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Temperature-related Cauchy–Born rule for multiscale modeling of crystalline solids

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Abstract

In this study, we develop a temperature-related Cauchy–Born (TCB) rule for multiscale modeling of crystalline solids based on the assumptions that deformation is locally homogeneous and atoms have the same local vibration mode. When employing the TCB rule in the nanoscale continuum approximation, the first Piola–Kirchhoff stress can be explicitly computed as the first derivative of the Helmholtz free energy density to the deformation gradient. Since the Helmholtz free energy is temperature-dependent, multiscale methods consisting of the TCB rule embedded continuum model can be used to elucidate temperature-related physical phenomena at the nanoscale. Stress analyses of canonical ensembles verify the continuum approximation with the TCB rule by comparing the calculated Cauchy stresses with the outcomes of molecular dynamics simulations. As an application of the TCB rule in multiscale modeling, the nanoscale meshfree particle method with the TCB rule demonstrates the same crack propagation phenomenon in a nanoplate as molecular dynamics. This example shows that the temperature effects are significant on the crack propagation speed when the temperature is in a particular range.

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1. Introduction

Although molecular systems with billions of atoms [1,2] can be modeled using molecular dynamics (MD) with current high-performance computing techniques, limitations of MD are always found on both length and time scales. These limitations prevent us from studying certain phenomena such as material failure. With the development of nanotechnology, multiscale methods have been of interest as a potential alternative for MD since they are feasible for simulating large nanoscale systems. Efficient multiscale methods are expected to cover a range of physical domains of different length scales from atomic to microscopic/mesoscopic to macroscopic scales.

One type of multiscale methods is hierarchical multiscale modeling, such as the quasicontinuum method [3,4], in which continuum methods are used to simulate a large group of atoms. The continuum approximation is based on the properties of a subscale model, such as an MD model. With the other type, concurrent multiscale methods use an appropriate model in different subdomains to treat each length scale simultaneously. One of the pioneering works was done by Abraham et al. [5], who developed a methodology called macro-atomistic-ab initio-dynamics (MAAD). Their method coupled a tight-binding quantum mechanical calculation, molecular dynamics and a finite

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element method together for different subdomains. Some concurrent methods, such as the bridging domain coupling method [6,7], couple a molecular model and a continuum model. Other multiscale methods can be found in [8–10].

In multiscale modeling of crystalline and amorphous solids, the intrinsic properties of the material are sought at the atomic level and embedded in the continuum model according to a homogenization procedure such as the Cauchy–Born (CB) rule [11,12]. It is assumed that the deformations are sufficiently small so that voids or dislocations do not develop in the continuum domain. The conventional CB rule states that the deformation is locally homogeneous, and the atomic-level lattice thereafter follows the deformation given by the macroscopically-imposed deformation gradient. Consequently, an undeformed lattice vector **A** in the reference configuration (with Lagrangian coordinates **X**) can be mapped into a deformed lattice vector **a** in the current configuration (with Eulerian coordinates **x**) by the deformation gradient **F** via $\mathbf{a} = \mathbf{F}\mathbf{A}$ where $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$. For single-layer curved crystalline sheets, the exponential CB rule [13,14] is available so that the deformation gradient can map the tangent space of the undeformed surface to the one of the deformed surface. However, the conventional CB rule assumes that the simulated systems are at zero temperature. Consequently, the nanoscale continuum approximations with the conventional CB rule have difficulties in demonstrating temperature-related physical phenomena at the nanoscale.

In this paper, we will propose a temperature-related Cauchy–Born (TCB) rule which can be implemented in most recently developed multiscale methods. This technique will be described in next section. Several examples will be given in Section 3 to verify the nanoscale continuum approximations embedded with the proposed TCB rule. The problem of crack propagation in a nanoplate will be studied using the nanoscale meshfree particle method with the TCB rule in Section 4, followed by the conclusions and discussion.

