Temperature-dependent Multi-scale Modeling of Surface Effects on Nano-materials

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Abstract

In this paper, a novel temperature-dependent multi-scale method is developed to investigate the role of temperature on surface effects in the analysis of nano-scale materials. In order to evaluate the temperature effect in the micro-scale (atomic) level, the temperature related Cauchy-Born hypothesis is implemented by employing the Helmholtz free energy, as the energy density of equivalent continua relating to the inter-atomic potential. The multi-scale technique is applied in atomistic level (nano-scale) to exhibit the temperature related characteristics. The first Piola-Kirchhoff stress and tangential stiffness tensor are computed, as the first and second derivatives of the free energy density to the deformation gradient, which are transferred to the macro-scale level. The Lagrangian finite element formulation is incorporated into the heat transfer analysis to develop the thermo-mechanical finite element model, and an intrinsic function is employed to model the surface and temperature effects in macro-scale level. The stress and tangential stiffness tensors are derived at each quadrature point by interpolating the data from nearby representative atom. The Boundary Cauchy-Born (BCB) elements are introduced to capture the surface, edge and corner effects. Finally, the numerical simulation of proposed model together with the direct comparison with fully atomistic model illustrates that the technique provides promising results for facile modeling of boundary effect on thermo-mechanical behavior of metallic nano-scale devices.

Keywords: Temperature-related Cauchy-Born; Hierarchical multi-scale modeling; Surface effects; Molecular dynamics; Nose-Hoover thermostat.

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1. Introduction

Nano-science and nano-technology have been attracted by many researchers in recent years. Nano-technology illustrates the novel properties of material at the atomistic-level, and produces a strong impact on the mechanical behavior of material. One of the most significant mechanisms of nano-scale materials is the surface stress effects, which is due to bonding environment of surface atoms. In general, the surface atoms have less neighboring atoms as compared to the bulk atoms. Thus, the surface atoms attempt to reach the equilibrium inter-atomic distances, which are different from those of the bulk atoms. The surface atoms are basically subjected to extra stresses compared to bulk atoms, called as the surface stresses (Sander 2003). Since the ratio of surface to volume at the nano-scale level becomes much higher than that of the macro-scale level, the importance of surface effect is more considerable at the atomistic level. It has been observed from the material bonding behavior that the surface stress can be happened as a result of the tensile and/or compressive nature, as shown in metals and silicon, respectively (Diao et al. 2003). In this study, the role of temperature on surface effects is investigated in the thermo-mechanical analysis of nano-scale materials.

Numerical simulation as a powerful tool contributes a significant role in nano-science and nano-technology. Although the molecular dynamics is a popular candidate in numerical simulation, it preserves the large time and length scale. The traditional continuum models are unable to capture the size-dependent elastic properties of nano-materials since they do not capture the nano-scale free surface effect, such as surface stresses. Multi-scale methods as a time efficient alternative provide a link between the molecular and continuum domains. The multi-scale methods use the continuum approximation to simulate a large group of molecules based on the properties of the atomistic model, such as the MD model. Various multi-scale techniques have been proposed by researchers, including the quasi-continuum by Shenoy et al. (1999), bridging domain by Xiao and Belytschko (2004) and bridging scale by Liu (2006). These methods are introduced to mitigate the inaccuracy of CB hypothesis wherever the atomic configuration reconfigures to an inhomogeneous structure. In multi-scale techniques, the continuum description is generally used in the region of nearly homogeneous deformation, while the atomistic configuration is applied in inhomogenous deformed regions.

In most multi-scale methods, it is assumed that the system occurs at zero temperature, and hence they are unable to represent the temperature dependent effects, due to deficiency in modeling the temperature effect at nano-scale. Recently, a multi-scale method was proposed by Liu and Li (2007), Sheng and Li (2009) and Li and Sheng (2010) to simulate the coupled, non-equilibrium thermo-mechanical processes. They coupled the multi-scale model with thermo-mechanical equations at the coarse scale, and employed the non-equilibrium molecular dynamics at the fine scale. In their works, each FE node in coarse scale was assumed as a
thermostat, and the atoms associated with each node were assumed to be in a local equilibrium state within one coarse scale time step. The coarse scale was solved by the FE method based on a coarse-grained thermodynamics model; whereas the fine scale was driven by the non-equilibrium molecular dynamics using the random force that is regulated by the inhomogeneous continuum filed through a No̧se–Hoover thermostat. The present study is focused on the development of a temperature-dependent multi-scale technique to capture the temperature influence on the surface stress.

The basis of surface effect is related to the nature of chemical bonding at the surface of structure. Sander (2003) demonstrated that the redistribution of electronic change as a result of the reduced atomic coordination near the surface, changes the binding of atoms. It was presented that the electron density is decreased near the surface edge and corners due to the fact that surface atoms have fewer bonding neighbors than atoms in material bulk. Consequently, as a result of the density difference between the surface and bulk electrons, the inter-atomic distance of external atoms decreases and the electron density increases; hence the interior part implements the stress on exterior boundaries. These surface stresses influence the self-healing behavior in nano-wires and their phase transformation (Diao et al. 2003; Park et al. 2005; Liang et al. 2005). The surface effects have been investigated by various researchers in the form of analytical and numerical models. Gurtin and Murdoch (1975, 1978) proposed a continuum theory for surface stresses in solid problems. Miller and Shenoy (2000) investigated the size dependency of material properties and the effective stiffness properties of a series of nano-structures, such as plates, bars and beams based on the augmented continuum theory. Their model was basically a special case of the general formulation of Gurtin and Murdoch, which indicates the size dependency of the effective stiffness of nano-structures due to the surface effects. The bulk and surface constants were calculated from the empirical atomistic potentials. Shenoy (2005) presented an approach to calculate the surface elastic constants through the atomistic model. Lim and He (2004) proposed a model based on the previous idea in order to capture the nonlinear size-dependent response of thin films with nano-dimen-sional thickness. Although the proposed model involved several advantages, the presence of some deficiencies disturbs the common use of augmented continuum as a general formulation. Dingreville et al. (2005) proposed an approach based on the surface free energy to derive the general formulation for the elastic behavior of nano-wires and nano-plates.

The surface Cauchy-Born (SCB) model was proposed by Park et al. (2006), in which the potential energy of system is decomposed into the bulk and surface components. They computed the potential energy in both parts of the domain using the Cauchy-Born (CB) hypothesis, and the surface constants, i.e. the stress and stiffness, were derived from the inter-atomic potential. They employed a nonlinear finite element model to simulate different nano-structures, such as metallic nano-wires and silicon nano-structures (Park and Klein 2008;
The SCB method presents the effect of surface and does not capture the edge and corner effects, which have significant influences on the mechanical properties of nano-structures, such as: nano-wires and nano-scale circuits, that have extensive applications in nano-electro-mechanical systems (NEMS) (Shidpour 2010; Lu et al. 2011). Recently, a multi-scale approach was presented by Abdolhosseini et al. (2011) based on the boundary Cauchy-Born (BCB) model, which takes the surface, edge, and corner effects into the computation. In BCB technique, the surface energy was obtained from the crystalline structure and inter-atomic potential. The BCB method was based on the Cauchy-Born hypothesis, in which the surface effect was modeled in the finite element method based on the intrinsic function of quadratures, called as an indicator of material behavior.

