratio is treated as 0.33 following Miller et al. (1998).

Accordingly, the critical energy release rate for the ductile fracture is expressed as

$$G_d = \left( K_{Ic}^\text{eff} \right)^2 \frac{a_{11}}{\sqrt{2}} \left[ \frac{a_{22}}{a_{11}} \right]^{1/2} + \frac{2a_{12} + a_{66}}{2a_{11}} \right]^{1/2}$$

where $a_{ij}$ ($i, j = 1, 2, 6$) is the elastic flexible component of the model and the critical energy release rate depends on the angle $\theta$ through the critical effective intensity factor $K_{Ic}^\text{eff}$. The minimum of $G_a$ is calculated as 0.9354 N/m for all possible values of $\theta$ and takes place in $\theta = 54.7^\circ$, 125.3$^\circ$, 234.7$^\circ$, and 305.3$^\circ$. It is noticed that $G_a$ is bigger than the minimum of $G_a$, which reveals that ductile fracture will occur at first in the example under consideration.

### 4.3. Slip orientation at the crack-tip

The critical energy release rate for the ductile fracture $G_d$ is minimum at $\theta = 54.7^\circ$, 125.3$^\circ$, 234.7$^\circ$, and 305.3$^\circ$, so that they can be regarded as four possible slip directions. But which angle is the final slip orientation?

Owing to the same resistance to slipping at every possible direction, the atomic shear stress can be considered as a criterion which determines the slip direction. The atomic stresses near the crack tip are computed according to Eq. (13). The shear stresses in the four possible slip directions, namely $\theta = 54.7^\circ$, 125.3$^\circ$, 234.7$^\circ$, and 305.3$^\circ$, are plotted in Fig. 4. For comparison, the elastic $1/\sqrt{r}$ curve is also presented in the figure. From the figure, it is found that the $1/\sqrt{r}$ dependence of the shear stress hold for different values of $\theta$, and its absolute value at $\theta = 234.7^\circ$ is bigger than the others, so it can be concluded that slip will occur in this direction at first. The coincidence is that the predicted slip direction is just perpendicular to the loading axis. This seems very counter intuitive, because it is usually given that the stresses are higher ahead of
the crack than to the sides. The simulation to mode I cracks in single crystals by Miller et al. (1998) made sure that, the intuition is right for a brittle orientation, but for ductile fracture, two Shockley dislocations emit normal to the crack plane.

Fig. 5 gives four pictures from the QC simulation of ductile fracture: (a) the equilibrium status before loading; (b) the deformation near the crack tip in the loading process; (c) further deformation before slipping; and (d) slip phenomena taking place at the tip of crack. For the convenience to observation, the pictures are rotated $54.74^\circ$ so that the crack looks horizontal. It is obvious from Fig. 5(d) that slip occurs approximately at $\theta = 234.7^\circ$. Fig. 6 plots an atomic picture with a slip plane as the contours, which agrees with the result concluded from Fig. 4.

5. Conclusions

The complex fracture behaviors of a single crystal with a mixed-mode crack are analyzed by the QC method, the critical energy release rates for brittle and ductile fracture are computed and compared, and the slip direction is determined. The following conclusions are concluded from the numerical analysis at the atomic scale: (1) the atomic stress fields around the crack tip have still singularity of the $1/\sqrt{r}$ form; (2) crack propagation or dislocation emission can be theoretically predicted by comparing the energy release rates for two types of fracture; and (3) slip occurs at first in the direction where the smallest energy release rate for ductile fracture and the biggest shear stress lie.

Fig. 4. Curves of the atomic shear stresses versus $r$ at four possible slip directions.

Fig. 5. Pictures from the QC simulation of ductile fracture.
Acknowledgments

This work is supported by Programs for New Century Excellent Talents in University (NCET-06-0645) and for Distinguished Young Scholars of Hubei Province (2007ABB010).

Appendix A

The atomic elastic constants are calculated by Eq. (12) and expressed as a matrix, having the unit of GPa.

\[
\begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{21} & C_{22} & C_{23} & 0 & 0 & 0 \\
C_{31} & C_{32} & C_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{66}
\end{bmatrix}
\]

\[
= \begin{bmatrix}
321.5 & 154.3 & 66.15 & 0 & 0 & 0 \\
154.3 & 233.3 & 154.3 & 0 & 0 & 0 \\
66.15 & 154.3 & 321.5 & 0 & 0 & 0 \\
0 & 0 & 0 & 127.8 & 0 & 0 \\
0 & 0 & 0 & 0 & 39.50 & 0 \\
0 & 0 & 0 & 0 & 0 & 127.8
\end{bmatrix}
\]

The subscripts of the atomic elastic constants here are related to those of the atomic elastic constant tensor in Eq. (12) by

\[
\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \end{bmatrix} = \begin{bmatrix} 11 & 22 & 33 & 23 & 31 & 12 \end{bmatrix}.
\]

The corresponding atomic elastic flexible constants can be calculated by \([a] = [c]^{-1}\).

References