2. Temperature-related Cauchy–Born rule

Generally, in a nanoscale continuum model with the finite element method, the potential energy depends on the elongations and angle changes of the atomic bonds underling the continuum meshes via the conventional CB rule. Therefore, the total potential of the continuum model, also called the strain energy, in the reference configuration Ω_0 is defined by

$$W^{\mathrm{C}} = \int_{\Omega_0} w_C(\mathbf{F})\,\mathrm{d}\Omega_0 \tag{1}$$

where w_C is the strain energy per unit volume. Then, the first Piola–Kirchhoff stress, **P**, can be obtained from the strain energy density via non-linear continuum mechanics [15] by

$$\mathbf{P} = \frac{\partial w_C(\mathbf{F})}{\partial \mathbf{F}} \tag{2}$$

The above equation is usually used as a constitutive relation implemented into continuum models in multiscale modeling of crystalline solids.

It has been shown that physical phenomena at the nanoscale, especially nanostructured material failure, are temperature-related. Therefore, it is important to consider temperature effects in the continuum model when performing multiscale modeling and simulations. Temperature effects can be introduced by employing potentials that incorporate the entropy due to lattice vibration, for example, in a local Einstein description [16,17]. This is conceptually similar to the coarse graining of vibrations in first-principles thermodynamics [18]. In this paper, we propose a temperature-related Cauchy–Born (TCB) rule for the continuum model in multiscale methods. Similar to what were proposed by Shenoy et al. [16] and Diestler et al. [19,20], we consider the Helmholtz free energy, which was called the effective energy in [16,19,20], instead of the potential energy. In their previous research works, Shenoy et al. [16] incorporated a free energy minimization technique into the quasicontinuum method, while Diestler and his co-workers calculated isotropic stresses using the pseudoatomic Hamiltonian. As a difference, we modify Eq. (2) to calculate the continuum-level Piola–Kirchhoff stress for continuum approach to finite-temperature nanosystems so that it can be easily implemented into most multiscale methods.

In this paper, the vibration of an atom in a crystalline solid is assumed to be harmonic. To simplify the harmonic approximation, we neglect all terms that couple vibration of different atoms. Then, the Helmholtz free energy, F_{H}, of a crystalline solid, which contains N atoms at a temperature of T, is given by [21]

$$F_{\mathrm{H}} = \varphi(\mathbf{x}) + \kappa_{\mathrm{B}} T \sum_j \ln\left[2\sinh\left(\frac{\hbar\omega_j}{4\pi\kappa_{\mathrm{B}}T}\right)\right] \tag{3}$$

where $\varphi(\mathbf{x})$ is the potential energy of the atoms in their equilibrium positions, **x**, at a temperature of 0 K; $\hbar$ is Planck's constant; κ_{B} is the Boltzmann constant. The sum over j includes all the non-zero vibrational modes of the system. The frequencies, ω_j, are the eigenvalues of the dynamical matrix

$$D_{I\alpha J\beta} = \frac{1}{\sqrt{m_I m_J}}\left(\frac{\partial^2 \varphi}{\partial x_{I\alpha}\partial x_{J\beta}}\right) \tag{4}$$

where $x_{I\alpha}$ is the vibrational coordinate in direction α for atom I, and m_I is the mass of atom I. When taking a local harmonic model [22], the principal frequencies of atom I can be calculated by diagonalizing the local dynamical matrix. Therefore, Eq. (3) can be simplified to

$$F_{\mathrm{H}} = \varphi(\mathbf{x}) + n\kappa_{\mathrm{B}} T \sum_I^N \ln\left[\left(\frac{\hbar\overline{D}_I^{1/2n}}{2\pi\kappa_{\mathrm{B}}T}\right)\right] \tag{5}$$

where n is the number of degrees of freedom per atom; $\bar{D}_I = \left(\prod_j^n \omega_{Ij}\right)^2$ is the determinant of the local dynamical matrix of atom I.

The TCB rule keeps the assumption of locally homogeneous deformation as in the conventional CB rule. In addition, it is assumed that the atoms have the same local vibration mode at a given temperature. Consequently, the free energy, W_{H}, of the crystalline solid with the continuum model can be expressed as follows:

$$W_{\mathrm{H}}(\mathbf{F},T) = \int_{\Omega_0} w_C(\mathbf{F})\,\mathrm{d}\Omega_0 + n\kappa_{\mathrm{B}}T\sum_i^{N_q} n_i^q \times \ln\left[\frac{\hbar(\overline{D}(\mathbf{F}(\mathbf{X}_i^q)))^{1/2n}}{2\pi\kappa_{\mathrm{B}}T}\right] \tag{6}$$