The present study is focused on the development of a temperature dependent multi-scale technique to investigate the role of temperature on surface effects of nano-materials in order to illustrate the significance of temperature effects on nano-structures. To this aim, the hierarchical multi-scale model recently developed by senior author (Abdolhosseini et al. 2011) for crystalline nano-structures is extended to the temperature related multi-scale technique in order to model the surface effects in dynamic simulation of crystalline nano-structures at various temperatures. The procedure is applied based on the temperature-related Cauchy-Born (TCB) hypothesis, in which the free energy of system is employed instead of the potential energy. Since the TCB rule is in the basis of the bulk atomic unit cell with no free surface effects, the information at each quadrature point is computed by using a smoothing procedure from closely representative atom. The non-linear finite element method is applied together with the heat transfer analysis to model the surface and temperature effects at macro-scale level. Based on the thermo-mechanical finite element simulation, the deformation gradient is obtained at each quadrature point in macro-scale domain. The deformation gradient is then transferred to nearby representative atom in order to calculate the first Piola-Kirchhoff stress and tangential stiffness tensors from the TCB rule in atomistic level. Finally, the reference BCB elements are introduced to capture the stresses at the surface, edge and corner of structures.

The paper is organized in the following sections; In section 2, the concept of temperature-related Cauchy-Born hypothesis is demonstrated. The Piola-Kirchhoff stress and tangential stiffness tensors are derived in this section based on the temperature dependent Cauchy-Born hypothesis. In order to model the real metallic behavior in nano-structures, the Sutton-Chen many-body potential is proposed for the calculation of stress and elasticity tensors. In section 3, the Lagrangian finite element formulation is presented in the framework of thermo-mechanical formulation. In section 4, the concept of multi-scale method together with the homogenization technique according to the boundary Cauchy-Born model are comprehensively demonstrated. Also presented in this section are the reference surface, edge and corner elements. Based on the proposed surface Cauchy-Born model, the coupled thermo-mechanical
behavior of nano-structures is presented in section 5. In order to verify the validity of proposed model, the results at various temperatures are directly compared with those of fully atomistic models. Finally, some concluding remarks are given in section 6.

2. Temperature related Cauchy-Born Hypothesis

The Cauchy-Born hypothesis is a homogenization assumption in the molecular theory of elasticity, in which the atomic positions are related to the continuum field through the deformation gradient. In this theory, it is assumed that the deformations are quite small, and if the solid state materials are subjected to small loading, the crystalline lattice is stable; so the CB is valid until the solid to solid phase transformation occurs. It is presumed that if the boundaries of a defect-free and single-crystalline infinite lattice are subjected to a homogeneous deformation, the entire lattice deforms according to the mentioned deformation gradient, so the atomistic-level lattice follows the deformation given by the macroscopically imposed deformation gradient (Ericksen 1984). The evaluation of Cauchy-Born hypothesis has been investigated by various researchers, including: a criterion for passing from the atomistic to continuum model by Friezecke and James (2000), a continuum based inter-atomic potentials theory by Zhang et al. (2002), an atomistic based finite deformation model by Arroyo and Belytschko (2002), a validity CB criterion for cubic lattice model by Friezecke and Theil (2002), a yield criterion for carbon nano-tubes by Jiang et al. (2003), and the failure and validity surfaces for 2D and 3D FCC lattices by Khoei et al. (2009) and Aghaei et al. (2009). The above theories were based on the molecular dynamics, or often atomistic simulation; however they are limited to zero temperature and do not accounted for the effect of temperature.

The effect of temperature in CB hypothesis has been performed by the local harmonic approximation relating the entropy to the vibration frequencies of the system. The instant temperature in molecular dynamic simulation is defined by the summation of kinetic energy over all degrees of freedom divided by the number of degrees of freedom. Jiang et al. (2005) established a finite temperature continuum theory directly from the inter-atomic potentials and studied several temperature-related material properties based on the Brenner inter-atomic potential and its second generation potential for carbon. Xiao and Yang (2006) proposed a temperature-related Cauchy-Born (TCB) rule for modeling of crystalline solids based on the assumptions that the deformation is locally homogeneous and atoms have the same local vibration mode. They implemented the TCB rule into the mesh-free particle method to investigate the temperature effects on nano-structure materials. A multi-scale model based on finite element method was proposed by Tang et al. (2006) and Tang and Aluru (2006; 2008) for mechanical analysis of silicon nanostructures at finite temperature, which does not require the
local harmonic approximation. Their multi-scale was derived by the extension of the quasi-continuum approach based on the classical continuum mechanics, and the constitutive response of the system was determined by employing an atomistic description. The constitutive response was determined by using the Helmholtz free energy density, in which the static part of the Helmholtz free energy density was obtained from the interatomic potential, and the vibrational part was calculated by using the theory of quantum-mechanical lattice dynamics. Yang and Xiao (2008) studied the material stability of nano-structures via the continuum linearized stability analysis with the TCB rule and shown that the nano-structure materials are more stable at lower temperatures. Yun and Park (2008) developed a temperature-related Cauchy-Born rule for multi-scale modeling of crystalline solids to investigate the surface stress effects of nano-materials. Recently, Khoei et al. (2011b) presented the temperature effects and validity of temperature-related Cauchy-Born hypothesis in three-dimensional lattice structures by comparatively analyzing results of the continuum mechanics calculation and molecular dynamics simulations.

According to the CB hypothesis, if \( a \) denotes a lattice vector in the material configuration and \( a \) indicates the same vector in the spatial configuration, the CB rule demonstrates that the relation between these two vectors can be established through the deformation gradient \( F \) by

\[
A = F \cdot a
\]

From the mathematical point of view, an approximation error entails in the above equation since the lattice vectors have finite lengths. However, it can be applicable as long as the lattice deformation is homogeneous in the scale of lattice vectors. In fact, the CB hypothesis must be employed wherever a description of underlying atomic structure is valid. This issue has been recently investigated by Khoei et al. (2009) and Aghaei et al. (2009) at zero temperature and by Khoei et al. (2011b) for a temperature-related CB hypothesis to derive the validity surfaces of CB rule. They produced a criterion for the validity of CB hypothesis by comparatively investigating the atomistic and continuous models, in which the crystalline lattice deforms homogeneously.

### 2.1. The Piola-Kirchhoff stress and tangential stiffness tensor

In order to derive the Piola-Kirchhoff stress and tangential stiffness tensor, the hyperelastic theory is used to model the homogeneous deformation of crystalline structure since the rate of recoverable strain energy is identical to the rate of work done on the structure. The first Piola-Kirchhoff stress \( P \) can be obtained using the strain energy \( W_c \) in the non-linear continuum mechanics as
in which the strain energy can be calculated using the inter-atomic potential for the crystalline structures. It was shown by molecular dynamics simulations that the temperature affects the strength of nano-structures \cite{xiao2006; khoei2011a}. Consequently, a temperature-related homogenization technique is required to consider the temperature effects in the continuum model when performing the multi-scale modeling of physical phenomena at nanoscale level, and as a result the potential that incorporates the entropy due to the lattice vibration must be applied. In this study, the Helmholtz free energy, called the effective energy, is implemented instead of the potential energy, in which the atoms at finite temperature occupy new positions due to the thermal vibrations. The Helmholtz free energy is the amount of thermodynamic energy which can be converted into the work at the constant temperature and volume. In continuum approach with the TCB rule, we assume that the atoms of a crystalline solid have locally homogeneous deformation with the same vibration mode as in the CB rule at a specified temperature. Thus, all local atoms have similar dynamical matrix, which is the function of deformation gradient. A similar approach was performed by \textit{Yun and Park (2008)} and \textit{Tang and Aluru (2008)} through a local-harmonic approximation of the free energy.

