A Temperature-related Homogenization Technique for Nanoscale Continuum Approximation

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ABSTRACT

A new homogenization technique, the temperature-related Cauchy-Born (TCB) rule, is proposed in this paper with the consideration of the free energy instead of the potential energy. Therefore, temperature effects at the nanoscale can be investigated using continuum approximation with the implementation of the TCB rule. The TCB rule is verified via stress analyses of several crystalline solids. We also implement the TCB rule into the meshfree particle method to investigate crack propagation in a nanoplate.

Keywords: homogenization, temperature, Cauchy-Born; meshfree, free energy

1 INTRODUCTION

Multiscale modeling and simulation of nanostructured materials has been of interest in the area of computational nanotechnology due to the limitations of molecular dynamics. Multiscale methods can be classified into two types: hierarchical multiscale methods and concurrent multiscale methods. Hierarchical multiscale methods employ continuum approximations to approach the nanoscale. Concurrent multiscale methods couple different length scales, and appropriate numerical methods are employed in various scales to perform simulation simultaneously.

Whether hierarchical or concurrent multiscale methods are used for modeling crystalline solids, continuum approximation is conducted through a homogenization technique such as the Cauchy-Born (CB) rule [1]. The CB rule assumes that there are locally homogeneous deformations in the continuum domain so that the constitutive relation is derived from atomic-level potential. Consequently, the homogenization technique provides a link between molecular and continuum models. However, the continuum model is usually assumed to be at a zero temperature. As a result, temperature effects at the nanoscale cannot be investigated via most currently-existed continuum approximation.

In this paper, we propose a new homogenization technique, called the temperature-related Cauchy-Born (TCB) rule, for the continuum model in multiscale methods. Using the work of Shenoy et al. [2] and Diestler et al. [3] as a referent, we consider the Helmholtz free energy, i.e. the effective energy in [2, 3]. Consequently, in the continuum domain the energy contains not only the potential energy due to deformation of molecular structures but also the thermal energy due to vibration of atoms. A stress-strain relation is given in the paper as a generalized constitutive law that can be employed in the continuum model of multiscale methods.

2 TEMPERATURE-RELATED CAUCHY-BORN RULE

Generally, in a nanoscale continuum model, the potential energy depends on the elongations and angle changes of the atomic bonds underlying the discretized continuum domain via the conventional CB rule [1]. The CB rule states that the deformation is locally homogeneous. Therefore, the atomic-level lattice follows the deformation given by the macroscopically imposed deformation gradient. Consequently, the total potential energy, also called the strain energy of the continuum model, in the reference configuration Ω_0 is defined by

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

where w_C is the strain energy per unit volume, and $\mathbf{F}$ is the gradient of deformation. Based on nonlinear continuum mechanics [4], the first Piola-Kirchhoff stress, $\mathbf{P}$, is obtained from the first derivative of the strain energy density to the gradient of deformation

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

The above equation usually serves as a constitutive relation implemented into continuum models in either hierarchical or concurrent multiscale modeling of crystalline solids. However, it is temperature-independent.

In the proposed Temperature-related Cauchy-Born (TCB) rule, we consider the Helmholtz free energy, i.e. the effective energy in [2, 3], rather than the potential energy at the nanoscale. The TCB rule assumes: 1) atoms have locally homogeneous deformation; 2) atoms have the same local vibration modes; 3) the vibration of an atom is harmonic; and 4) coupled vibration of different atoms is negligible. In the continuum model of a crystalline solid

NSTI-Nanotech 2007, www.nsti.org, ISBN 1420061828 Vol. 1, 2007

that contains N atoms at a temperature field of $T(\mathbf{X})$, the total free energy, W_H, is written as

$$W_H(\mathbf{F},T)=\int_\Omega w_C(\mathbf{F})d\Omega+n\kappa_B\int_\Omega \rho_n T\ln\left[\frac{\hbar\left(\overline{D}(\mathbf{F})\right)^{\frac{1}{2n}}}{\kappa_B T}\right]d\Omega$$
$$=\sum_i^{N_q} w_C\left(\mathbf{F}_i^q\right)A_i+n\kappa_B\sum_i^{N_q} n_i^q T_i^q\ln\left[\frac{\hbar\left(\overline{D}\left(\mathbf{F}_i^q\right)\right)^{\frac{1}{2n}}}{\kappa_B T_i^q}\right] \quad (3)$$

where ρ_n is the number of atoms per unit volume; N_q is the number of quadrature points in the continuum model; and A_i is the volume associated with one quadrature point, X_i^q, which represents n_i^q atoms. The first term on the RHS of the above equation is the continuum level strain energy when temperature is equal to zero. In the continuum model, the deformation gradient and the temperature are evaluated at each quadrature point. With the TCB technique, all the bonds and atoms in A_i are assumed to be at the same deformation and the same temperature.