where N_q is the number of quadrature points in the continuum model in which one quadrature point, X_i^q, represents n_i^q atoms. In the continuum model, the deformation gradient is evaluated at each quadrature point. It should be noted that temperature does not need to be a global constant. The temperature field can be discretized in the continuum model and temperature can also be evaluated at each quadrature point. The continuum-level strain energy density in the first term on the RHS of the above equation can still be calculated via the conventional CB rule, which is compatible with the TCB rule. Then, the first Piola–Kirchhoff stress can be obtained from the first derivative of the free energy density, w_{H}, which is a function of the temperature and the deformation gradient:

$$\mathbf{P}(\mathbf{F},T) = \frac{\partial w_{\mathrm{H}}(\mathbf{F},T)}{\partial \mathbf{F}} \tag{7}$$

The above equation can serve as a temperature-related constitutive relation for the nanoscale continuum modeling of crystalline solids. In other words, the TCB rule can be used to replace the conventional CB rule in multiscale methods so that temperature effects can be considered in order to study temperature-dependent physical phenomena of nanostructured materials.

3. Verifications

To verify the developed TCB rule, we perform stress analyses of a one-dimensional molecule chain and a two-dimensional crystalline solid at any given deformation gradients and temperatures. With the nanoscale continuum approximation and the TCB rule, the first Piola–Kirchhoff stress can be calculated via Eq. (7). Then, the continuum-level Cauchy stress, $\boldsymbol{\sigma}^{\mathrm{C}}$, can be computed via $\boldsymbol{\sigma}^{\mathrm{C}} = J^{-1}\mathbf{F}\cdot\mathbf{P}^T$ where $J = \det(\mathbf{F})$ is the determinant of deformation gradient $\mathbf{F}$ [15]. The calculated continuum-level Cauchy stresses will be compared with the atomic-level Cauchy stresses obtained from molecular dynamics simulations. In molecular dynamics simulations, the periodic boundary condition and the Berendsen thermostat [23] are used, and the simulated systems are canonical ensembles undergoing any given deformations and temperatures. Then, the atomic-level Cauchy stresses [24], $\boldsymbol{\sigma}^{\mathrm{A}}$, of the simulated molecular system with the volume of Ω can be calculated via

$$\boldsymbol{\sigma}^{\mathrm{A}} = \frac{1}{\Omega}\sum_I\left(\frac{1}{2}\sum_{J(\neq I)}\mathbf{r}_{IJ}\otimes\mathbf{f}_{IJ}\right), \quad \mathbf{f}_{IJ} = \frac{\partial\varphi(r_{IJ})}{\partial r_{IJ}}\frac{\mathbf{r}_{IJ}}{r_{IJ}} \tag{8}$$

where $\mathbf{r}_{IJ}(=\mathbf{r}_J - \mathbf{r}_I)$ represents interatomic distance between atoms J and I, and $\otimes$ denotes the tensor product of two vectors. The sign convention adopted here for interatomic forces, $\mathbf{f}_{IJ}$, is positive for attraction and negative for repulsion. Accordingly, a positive stress indicates tension and a negative stress indicates compression. We should note here that the Monte Carlo method could result in the same state of stresses as molecular dynamic simulations for canonical ensembles.

We first consider a one-dimensional molecule chain, which contains 100 atoms, each of which has a mass of 1.993×10^{-26} kg. The following Lennard–Jones 6–12 potential function is employed to describe the interatomic interaction between nearest neighbored atoms

$$\varphi(l) = 4\varepsilon\left[\frac{1}{4}\left(\frac{l_0}{l}\right)^{12} - \frac{1}{2}\left(\frac{l_0}{l}\right)^{6}\right] \tag{9}$$

where $l_0 = 1$ nm is the undeformed bond length, and $\varepsilon = 8.25\times10^{-18}$ J is the depth of the energy well. When this molecular chain is under a deformation gradient of F, the length of the deformed bond is $l = Fl_0$ since the deformation is assumed to be homogeneous. The dynamic matrix for each atom can also be calculated, and they are the same based on the assumption of the TCB rule. A simple formula can be obtained to compute the continuum-level Cauchy stress via Eqs. (6) and (7), and it is

$$\boldsymbol{\sigma}^{\mathrm{C}} = P = \varphi'(l) + \frac{\kappa_{\mathrm{B}}T}{2}\frac{\varphi'''(l)}{\varphi''(l)} \tag{10}$$

Fig. 1 shows the comparison of atomic-level and continuum-level Cauchy stresses with temperatures when a given deformation gradient is applied on the molecule chain.