\[
P = \frac{\partial W_c}{\partial F} \quad (2)
\]

The vibration of atom in a crystalline solid is assumed to be harmonic, so the Helmholtz free energy \( W_H = W_c - TS \) depends on the atomic bond length \( r \), temperature \( T \), and the entropy \( S \). The entropy \( S \) in the Helmholtz free energy can be calculated from the quasi-harmonic approximation expressed for the system of size \( N \) as

\[
S = -k_B \sum_{j=1}^{3N} \ln \left[ 2 \sinh \left( \frac{h \omega_j}{4 \pi k_B T} \right) \right] \quad (3)
\]

The vibration of atom in a crystalline solid is assumed to be harmonic, so the Helmholtz free energy \( W_H \) of a crystalline solid, which contains \( N \) atoms at temperature \( T \), can be defined as \cite{rickman2002}

\[
W_H = W_c(x) + k_B T \sum_j \ln \left[ 2 \sinh \left( \frac{h \omega_j}{4 \pi k_B T} \right) \right] \quad (4)
\]

where \( W_c(x) \) is the potential energy of atoms in their equilibrium at the position \( x \) at zero temperature, \( h \) is the Planck constant and \( k_B \) is the Boltzmann constant. The sum over \( j \) includes all non-zero vibrational modes of the system. The frequencies \( \omega_j \) are the Eigen values of dynamical matrix, i.e.

\[
D_{\text{aff}} = \frac{1}{\sqrt{m_i m_j}} \left( \frac{\partial^2 W_0}{\partial X_{ia} \partial X_{j\beta}} \right) \quad (5)
\]
where $X_{ia}$ is the vibrational coordinate at the direction $\alpha$ for atom $I$, and $m_I$ is the mass of atom $I$. Equation (4) can be simplified as

$$W_H = W_C(x) + n k_B T \sum_{i=1}^{N} \ln \left( \frac{h D_i^{\frac{1}{2n}}}{2\pi k_B T} \right)$$

(6)

where $D$ is the determinant of local dynamical matrix.

The Sutton-Chen many-body potential is chosen here for the calculation of potential energy defined as (Sutton and Chen 1990)

$$w_0 = w_{0i} = \varepsilon \frac{1}{\Omega_{0i}} \left[ \frac{1}{2} \sum_{j \neq i} \left( \nu(r_{ij}) - c \sqrt{\rho_i} \right) \right]$$

(7)

where $\nu(r_{ij}) = a/r_{ij}^n$ and $\rho_i = \sum_{j \neq i} (a/r_{ij})^m$. In above relation, $\Omega_{0i}$ is the local atomic volume in relaxed and underformed configuration of the lattice structure associated with atom $i$, $w_{0i}$ is the potential energy of atom $i$, $r_{ij}$ is the inter atomic distance between the host and its neighbor $j$, $a$ is the lattice parameter and $m$, $n$, $c$ and $\varepsilon$ are the potential parameters. These constants are obtained for various materials by Sutton and Chen (1990).

In hyperelasticity, the stress tensor is derived by differentiating the strain energy of deformed material with respect to the deformation gradient. Hence, the first Piola-Kirchhoff stress tensor $P_{ij}$ can be calculated as the first derivative of free energy density $W_H$, which is a function of temperature and deformation gradient, as

$$P_{ij}(F, T) = \frac{\partial W_H(F, T)}{\partial F_{ij}}$$

(8)

in which the above definition is derived for three-dimensional lattice structure as

$$P = \frac{\partial W_C}{\partial F^T} + \frac{k_B T}{\sqrt{3} D r_0^2} \frac{\partial D}{\partial F^T}$$

(9)

where $F$ is the deformation gradient and $r_0$ is the initial distance between atoms. Since the first Piola-Kirchhoff stress tensor is not a symmetric tensor, there is of little interest to obtain the internal forces in terms of the nominal stress $P_{ij}$. So the Cauchy stress can be calculated, as an Eulerian measure, and the symmetric tensor can be defined as

$$\sigma_{ij} = \frac{1}{J} F_{ik} P_{kj}$$

(10)

where $J$ is the determinant of deformation gradient tensor, known as Jacobian.

8
In hyperelasticity, the first elasticity tensor can be derived based on the second derivative of strain energy density with respect to the deformation gradient as

\[ C_{ijkl}^1 = \frac{\partial^2 w_H(F,T)}{\partial F_{ji} \partial F_{lk}} \tag{11} \]

Substituting relation (6) in (11) results in

\[ C_{ijkl}^1 = \frac{\partial^2 W_c}{\partial F_{ji} \partial F_{lk}} + \frac{k_B T}{2D} \frac{\partial^2 \bar{D}}{\partial F_{ji} \partial F_{lk}} - \frac{k_B T}{2D^2} \frac{\partial \bar{D}}{\partial F_{ji}} \otimes \frac{\partial \bar{D}}{\partial F_{lk}} \tag{12} \]

in which the first term of elasticity tensor is derived by considering the strain energy density regardless of temperature effect as

\[
\frac{\partial^2 W_c}{\partial F_{ji} \partial F_{lk}} = \frac{\varepsilon}{2\Omega_o} \left\{ \sum_{q \neq p} \left[ \left( \frac{\partial^2 v(r_{pq})}{\partial r^2_{pq}} \frac{\partial r_{pq}}{\partial F_{lk}} - c \frac{\partial^2 \rho_p}{\partial r_{pq} \partial F_{lk}} \frac{\partial r_{pq}}{\partial F_{ji}} \right) + \frac{c}{2\rho_p \sqrt{\rho_p}} \left( \sum_{q \neq p} \frac{\partial \rho_p}{\partial r_{pq}} \frac{\partial r_{pq}}{\partial F_{lk}} \right) \right] \right\} + \frac{c}{2\rho_p \sqrt{\rho_p}} \left( \sum_{q \neq p} \frac{\partial v(r_{pq})}{\partial r_{pq}} - c \frac{\partial \rho_p}{\partial r_{pq}} \frac{\partial r_{pq}}{\partial F_{ji}} \right) \frac{\partial^2 r_{pq}}{\partial F_{ji} \partial F_{lk}} \tag{13} \]

where the term \( \frac{\partial^2 r_{pq}}{\partial F_{ji} \partial F_{lk}} \) can be calculated as

\[
\frac{\partial^2 r_{pq}}{\partial F_{ji} \partial F_{lk}} = \frac{r^2_{pq} \delta_{ji} - r^3_{pq}}{r^3_{pq}} F_{kk}^{-1} F_{il}^{-1} \tag{14} \]

where \( \delta \) is the Kronecker delta in indicial notation.