Consequently, the strain energy density, w_C, and the dynamic matrix can be calculated using the unit cell model for each quadrature point. As a difference from other research [2, 3], we modify Eq. (2) to calculate the continuum-level first Piola-Kirchhoff stress for continuum approach to finite-temperature nano systems as follows,

$$\mathbf{P}(\mathbf{F},T)=\frac{\partial w_H(\mathbf{F},T)}{\partial\mathbf{F}} \quad (4)$$

where w_H is the free energy density, and it is a function of the deformation gradient and the temperature. Eq. (4) can serve as a temperature-dependent constitutive relation that can be implemented in most hierarchical and concurrent multiscale methods to investigate temperature-related physical behavior of nanostructured materials

3 VERIFICATION OF THE TCB RULE

To verify the proposed TCB rule, we perform stress analyses of a crystalline solid with two-dimensional triangular lattice at any given deformation gradient and temperature using the continuum approximation with the TCB rule. Then, we compare the continuum-level Cauchy stresses with the atomic-level ones from molecular simulations. It should be noted here that the simulated objects are assumed to be canonical ensembles subject to any given deformation and temperature. The atomic-level Cauchy stresses [5], $\boldsymbol{\sigma}^A$, of the simulated object is calculated via

$$\boldsymbol{\sigma}^A=\frac{1}{V}\sum_I\left(\frac{1}{2}\sum_{J(\neq I)}\mathbf{r}_{IJ}\otimes\mathbf{f}_{IJ}\right),\ \mathbf{f}_{IJ}=\frac{\partial\varphi(r_{IJ})}{\partial r_{IJ}}\frac{\mathbf{r}_{IJ}}{r_{IJ}} \quad (5)$$

where V is the total volume; $\mathbf{r}_{IJ}(=\mathbf{r}_J-\mathbf{r}_I)$ and $\mathbf{f}_{IJ}$ represent the interatomic distance and force between atoms J and I, respectively; $\otimes$ denotes the tensor product of two vectors. The sign convention adopted here for $\mathbf{f}_{IJ}$ that is positive for attraction and negative for repulsion. Accordingly, a positive stress indicates tension and a negative stress indicates compression.

When employing the continuum approximation with the TCB rule, the first Piola-Kirchhoff stress, $\mathbf{P}$, is calculated via Eq. (4) Then, the continuum-level Cauchy stress, $\boldsymbol{\sigma}^C$, is computed [4] as

$$\boldsymbol{\sigma}^C=J^{-1}\mathbf{F}\cdot\mathbf{P}^T,\ J=\det(\mathbf{F}) \quad (6)$$

where J is the determinant of deformation gradient $\mathbf{F}$.

The simulated nanoplate contains 1116 atoms, and its length and width are 30 nm, respectively. Each atom has a mass of $12amu$. We employ the following Lennard-Jones 6-12 potential function to describe the interatomic interaction between nearest neighbored atoms

$$\varphi(l)=4\varepsilon\left[\frac{1}{4}\left(\frac{l_0}{l}\right)^{12}-\frac{1}{2}\left(\frac{l_0}{l}\right)^{6}\right] \quad (7)$$

where l is the deformed bond length, $l_0=1nm$ is the undeformed bond length, and $\varepsilon=8.25aJ$ is the depth of the energy well.

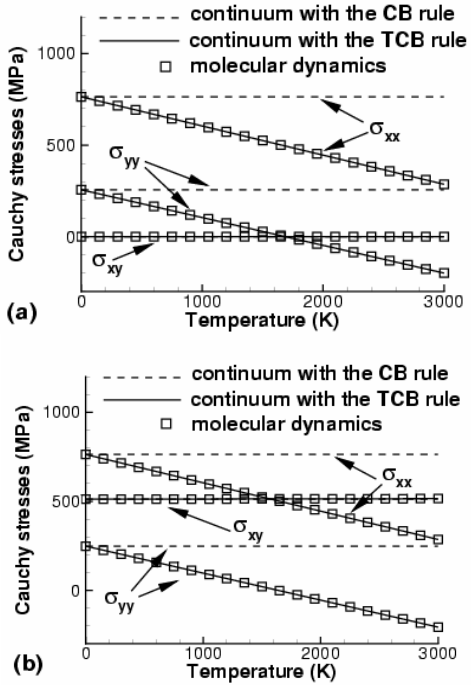

Figure 1. Comparison of Cauchy stress components at various temperatures in a two-dimensional Lennard-Jones crystal subjected to the following deformation gradients: (a) F_{11} = 1.001, F_{12}=F_{21} = 0.0, F_{22} =1.0; and (b) F_{11}=1.001, F_{12} = 0.002, F_{21}=0.0, F_{22}=1.0