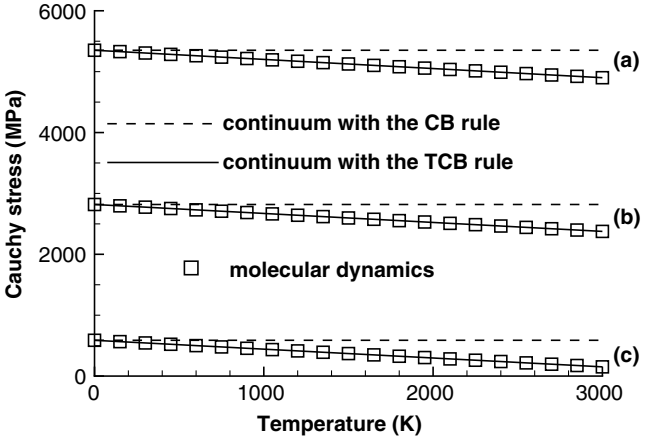

Fig. 1. Comparison of Cauchy stresses of a molecular chain when the deformation gradients are (a) $F = 1.001$, (b) $F = 1.005$ and (c) $F = 1.01$.

Molecular dynamics elucidates that the lower stress is obtained at a higher temperature due to the thermal expansion. However, since the continuum approximation with the conventional CB rule does not include temperature effects, its derived Cauchy stresses are independent of the temperature and become a constant in Fig. 1. When the TCB rule is employed, the Cauchy stresses are temperature-related and are in accord with molecular dynamics results very well.

We then study a plate of two-dimensional Lennard–Jones crystal with a triangular–hexagonal lattice as shown in Fig. 2. This nanoplate contains 1116 atoms, and its length and width are 30 nm. The interatomic Lennard–Jones 6–12 potential and its parameters are the same as in Eq. (9). When the nanoplate undergoes a deformation gradient, $\mathbf{F} = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}$, all the unit cells are assumed to be deformed identically, and all the atoms have the same harmonic vibration mode via the TCB rule. Therefore, the strain energy density at the temperature of 0 K can be calculated from the potential of the unit cell, as well as the dynamic matrix of the atom located in the center of the unit cell. Both of them can be expressed in terms of the given deformation gradient and temperature. Then, the continuum-level Cauchy stress of the nanoplate can be computed.

Fig. 3 shows the comparison of each component of Cauchy stresses with temperature when a small deformation is given. If temperature effects are considered, the continuum-level normal stresses, calculated based on the TCB rule, decrease with the increasing temperature. The results match the molecular dynamics solutions very well. The continuum approximation with the conventional CB rule gives constant normal stresses without the consideration of temperature effects. Since shear stresses are not influenced by temperature, their magnitudes can be obtained from continuum approximations with the conventional CB or TCB rule and supported by molecular dynamics simulations.

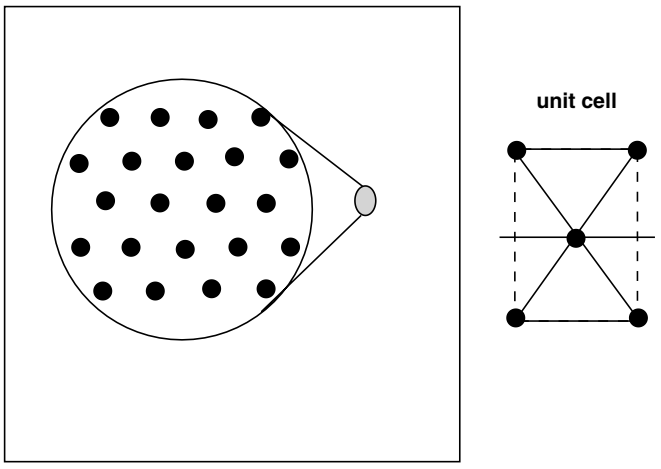

Fig. 2. A two-dimensional Lennard–Jones crystal with a triangular–hexagonal lattice.