In relation (12), the next terms of elasticity tensor are the temperature related parts and describe the influence of temperature on material stability. In order to derive the first and second derivatives of the determinant of dynamical matrix, the off-diagonal terms of matrix can be ignored, so the determinant of dynamical matrix can be written as

\[ \bar{D} = D_{11} D_{22} D_{33} \tag{15} \]

The first derivative of the determinant of dynamical matrix with respect to the deformation gradient, given in equation (12), can be obtained as

\[ \frac{\partial \bar{D}}{\partial F_T} = D_{11} D_{22} \frac{\partial D_{33}}{\partial F_T} + D_{11} D_{33} \frac{\partial D_{22}}{\partial F_T} + D_{22} D_{33} \frac{\partial D_{11}}{\partial F_T} \tag{16} \]

and the second derivative of the determinant of dynamical matrix with respect to the deformation gradient can be derived as
In the updated Lagrangian formulation of finite element method proposed here, the Truesdell elasticity tensor is used, which can be derived from the first elasticity tensor using the following relation

\[
C^{(1)}_{ijkl} = \frac{1}{F_{im}F_{jn}} C_{m,jnk}^{(1)} - \delta_{jk} \sigma_{il} \tag{18}
\]

The Piola-Kirchhoff stress and elasticity tensor defined through equations (8–11) represent the nonlinear continuum formulation, which can be applied in the metallic lattice structure. In order to employ this continuum formulation in the boundary value problem, the nonlinear finite element method is derived by evaluating the deformation gradient and temperature at each quadrature point, as described in the next section.

3. Nonlinear Finite Element Analysis of Thermo-mechanical Problem

3.1. Nonlinear finite element formulation

The nonlinearities in FEM arise from two main sources; the constitutive and geometric nonlinearities, in which the latter is mainly due to large deformation. Whether the displacement is small or large, the equilibrium equation between the internal and external forces is absolutely mandatory. In general, the equilibrium equation of a body can be written as

\[
\frac{\partial \sigma_{ij}}{\partial x_j} + \rho \dot{b}_i = \rho \dot{\nu}_i \tag{19}
\]

where \( \rho \) is the material density and \( \dot{b}_i \) is the body force. According to the virtual work theorem, the above equation can be converted to its weak-form by multiplying equation (19) to the virtual velocity field \( \delta \nu_i \), and integrating over the entire body, i.e.

\[
\int_{\Omega} \delta \nu_i \left( \frac{\partial \sigma_{ij}}{\partial x_j} + \rho \dot{b}_i - \rho \dot{\nu}_i \right) \, d\Omega = 0 \tag{20}
\]

Applying the Divergence theorem, the weak form of equation (20) can be written as

\[
\int_{\Omega} \frac{\partial (\delta \nu_i)}{\partial x_j} \sigma_{ij} \, d\Omega - \int_{\Omega} \delta \nu_i \rho \dot{b}_i \, d\Omega - \int_{\Gamma} \delta \nu_i \tau_i \, d\Gamma + \int_{\Omega} \delta \nu_i \rho \dot{\nu}_i \, d\Omega \tag{21}
\]
where \( t_i \) is the traction vector applied on the surface boundary. In order to develop a finite element formulation, equation (21) can be solved numerically using the spatial discrete domain. If the coordinate of nodal point \( I \) at time \( t \) is denoted by \( x_i(t) \), the coordinate of an arbitrary point \( x_i(X,t) \) can be obtained by means of shape functions \( N_i(X) \) as

\[
x_i(X,t) = N_i(X) x_i(t)
\]  

(22)

where indices \( I \) and \( i \) denote the node number and the Cartesian direction, respectively. In the above equation, \( X \) denotes the nodal coordinate in the undeformed configuration. The shape functions \( N_i(X) \) can be used to derive the displacement, velocity and acceleration at any arbitrary point of domain. The discretization process can be similarly applied to the virtual velocity \( \delta v_i \) in equation (21); so it can be rewritten as

\[
\int_\Omega \frac{\partial N_i}{\partial x_j} \sigma_{ij} \, d\Omega - \int_\Omega N_i \rho b_i \, d\Omega - \int_\Gamma N_i t_i \, d\Gamma + \int_\Omega N_i \rho \dot{v}_i \, d\Omega = 0
\]  

(23)

In the above equation, the first integral indicates the internal forces \( f^{\text{int}} \), and the sum of next two terms represent the external forces \( f^{\text{ext}} \). The last integral demonstrates the inertial forces due to the acceleration of system, which can be ignored in the simulation of quasi-static process. The nonlinear finite element equation (23) can be solved by an iterative approach due to intrinsic nonlinear nature of the governing equations.

In order to derive the updated Lagrangian formulation of nonlinear finite element method, the first term of equation (23) can be rewritten in term of objective Eulerian measure. Manipulating the internal forces \( f^{\text{int}} \) by the means of basic continuum mechanics relations, the Eulerian description can be written as

\[
\hat{f}^{\text{int}}_i = \int_\Omega \frac{\partial N_i}{\partial x_k} \left( \sigma_{kl}^{\text{pc}} + \sigma_{kl} L_{ii} \right) \, d\Omega
\]  

(24)

where \( \hat{f}^{\text{int}}_i \) is the incremental internal force at node \( I \) of \( i^{\text{th}} \) direction and \( \sigma_{kl}^{\text{pc}} \) is the objective rate of Cauchy stress tensor. Equation (24) is mainly consisted of two distinct parts; the incremental material internal force \( f^{\text{mat}} \), and the incremental geometric internal force \( f^{\text{geo}} \) defined as

\[
\dot{f}^{\text{mat}}_i = \int_\Omega \frac{\partial N_i}{\partial x_k} \sigma_{kl}^{\text{pc}} \, d\Omega
\]

\[
\dot{f}^{\text{geo}}_i = \int_\Omega \frac{\partial N_i}{\partial x_k} \sigma_{kl} L_{ii} \, d\Omega
\]  

(25)
where $L$ is the velocity gradient tensor, i.e. $L_{ij} = \partial v_i / \partial x_j$. In above relation, the objective rate of Cauchy stress $\sigma^{\text{vc}}$ can be expressed in terms of conjugate strain measure, i.e. the rate of deformation tensor and Truesdell elasticity tensor as $\sigma^{\text{vc}}_{ij} = C_{ijkl} \sigma^{\text{T}}_{kl}$. Inserting this relation into equation (25) and manipulating the notation $D_{kl}$ as the symmetric part of velocity gradient tensor, and considering the symmetry of Truesdell elasticity tensor, equation (25) can be rewritten as

$$
\dot{f}_{li}^{\text{mat}} \triangleq \int_{\Omega} \frac{\partial N_l}{\partial x_k} C_{kl}^{\sigma} \frac{\partial v_i}{\partial x_l} \, d\Omega
$$

$$
\dot{f}_{li}^{\text{geo}} \triangleq \int_{\Omega} \frac{\partial N_l}{\partial x_k} \sigma_{kl} \frac{\partial v_i}{\partial x_l} \, d\Omega
$$

By implementation of discretization technique to the term of velocity gradient in equation (26), the material and geometric stiffness matrices can be derived as

$$
\dot{f}_{li}^{\text{mat}} = \left[ \int_{\Omega} \frac{\partial N_l}{\partial x_k} C_{kl}^{\sigma} \frac{\partial N_j}{\partial x_l} \right] v_{jj} \quad \text{or} \quad \dot{f}_{li}^{\text{mat}} = K_{lij}^{\text{mat}} v_{jj}
$$

$$
\dot{f}_{li}^{\text{geo}} = \left[ \int_{\Omega} \frac{\partial N_l}{\partial x_k} \sigma_{kl} \frac{\partial N_j}{\partial x_l} \delta_{ij} \, d\Omega \right] v_{jj} \quad \text{or} \quad \dot{f}_{li}^{\text{geo}} = K_{lij}^{\text{geo}} v_{jj}
$$

The integrals of material and geometric stiffness matrices must be evaluated numerically. Among varieties of different approaches, two techniques are more prevalent; the Newton-Cotes and Gauss methods. Despite the lower precision of Newton-Cotes method, it provides the opportunity to choose the position of quadratures, which can be helpful wherever their configuration is a primary concern in numerical solution. As a practical guideline in the solution of equation (23), the total external force is divided into several increments, in which each incremental load is implemented at the beginning of each step. In order to implement the equivalent continuum presented in previous section, we need to make two main changes in a conventional nonlinear finite element. Firstly, in the calculation of material stiffness matrix $K_{lij}^{\text{mat}}$, the Truesdell stiffness matrix must be calculated using equation (18). Secondly, in the evaluation of geometric stiffness matrix $K_{lij}^{\text{geo}}$, the Cauchy stress must be calculated from equation (10).