Figure 1 shows the comparison of each component of Cauchy stresses at various temperatures when two different deformation gradients are given. We also calculate Cauchy stresses using the continuum model with the conventional CB rule to demonstrate the advantages of the TCB rule. The continuum approximation with the conventional CB rule gives constant stresses at different temperatures since temperature effects are not considered in the CB rule. If temperature effects are considered, the continuum-level normal stresses, calculated based on the TCB rule, decrease with the increasing temperature due to thermal expansion. The results agree with the molecular dynamics solutions. Shear stresses calculated from continuum approximations with either the conventional CB or the TCB rule are supported by molecular dynamics simulation because temperature has no effects on shear stresses.

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 Figure 2, the dimensions of this nanoplate are: length $800nm$ and width $280nm$, and the nanoplate contains 256,961 atoms with the mass of $1.0\times10^{-22}kg$. An edge crack is initiated in the middle of the plate by taking out a number of bonds, and the initial crack length is $20nm$. For simplification, the crack is restricted to propagate along the weak interface by assuming that only weakened bonds can be broken. We use a harmonic potential function to describe interatomic interactions between nearest neighboring atoms, except weakened bonds. A Lennard-Jones potential with a cutoff distance of 2.0nm, as described in Eq. (7), is used for weakened bonds.

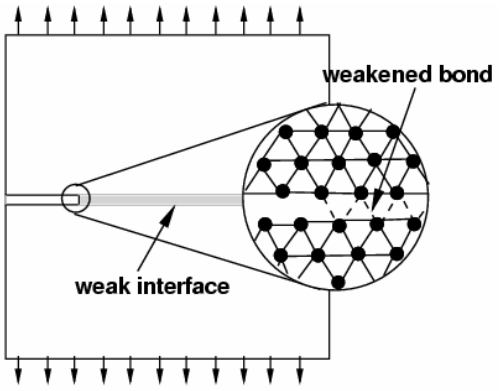

Figure 2. A nanoplate with the triangular-hexagonal lattice containing an initial edge crack.

In this example, the nanoscale meshfree particle method is employed with the implementation of the TCB rule. 13,600 particles are considered in the meshfree particle model. The cohesive model is used in this letter for the weak interface, and the cohesive traction, $\boldsymbol{\tau}$, can be derived as

$$\boldsymbol{\tau}=\frac{\partial\hat{w}_H(\boldsymbol{\delta},T)}{\partial\boldsymbol{\delta}},\ \boldsymbol{\delta}=\mathbf{u}^+-\mathbf{u}^- \tag{8}$$

where $\mathbf{u}^+$ and $\mathbf{u}^-$ are displacements of upper and lower facets of the weak interface, i.e. the cohesive zone, respectively. $w_{eff}(\boldsymbol{\delta},T)$ is the free energy per length along the weak interface and can be calculated similarly to Eq. (3).

In this example, the nanoplate is loaded in mode I via prescribed displacements as shown in Figure 2. The loaded strain rate is 1×10^{-8} per fs. We study the effects of temperature on crack speed, and three different temperatures, 100K, 300K and 1000K, are considered. Figure 3 shows the evolution of crack speeds when the nanoplate is at a given temperature. We can see that cracks start to propagate around 0.3ns and crack speeds become constants within 0.1ns. The terminal constant crack speeds are 600m/s, 1100m/s and 1350m/s for 100K, 300K and 1000K, 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 1000K. When considering higher temperatures, such as 2000K, 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 1000K. 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 globally constant temperature. Figure 3 also shows that the same phenomenon can be observed when performing molecular dynamics simulations.

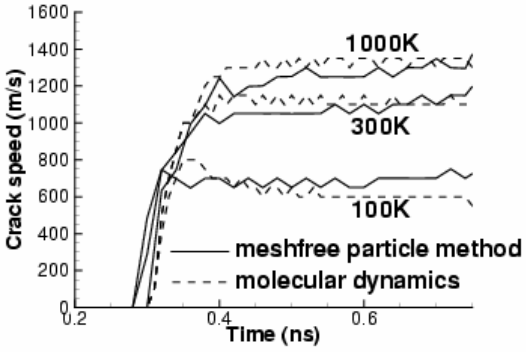

Figure 3. Comparison of crack propagation speed with different temperatures

NSTI-Nanotech 2007, www.nsti.org, ISBN 1420061828 Vol. 1, 2007

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