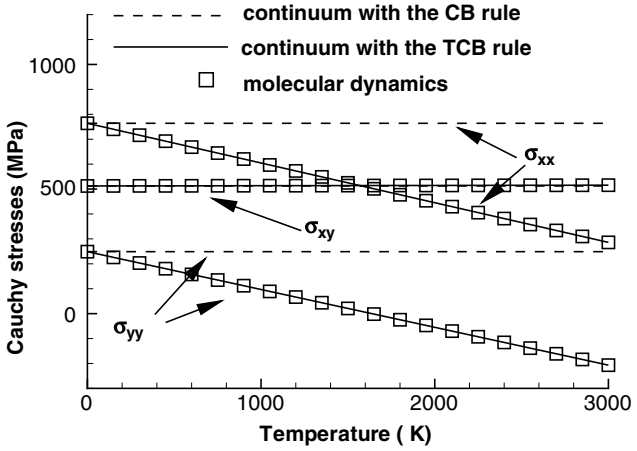

Fig. 3. Comparison of Cauchy stress components with temperature in the two-dimensional Lennard–Jones crystal undergoing the following deformation gradient: $F_{11} = 1.001$, $F_{12} = 0.002$, $F_{21} = 0.0$, $F_{22} = 1.0$.

4. Crack propagation in a nanoplate

As one application of the TCB rule in multiscale modeling of crystalline solids, we use the meshfree particle method with the TCB rule to simulate crack propagation in a nanoplate with the triangular–hexagonal lattice. As shown in Fig. 4, the dimensions of this nanoplate are length 800 nm and width 280 nm, and the nanoplate contains 256,961 atoms with the mass of 1.0×10^{-22} kg. An edge crack is initiated in the middle of the plate by taking out a number of bonds, and the initial crack length is 20 nm. For simplification, the crack is restricted to propagate along the weak interface by assuming that only weakened bonds can be broken. Buehler et al. [25] studied a similar problem and pointed out that a local hyperelastic zone

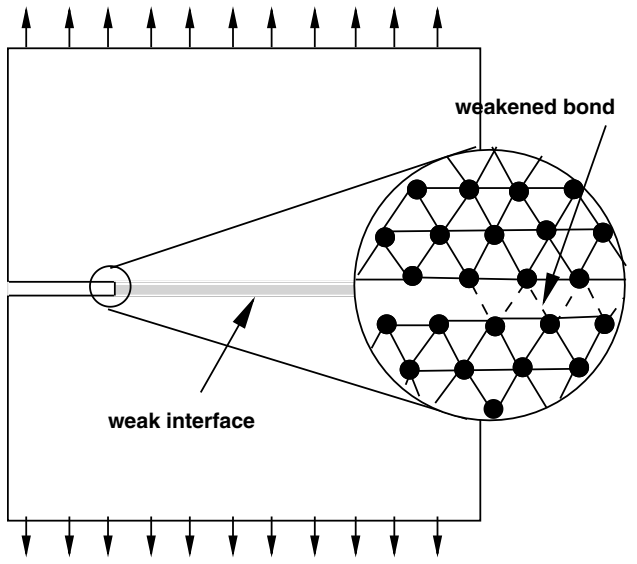

Fig. 4. A nanoplate with the triangular–hexagonal lattice containing an initial edge crack.

around the crack tip can influence the velocity of the crack. They used biharmonic potential functions with various cut-off distances. As a difference, we use a harmonic potential function to describe interatomic interactions between nearest neighboring atoms, except weakened bonds. The harmonic potential function is

$$\varphi_1(r) = \frac{1}{2}k(r - r_0)^2 \tag{11}$$

where the length of undeformed bond is $r_0 = 1$ nm, and the spring constant is $k = 594.0$ N/m. A Lennard–Jones potential with a cut-off distance of 2.0 nm, as described in Eq. (9), is used for weakened bonds. It should be noted here that the tangential stiffness of the weakened bond is equal to the spring constant, k.

We already developed a hierarchical multiscale method by implementing the conventional CB rule into the meshfree particle methods [26]. In this example, the nanoscale meshfree particle method is employed with the implementation of the TCB rule. There are 13,600 particles in the meshfree particle model. The nodal integration scheme is used so that particles are quadrature points. The cohesive model [27] is used in this paper for the weak interface, and the cohesive traction, $\boldsymbol{\tau}$, can be derived as

$$\boldsymbol{\tau} = \frac{\partial \widehat{w}_{\mathrm{H}}(\boldsymbol{\delta}, T)}{\partial \boldsymbol{\delta}}, \quad \boldsymbol{\delta} = \mathbf{u}^+ - \mathbf{u}^- \tag{12}$$

where $\mathbf{u}^+$ and $\mathbf{u}^-$ are displacements of upper and lower facets of the weak interface, i.e., the cohesive zone, respectively. $\widehat{w}_{\mathrm{H}}(\boldsymbol{\delta}, T)$ is the free energy per length along the weak interface and can be calculated similarly to Eq. (6).