### 3.2. Thermo-mechanical FE formulation

In order to derive the thermo-mechanical finite element formulation, the Lagrangian finite element technique, presented in previous section, is incorporated into the heat transfer formulation. The governing equation of heat conduction is derived for a continuous medium from the principle of conservation of heat energy over an arbitrary fixed volume. Based on this
principle, the heat increase rate of the system is equal to the summation of heat conduction rate and heat generation rate in a fixed volume. The empirical relationship of the Fourier law of heat conduction states that for a surface with the unit normal vector \( n \), the rate of heat conduction across the surface, per unit area, in the direction \( n \) can be obtained as

\[
q = -k (\text{grad} T) \cdot n = -k \frac{\partial T}{\partial n}
\]

(28)

where \( k \) is the thermal conductivity which is a property of the medium and \( q \) is the flux of heat in direction \( n \), with \( n \) denoting the outward unit normal to surface \( \Gamma \). Hence, the rate of heat conduction into the domain \( \Omega \) across the surface \( \Gamma \) can be given by

\[
\int_{\Gamma} -q \, d\Gamma = \int_{\Gamma} k(\text{grad} T) \cdot n \, d\Gamma = \int_{\Omega} \text{div}(k \text{ grad } T)d\Omega
\]

(29)

The heat conduction equation can therefore be written as

\[
\rho c \frac{\partial T}{\partial t} = \text{div}(k \text{ grad } T) + Q
\]

(30)

where \( c \) and \( Q \) are the specific heat capacity and heat generation rate of system. The implementation of appropriate boundary conditions leads to a unique solution of the heat conduction over an arbitrary domain. The typical boundary condition is based on the Dirichlet condition which can be specified as the constant temperature at the boundaries of domain.

In order to solve the heat conduction equation (30), the standard finite element Galerkin discretization process is used by approximating the temperature field as

\[
T(x, y, z, t) = \sum_{i=1}^{m} N_i(x, y, z) T_i(t)
\]

(31)

where \( N_i \) is the shape function and \( T_i(t) \) is the nodal temperature. Applying the FE Galerkin discretization into the heat conduction equation (30) results in

\[
C \dot{T} + HT = g
\]

(32)

where \( C \) is the capacity matrix, \( H \) is the conductivity matrix and \( g \) is the thermal loading vector. In order to discretize the system of equation in time, the time stepping procedure is employed based on the \( \theta \) method. Applying the time stepping method in equation (32), we have

\[
(C + \theta \Delta t \, H) T^{n+1} = (C - (1 - \theta) \Delta t \, H) T^n + \Delta t \, g^n
\]

(33)

where
\[ C_{ij} = \int_{\Omega} pc N_i N_j \, d\Omega \]  

\[ H_{ij} = \int_{\Omega} \left[ k_x(T) \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + k_y(T) \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + k_z(T) \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right] \, d\Omega + \int_{\Gamma_{\alpha}} \alpha N_i N_j \, d\Gamma_{\alpha} \]  

\[ g_i = \int_{\Omega} Q N_i \, d\Omega - \int_{\Gamma_q} q N_i \, d\Gamma_q + \int_{\Gamma_{\alpha}} \alpha N_i T_{\alpha} \, d\Gamma_{\alpha} \]  

where \( q \) and \( \Gamma_q \) are the heat flux and the surface boundary of heat flux, respectively, \( \alpha \) and \( \Gamma_{\alpha} \) are the convection heat transfer coefficient and the surface boundary of heat transfer, respectively, and \( T_{\alpha} \) is the atmospheric temperature.

In the basis of heat conduction finite element equation (33), the distribution of temperature can be achieved at the selected time intervals. The thermal expansion/contraction strain \( \Delta \varepsilon \) due to changes of temperature can then be obtained by using \( \Delta \varepsilon = \alpha \Delta T \), with \( \alpha \) denoting the thermal coefficient. The value of thermal strain can be calculated at each quadrature point, and used as the external forces in the nonlinear finite element analysis. Finally, the deformation gradient can be evaluated using the nonlinear FE model in macro-scale level.

4. Boundary Cauchy-Born Model

In order to illustrate the effect of surface stress with temperature, a fully atomistic model and its equivalent continuous model are implemented in the nonlinear finite element method. The temperature-related Cauchy stress and the temperature dependent Truesdell elasticity tensor are evaluated at each integration point in atomistic model. The Lagrangian thermo-mechanical finite element formulation is then employed to evaluate the temperature and deformation gradient at each integration point in continuum model. It is obvious that the position of integration points in the continuous model may not coincide with atomic positions in the atomistic model. In such case, if the integration point is placed within the bulk of structure, i.e. it is far enough from the proximity of surface, the integration point experiences similar material properties of surrounding atoms. Since the integration point needs to demonstrate the material behavior of surrounding atoms, the properties of the quadrature point can be assumed equal to the representative atom in the bulk of material. In fact, the representative atom is chosen to define all possible neighbors within the cut-off radius of simulation. This assumption is implicitly expressed in all multi-scale methods based on the CB hypothesis (Shenoy et al. 1999; Park et al. 2006). If the integration point approaches to the surface of structure, the above assumption becomes invalid. In reality, a quadrature point adjacent to the surface of structure has different neighboring list of atoms. Hence, the representative atom is incapable of capturing the specific characteristics of the integration point near the surface.
Consequently, a model with inhomogeneous nature of atomic medium is required near the surface to describe the surface effect in nano-structure properly. The Boundary Cauchy-Born (BCB) model is a novel technique, which has been recently presented by senior author (Abdolhosseini et al. 2011). In this technique, the quadrature point reflects the governing circumstances on lattice structure by means of interpolating information, i.e. the Cauchy stress and Truesdell elasticity tensor, from possible atomic positions near to the integration point.

In order to efficiently implement the technique, the concept of boundary CB element is defined by introducing the surface, edge, and corner elements. An applicable and suitable approach for simulation of structure with complicated shapes and geometries are provided by combining the concept of boundary CB element with the reference boundary CB element. In order to avoid the repetitious definition of a single conceptual object and use this object anywhere necessary, the reference boundary CB elements are defined, in which all information are calculated and then mapped to real elements that have arbitrary spatial configuration. Due to considerable variation of material properties from the surface to the center of crystalline structure, the reference boundary CB elements are defined with more quadrature points in perpendicular direction to the surface. Furthermore, in order to efficiently capture the surface effect, an appropriate cut-off radius of atomistic model is applied by considering 7 shells of atomic neighbors. In this case, 134 atoms are specified in the calculation of representative atom in the bulk of structure. This cut-off radius means that those atoms exposed to surface effects are up to the third atomic layer and, those of the fourth layer can be considered as the bulk atoms.

In the Boundary Cauchy-Born (BCB) model, the integration point inherits information from the atoms of upper and lower layers. According to the number of element sides on the surface of structure, three types of boundary CB elements are implemented, including: the surface element, the edge element, and the corner element. In the reference surface element, one side of element is only placed on the surface of structure, as shown in Figure 1. In this element, the surface of element is chosen perpendicular to the global $z$ -direction. According to Figure 1, each atom located in layer $L_1$ is identical to the representative bulk atom, since it has 134 neighboring atoms. However, those atoms located in layers $L_2$, $L_3$ and $L_4$ have different neighbors with less than 134 atoms. It must be noted that the density of neighbors around each atom is absolutely different in $z$ -direction. In other words, each atom of layer $L_2$ does not include the upper neighboring atoms, while the atom in layer $L_3$ acquires part of its upper neighbors. Since one side of element is only located on the surface, all atoms of each layer have identical neighbor lists and consequently, identical properties. Considering a quadrature point between the layer $L_1$ and $L_4$, as shown in Figure 1, if the required information of this quadrature is called by $\mu$, it can be calculated by a linear interpolation of data between two adjacent atomic layers $L_1$ and $L_4$ as
\[ \mu_Q = \frac{z_1}{z_1 + z_2} \mu_{L_4} + \frac{z_2}{z_1 + z_2} \mu_{L_1} \]  

(37)

where \( \mu_Q, \mu_{L_1} \) and \( \mu_{L_4} \) denote the desired characteristic at the quadrature and representative atoms of layers \( L_1 \) and \( L_4 \), respectively. As shown in Figure 1, \( z_1 \) and \( z_2 \) represent the distance from layers \( L_4 \) and \( L_1 \), respectively. In order to achieve an efficient number of integration points and atomic layers, four atomic layers are chosen within the reference surface element, so the size of element in the surface direction is less than twice the lattice parameter.

In the reference edge element, two surfaces of element are placed on the surface of structure, which are perpendicular to the global \( x^- \) and \( z^- \) directions. In this element, the concept of atomic layers cannot be used, and each atom has its own neighboring list, which distinguishes it from other atoms. As shown in Figure 2, there are four representative atoms within the proximity of each quadrature in one surface, which is perpendicular to the intersection of two surface sides. It must be noted that the accuracy of computation in reference boundary elements can be increased by choosing the quadrature points close to representative atoms based on the Newton-Cotes method. If the quadrature point approaches to the representative edge atoms, its properties must be similar to the nearby representative edge atom. Since four representative atoms are chosen within the proximity of each quadrature point, the conventional two-dimensional shape functions of rectangular element can be utilized to interpolate the desired properties of quadrature point. This property can be derived as

\[ \mu_Q = \mu_{L_i} N_{L_i}(x_Q, z_Q) + \mu_{L_j} N_{L_j}(x_Q, z_Q) + \mu_{L_k} N_{L_k}(x_Q, z_Q) + \mu_{L_l} N_{L_l}(x_Q, z_Q) \]  

(38)

where \( N_{L_i}(x_Q, z_Q) \) are the shape functions of representative atoms \( L_i \) at each quadrature point, and \( i, j, k \) and \( l \) denote the nearby representative atoms, which are located on the vertices of a virtual square with side lengths equal to half lattice parameter. It must be noted that since there are two surface sides in this type of element, the quadrature points must be increased in both directions.

In the reference corner element, there are three sides of element located on the surface of structure, in which the material properties are changed in all three directions. Hence, the number of quadratures must be increased in all directions, so eight atoms are specified near each quadrature point. Since the quadrature should have similar characteristics with its representative nearby atom, its characteristics can be computed based on the interpolation shape functions of a cubic element. The property of each quadrature can be evaluated as

\[ \mu_Q = \sum_{i=1}^{8} \mu_{L_i} N_{L_i}(x_Q, y_Q, z_Q) \]  

(39)
where \( N_{l_i}(x_Q, y_Q, z_Q) \) is the value of shape function at the quadrature point.

### 4.1. The temperature-related BCB model

The computational algorithm of temperature-related hierarchical multi-scale modeling of surface effects, described in preceding sections, is numerically implemented into the nonlinear thermo-mechanical finite element code. In order to implement the Boundary Cauchy-Born (BCB) model in the finite element mesh of macro-scale level, the BCB elements are employed based on the types of surface elements by introducing the quadratures, their direction, representative atoms, and their characteristics. In order to map the information obtained from the reference element to the standard element, the rotation matrix is computed for each reference element. The main variables that need to be transferred to the standard configuration, include the Cauchy stress and the Truesdell elasticity tensor, i.e.

\[
\sigma_{ij} = Q_{mi} Q_{nj} \sigma^*_{mn} \tag{40}
\]

\[
C_{ijkl} = Q_{mi} Q_{nj} Q_{kp} Q_{lq} C^*_{mnpq} \tag{41}
\]

where \( Q \) denotes the rotation tensor, and \( C^*_{mnpq} \) and \( \sigma^*_{mn} \) indicate the calculated values in reference element.

In the macro-scale simulation, the temperature of surface boundary is increased at each time step using a specified temperature rate. The heat transfer analysis is then performed to obtain the distribution of temperature throughout the body at each time step. This temperature distribution can be obtained using the temperature gradient computed from the surface boundary with higher temperature to the bulk of structure with lower temperature. By obtaining the temperature distribution in the body, the thermal expansion/contraction strain can be evaluated at each quadrature point using the thermal coefficient, and the initial values of strain can be employed as equivalent nodal forces on the structure. The equivalent nodal forces of thermal expansion/contraction strain are then implemented to solve the system using the nonlinear finite element simulation at each time step in an iterative manner. The above simulation leads to the values of displacement and temperature at the macro-scale level. The macroscopic values of the deformation gradient tensor \( F \) and temperature \( T \) obtained at the nodal points can be used as the initial boundary conditions of the micro-scale simulation. Based on the molecular dynamics analysis, the values of stresses and elasticity tensors can be obtained by using the temperature-related Cauchy Born homogenization technique, described in Section 2, to evaluate the first Piola-Kirchhoff stress and the Truesdell elasticity tensors at each quadrature point. At this stage, the convergence criteria must be controlled in the
nonlinear finite element simulation. If the convergence is satisfied, the solution of current time step is completed and the analysis can be carried out at the next time step. This process is continued until the temperature of surface boundary reaches the specified temperature. The computational procedure of the temperature-dependent multi-scale BCB model is presented in Table 1.

5. Numerical Simulation Results

5.1. Temperature stability of tangential stiffness tensor

Consider the diagonal deformation gradient matrix $F$ as

$$
F = \begin{bmatrix}
\lambda_1 & 0 & 0 \\
0 & \lambda_1 & 0 \\
0 & 0 & \lambda_1
\end{bmatrix}
$$

(42)

where $\lambda_1$ is in the range of 0.85 to 1.15. According to this deformation gradient, the elasticity tensor can be calculated using the second derivative of free energy at various temperatures. Figure 3 illustrates the effect of temperature on the first tangential stiffness matrix. As shown in this figure, the elasticity tensor is stable at zero temperature for various deformation gradients, however – it becomes drastically unstable by increasing the temperature, in which the range of instability expands due to increase of temperature.