In this example, the nanoplate is loaded in mode I via prescribed displacements as shown in Fig. 4. The loaded strain rate is 1×10^{-8} fs^{-1}. We study the effects of temperature on crack speed, and three different temperatures, 100, 300 and 1000 K, are considered. Fig. 5 shows the evolution of crack speeds when the nanoplate is at a given temperature. We can see that cracks start to propagate around 0.3 ns and crack speeds become constants within 0.1 ns. The terminal constant crack speeds are 600, 1100 and 1350 m/s for 100, 300 and 1000 K, respectively. It can be seen that high temperature results in high crack propagation speed. All the calculated crack speeds are lower than the Rayleigh wave speed, although the speed can be 98% of the Rayleigh wave speed when temperature is 1000 K. When considering higher temperatures, such as 2000 K, the crack speed does not increase significantly and is still lower than the Rayleigh wave speed. In this example, our simulations demonstrate that the temperature has significant effects on the crack propagation speed when it is lower than 1000 K. Otherwise, the temperature effects are not significant. As a comparison, we also perform molecular dynamics simulations, and the Berendsen thermostat is used to maintain the nanoplate at a given temperature. Fig. 5 also shows that the same phenomenon can be observed when performing molecular dynamics simulations.

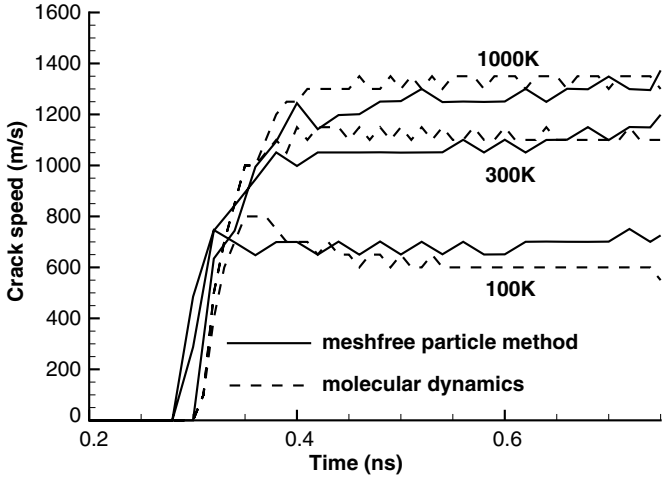

Fig. 5. Comparison of crack propagation speed with different temperatures.

5. Conclusions and discussion

We proposed a TCB rule which can be implemented in nanoscale continuum approximations to study temperature-dependent physical phenomena of crystalline solids. The examples showed that a continuum model with the TCB rule can elucidate similar phenomena as molecular dynamics for canonical ensembles. It should be noted here that continuum approximations with the TCB rule are not restricted to nanosystems with a globally constant temperature, even though all the above examples have such precondition. Since it is assumed that atoms have the same harmonic vibration mode locally in the TCB rule, the free energy can be evaluated at the discretized elements or particles with a locally constant temperature if finite element methods or meshfree particle methods are used, respectively. In these general cases, the energy equation has to be implemented in the continuum model to describe heat transfer behaviour.

It has been known that length scale has significant effects on dynamic fracture. Hierarchical multiscale methods with continuum modeling of fracture may have difficulties in elucidating physical phenomena of dynamic fracture at the nanoscale. For example, the above example cannot demonstrate the supersonic crack velocity which was observed in some molecular dynamics simulations [25]. Therefore, concurrent multiscale methods are of interest since they can provide an appropriate multiple-length-scale model in which molecular dynamics is used to simulate crack propagation while the rest is modeled by continuum mechanics as the elastic media. However, the coupling of the models may introduce some serious difficulties due to large variance in length scales. The development of an efficient failure model for hierarchical multiscale method will stimulate our further research on multiscale modeling and simulations.

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