In order to present the effect of temperature dependent elasticity tensor in the temperature-related multi-scale model, a nano-scale ring is simulated by using the BCB technique. The internal and external radii of the ring are 205.5 and 244.4 Å, respectively, and the height is 38.9 Å. The Sutton-Chen inter-atomic potential is used in the model and the silver constants are employed in numerical analysis. The finite element model is constructed of 1000 twenty-noded quadratic hexahedral elements. In Figure 4, the evolution of stress $\sigma_x$ contours are shown using the temperature-related multi-scale model for two different cases, i.e. the elasticity tensor with no temperature effect and the temperature-related elasticity tensor. Obviously, by increasing the temperature, the temperature-related elasticity tensor displays different behavior. Clearly, the ring becomes harden at 165°K, as shown in Figure 4(d), and the system freezes completely at 195°K, as shown in Figure 4(f).

The effect of temperature dependent elasticity tensor is also investigated for a nano-scale cube, as shown in Figure 5. A cubic specimen with the length of 81.6 Å is modeled to illustrate the surface effects in the temperature-related multi-scale model. Obviously, similar behavior occurs for the nano-scale cube while applying the temperature dependent elasticity tensor into
the model. As can be also observed in Figure 3, the system becomes stiffer at lower
temperatures for various deformation gradients. The physical interpretation of this observation
can be related to the principal frequencies of atoms and the eigen-values of dynamic matrix.
Yang and Xiao (2008) presented that the stability of material strongly depends on the roots of
following equation

\[-\rho_0 \omega^2 g_l + \kappa^2 C_{ijkl} n_j^0 n_l^0 g_k = 0\] 

where $n^0$ is the normal direction with respect to initial configuration and $\kappa$ and $\rho_0$ are the
wave number and initial density, respectively. The roots of above equation can be obtained by

\[\det \left[ \omega^2 \delta_{ik} - \frac{\kappa^2}{\rho_0} A_{ik} \right] = 0\] 

where $A_{ik} = C_{ijkl} n_j^0 n_l^0$. In three-dimensional deformation gradient, the roots of this equation
are the function of temperature. In the instability condition, the principal frequencies of atoms
are in the resonance mode and the structure becomes unstable; as a result the model becomes
harden and the stresses decrease gradually. The resonance modes of vibration are related to
the temperature and increase directly with the temperature.

5.2. Temperature effect on surface stress

In this section, two examples proposed in previous section are simulated by the temperature
dependent multi-scale technique and the results are compared with fully atomistic model in
order to evaluate the capability of temperature-related boundary Cauchy-Born (BCB) model.
Both examples are performed in three-dimensional crystalline structure. The first example is
chosen to demonstrate the temperature effect on surface stresses in the nano-scale cube. An
finite FCC crystal is simulated by increasing the temperature, and the results of multi-scale
simulation are compared with the molecular dynamics model. In order to control the increase
of temperature in the nano-cube, the Nose-Hoover thermostat is employed. The temperature
of cube is increased by the rate of 1°K per 100 steps. The MD sample is consisted of 32000
atoms. The evolution of stress components is performed at the center, surface and edge lines
of the cube, as shown in Figure 6. In Figure 7, the contours of stress component $\sigma_x$ are shown
for the molecular dynamics and boundary Cauchy-Born models at various temperatures.
Obviously, the temperature-related BCB model can effectively capture the surface effect in
nano-cube, particularly the highest values of stress can be observed along the edges of cube.
Clearly, the stress concentration at the edges of BCB model is in complete agreement with that
obtained by the MD model at various temperatures. As can be seen in Figure 7, the effect of
BCB stresses reduces at higher temperatures due to the volume expansion, in which the values of stresses at the edges of cube converge to the values of surface stresses.

In Figure 8, the evolution of stress $\sigma_x$ is shown along the line passed through the center of cube for the BCB model at various temperatures. Clearly, it shows that the stress is positive at the boundaries of cube, and reduces to the negligible negative value when approaching to the center of cube. The physical interpretation of this observation reveals that the outer surface of cube is stretched by the inner part to increase the electron density at the boundary atoms, and the inner core is compressed by the outer surface according to the third Newton law. It can also be observed that the values of boundary stress decrease by increasing the temperature and the values of stress increase slightly at the center of cube. In fact, the cube expands and the distances between neighboring atoms increase at higher temperatures. Since there is an inverse relationship between the energy and atomic distance, the strain energy relating to atomic bonding reduces and the deficiency of atomic coordination near the surface is not noticeable. Furthermore, the significance of temperature dependent part of the Helmholtz free energy is obvious at higher temperatures. As a result, the role of the first part of strain energy relating to atomic bonding in the total energy becomes less important and the surface effects due to the reduction of atomic coordination are not substantial near the surface.

In Figure 9, the evolution of stress $\sigma_x$ is presented along the line passed through the surface of cube at various temperatures. The results demonstrate that the values of stress are high at the center of surface and reduce by increasing the temperature. The stress values decrease by approaching to the edges of cube, and in a few angstroms it shows the stress concentration at the edges of cube at zero temperature, however – the stress concentration reduces by increasing the temperature up to 600°K and decreases drastically at the edge of cube for higher temperatures. In Figure 10, the evolution of stress $\sigma_x$ is presented along the line pass through the edge of cube. Clearly, the values of stress decrease by increasing the temperature, in which the surface effect diminishes at higher temperatures. In Figure 11, the evolutions of shear stress $\sigma_{xy}$ are plotted along the line passed through the surface of cube at various temperatures. Obviously, the most outstanding features of the boundary CB technique displays in modeling of surface effects, particularly at the edges of cubic specimen.

The second example is chosen to demonstrate the effect of temperature in boundary CB method by modeling the surface effects in curved structures. A nano-scale ring is simulated by the temperature-related BCB technique and the results are compared with molecular dynamics model, as shown in Figure 12. The Sutton-Chen inter-atomic potential is used in both models and the silver constants are employed in numerical analyses. The MD model is consisted of 130000 atoms which are extracted from a rectangular lattice in [1 0 0], [0 1 0] and [0 0 1] crystalline directions. The finite element models are constructed using 1000 twenty-noded
quadratic hexahedral elements. In both MD and BCB simulations, the temperature of outer surface is increased from zero to \(500^\circ K\), which can be transmitted to the inner part of the ring according to the thermal conductivity of thermo-mechanical analysis. In Figure 12, the distribution of stress \(\sigma_x\) contours are shown for the molecular dynamics and boundary Cauchy-Born models at various temperatures. The stress distributions at the surface and edges of BCB model are in complete agreement with those obtained by the MD model. Obviously, the planes parallel to \(z\)-axis are influenced by the surface effect, and the maximum values of stress occur in the circumferential plans parallel to \(x\)-direction. However, these stress values reduce by increasing the temperature in both MD and BCB models. In addition, the evolution of stress distribution with temperature on the surface and edges of the ring can be compared with those obtained for the nano-cube at higher temperatures. The above two examples adequately illustrate the efficiency of temperature dependent BCB model in modeling the behavior of surface stresses over the body of structure at different temperatures.

6. Conclusion

In the present paper, a novel temperature-related multi-scale method was developed based on the boundary Cauchy-Born model to evaluate the role of temperature on surface effects in the analysis of nano-materials. The temperature-related Cauchy-Born hypothesis was employed by applying the Helmholtz free energy, as the energy density of equivalent continua relating to the inter-atomic potential. The temperature-related multi-scale technique was applied in atomistic level to obtain the first Piola-Kirchhoff stress and tangential stiffness tensor, as the first and second derivatives of free energy density. The Lagrangian finite element formulation was applied into the heat transfer analysis to develop the thermo-mechanical finite element model. The stress and tangential stiffness tensors were computed at each quadrature by interpolating the data from nearby representative atoms. The Boundary Cauchy-Born elements were introduced to capture the surface, edge and corner effects.

In order to perform the multi-scale simulation, the temperature of surface boundary was first increased at each time step using a specified temperature rate in the macro-scale level. The heat transfer analysis was then performed to obtain the distribution of temperature throughout the body at each time step. The thermal expansion/contraction strain was obtained at each quadrature point, and the values of initial strain were computed as equivalent nodal forces on the structure. The equivalent nodal forces of thermal expansion/contraction strain were then applied to solve the system using the nonlinear finite element simulation at each time step. The macroscopic values of the deformation gradient and temperature obtained at the quadrature points were then used as the initial boundary conditions of the micro-scale
simulation. In the molecular dynamics analysis, the values of the first Piola-Kirchhoff stress and the Truesdell elasticity tensors were obtained by using the temperature-related Cauchy Born homogenization technique at each quadrature point. If the convergence was satisfied in the nonlinear finite element simulation, the analysis was continued in the next time step until the temperature of surface boundary reaches the specified temperature.

Finally, the proposed computational algorithm of temperature-related hierarchical multi-scale model was implemented into the nonlinear thermo-mechanical finite element code to numerically evaluate the surface effects at various temperatures in nano-scale materials. The stability analysis of elasticity tensor was investigated in multi-scale simulation at various temperatures for different deformation gradients. The stability analysis was carried out for a nano-scale cube and a nano-scale ring, and the results of the temperature-related elasticity tensor were compared with those obtained from the elasticity tensor with no temperature effect. It was shown that the system becomes stiffer at lower temperatures for various deformation gradients, however by increasing the temperature, the temperature-related elasticity tensor displays different behavior. In order to illustrate the authenticity of results obtained by the temperature-related BCB multi-scale model, two numerical examples were simulated at different temperatures and the results were compared with the fully atomistic model. It has been shown that the technique provides promising results for facile modeling of boundary effect on thermo-mechanical behavior of metallic nano-scale devices.

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Table 1. The computational procedure of the temperature-dependent multi-scale BCB model

For each time step $\Delta t = t_{n+1} - t_n$

i) Set the incremental prescribed displacements as initial boundary conditions for the thermo-mechanical analysis,

ii) Set the incremental prescribed temperatures as the surface boundary conditions for the heat transfer analysis,

iii) Set the type of BCB elements by introducing the quadratures, their direction, representative atoms, and their characteristics for the micro-scale computation,

iv) Continue the following steps for each iteration $i$ within the time step $(t_n, t_{n+1})$,

FE modeling of heat transfer analysis

v) Construct the capacity matrix $C$, the conductivity matrix $H$ and the thermal load vector $g$ for the evaluation of nodal temperatures at iteration $i$,

vi) Solve the heat conduction finite element equation (33) to obtain the values of temperature at each nodal point,

vii) Evaluate the thermal expansion/contraction strain $\Delta \varepsilon$ due to changes of temperature using $\Delta \varepsilon = \alpha_T \Delta T$,

viii) Set the values of thermal strain as the equivalent nodal forces for the nonlinear thermo-mechanical analysis,

FE modeling of thermo-mechanical analysis

ix) Construct the material and geometric stiffness matrices, $K^{mat}$ and $K^{geo}$ given in (27) using the values of stress tensor and elasticity tensor obtained from the atomistic model at previous iteration (xv),

x) Substitute the material and geometric stiffness matrices obtained from (ix) together with the values of thermal strain obtained from step (viii) into equation (23),

xi) Solve the thermo-mechanical finite element (23) to obtain the nodal displacements at iteration $i$,

xii) Set the deformation gradient tensor $F$ and temperature $T$ obtained from steps (vi) and (xii) as the initial boundary conditions of the micro-scale computation,

Molecular dynamics computation

xiii) Evaluate the first Piola-Kirchhoff stress tensor $P_{ij}$ and the first elasticity tensor $C_{ijkl}^1$ for each atom using relations (9) and (11) based on the deformation gradient tensor and temperature obtained from step (xii),

xiv) Obtain the Cauchy stress tensor and Truesdell elasticity tensor for each atom using the temperature-related Cauchy Born given in (10) and (18),

xv) Determine the Cauchy stress tensor and Truesdell elasticity tensor at each quadrature point by transferring the data from the atomistic model based on the concept of the surface, edge, and corner elements defined in (37–39),

Check the convergence criteria in the nonlinear thermo-mechanical analysis. If the convergence is satisfied, the analysis is carried out at the next time step.
Figure 1. Description of reference surface element and its configuration with respect to atomistic model

Figure 2. Description of reference edge elements and configuration of representative edge atoms with respect to integration points
Figure 3. The variations of stiffness tensor component (1, 1) with the deformation gradient at different temperatures
Figure 4.
Figure 4. Modeling of a nano-scale ring; The evolution of stress $\sigma_x$ contours in temperature-related Cauchy Born model at various temperatures; a) zero temperature, b) 140°K, c) 145°K, d) 165°K, e) 180°K, f) 195°K. (Figures at the left-hand-side display no temperature effect in elasticity tensor and figures at the right-hand-side represent the temperature-related elasticity tensor)
Figure 5.
Figure 5. The distribution of stress $\sigma_x$ contours for a nano-scale cube in the temperature-related CB model at various temperatures; a) $160^\circ$K, b) $170^\circ$K, c) $175^\circ$K, d) $180^\circ$K, e) $215^\circ$K. (Figures at the left-hand-side display no temperature effect in elasticity tensor and figures at the right-hand-side represent the temperature-related elasticity tensor)
Figure 6. Modeling of nano-scale cube; The evolution of stress components at the center, surface and edge lines of the cube
Figure 7.
Figure 7. The evolution of stress $\sigma_x$ contours for a nano-scale cube at various temperatures; a) zero temperature, b) $125^\circ K$, c) $250^\circ K$, d) $375^\circ K$, e) $500^\circ K$. A comparison between the molecular dynamics simulation and the temperature-related BCB multi-scale model.
Figure 8. The evolution of stress $\sigma_x$ along the line passed through the center of cube

Figure 9. The evolution of stress $\sigma_x$ along the line passed through the surface of cube
Figure 10. The evolution of stress $\sigma_x$ along the line passed through the edge of cube.

Figure 11. The evolution of shear stress $\sigma_{xy}$ along the line passed through the surface of cube.
Figure 12.
Figure 12. The evolution of stress $\sigma_x$ contours for a nano-scale ring at various temperatures; a) zero temperature, b) 125$^\circ$K, c) 250$^\circ$K, d) 375$^\circ$K, e) 500$^\circ$K. A comparison between the molecular dynamics simulation and the temperature-related BCB multi-scale model.