Computational Materials Science xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

The calculation of mechanical behavior for metallic devices at nano-scale based on Atomic–Continuum Coupled model

Bowen Li [a,*], Junzhi Cui [a], Xia Tian [b], Xingang Yu [c], Meizhen Xiang [d]

[a] Academy of Mathematics and System Science, Chinese Academy of Sciences, China
[b] College of Mechanics and Materials, Hohai University, China
[c] School of Physics, University of Chinese Academy of Sciences, China
[d] Institute of Applied Physics and Computational Mathematics, China

ARTICLE INFO

Article history:
Received 14 November 2013
Received in revised form 1 February 2014
Accepted 4 February 2014
Available online xxxx

Keywords:
Atomic–Continuum Coupled (ACC) model
Representative volume element (RVE)
Basic deformation element
Stress tensor
Single-crystal Cu nanowire

ABSTRACT

Atomic–Continuum Coupled (ACC) model is a nonlocal model which couples the continuum mechanics with atomic model. It is proposed by Xiang et al. (2011). The model is modified and improved to study the mechanical behavior for metallic devices at nano-scale in this paper. Some essential concepts coupling molecular dynamics with continuum mechanics are defined, such as representative volume element (RVE), atomic occupation coefficient, basic deformation element, deformation environment and so on. The computable formulae of some mechanical quantities, including deformation gradient, strain and stress tensor, etc., are derived in detail. And all those for the single-crystal Cu nanowire under tension and bending are numerically calculated. The results show the inhomogeneity of strain and stress tensor in Cu nanowire under tension and bending.

1. Introduction

The proposition of "Materials Genome Initiative" arouses scientist's enthusiasm to study the physical, chemical and mechanical behaviors of materials, especially on their relation between the physical quantities at different scales, to provide theoretical foundation for revealing the function and performance of materials.

As our attention is limited to macroscopic mechanical behavior of materials, continuum mechanics is inevitable. The thermodynamical behaviors of materials, such as the deformation gradient, strain, stress, elasticity tensor and temperature, are all treated as the continuous fields. On the other hand, as we focus on the micro-scale, the atomic model (e.g. Molecular Dynamics model) is adopted to probe the physical/mechanical performances and only the position and velocity of each atom is recorded. However, as the physical/mechanical behavior in meso-scale is probed from microns to nanometers, neither the continuum model nor the atomic model is quite effective. For this reason, so many scientists have developed some coupled multi-scale models. And those can be divided into two classes [1]: one is called mixing method, which directly or concurrently couples MD model with continuum one, such as quasi-continuum method (QC) proposed by Tadmor et al. [2] and Miller and Tadmor [3], coarse-grained molecular dynamics (CGMD) by Rudd and Broughton [4], bridging scale method by Wagner and Liu [5], the heterogeneous multi-scale methods by Engquist and E [6] and so on. The other is the generalized continuum model which is based on atomic interaction; see Eringen [7,8].

Xiang et al. [9,10] proposed the Atomic–Continuum Coupled (ACC) model which is based on the atomic interactive potential to construct nonlocal stress–strain relationship in a representative volume element between molecular dynamics and continuum mechanics. However, Xiang did not provide the well-defined computational method for it, and neither gave the numerical simulations for 3D micro-nano scale devices to verify its validity.

The effective algorithms on ACC model are systematically discussed, and numerical simulations for 3D metallic nanowire are shown in this paper. In particular, starting from the atomic model (MD), and then the position of each atom inside the RVE is utilized to construct basic deformation element, deformation environment and nonlocal stress–strain relation.

The rest of paper is arranged as follows: In Section 2, the basic concepts of ACC model for metallic micro-nanometer structure is introduced. In Section 3, the expressions of stress and strain tensor are given. In Section 4, the algorithms are described. In Section 5, some numerical results for single-crystal Cu nanowire under tension and bending are shown. The last section is the conclusion.

2. The essential concepts of ACC model

In this section, some essential concepts of ACC model are defined, including the decomposition of atomic motion, the atomic

* Corresponding author. Tel.: +86 18610881811.
E-mail address: libowen@lsec.cc.ac.cn (B. Li).

http://dx.doi.org/10.1016/j.commatsci.2014.02.002
0927-0256/

model, the representative volume element (RVE), basic deformation element and deformation gradient, etc.

2.1. Structural deformation of atomic cluster

The derivation of ACC model relies on the conservation of mass, momentum and energy. In continuum thermodynamics, structural deformation and thermal vibration are expressed by displacement and temperature fields, respectively. However, in atomic models, system state is only determined by atomic positions and their derivatives with respect to time t. In order to establish the coupled dynamic relationship between atomic model with continuum one, it is necessary to abstract the structural deformation part from atomic motion, it means that it is necessary to decompose the atomic motion into two parts: structural deformation and thermal vibration

$$\begin{aligned} x_\alpha &= \bar{x}_\alpha + \tilde{x}_\alpha \\ \dot{x}_\alpha &= \dot{\bar{x}}_\alpha + \dot{\tilde{x}}_\alpha \end{aligned},$$

where x_α and $\dot{x}_\alpha$ are the instantaneous position and velocity of atom α respectively, $\bar{x}_\alpha$ and $\dot{\bar{x}}_\alpha$ the structural deformation and velocity of atomic cluster at atom α, $\tilde{x}_\alpha$ and $\dot{\tilde{x}}_\alpha$ the thermal vibration components of atom α around $\bar{x}_\alpha$ and $\dot{\bar{x}}_\alpha$, respectively. In other words, $\bar{x}_\alpha$ represents the local deformation of microstructure, and $\tilde{x}_\alpha$ the high-frequency vibration in the vicinity of equilibrium position which have no effect upon structural deformation of atomic cluster, for the frequency corresponding to thermal vibration is much higher than one to the structural deformation.

In this paper, only the mechanical behavior for metallic nanowire is discussed. Hence, in order to eliminate the noises induced by atomic thermal vibrations, it is necessary to introduce the averaging operator for the position of each atom with respect to time t in a time period including present moment while computing the continuum mechanical quantities in ACC model. And it is very important to choose the suitable time interval. Generally speaking, the frequency of thermal vibration of nano-scale micro-structure is between 0.5 THz and 50 THz, while the frequency of micro-structural deformation is about 2 GHz at most, except for the vibration induced by laser [11–13]. If taking 0.5 THz as the lower limit of cut-off frequency, the time period greater than 2 ps (1/(0.5 THz)) is chosen for time averaging. In the tension and bending simulations of single-crystal Cu nanowire below, the period 2 ps is chosen to eliminate high-frequency thermal vibrations to obtain the micro-structural deformation component.

2.2. Atomic model

Suppose atomic interactions subject to Newton Second Law. Consider a local system which is composed of M atoms inside a structure. According to atomic theory, the potential function of the system can be expressed as

$$\begin{aligned} U(q_1, q_2, \ldots, q_M) &= \sum_\alpha V_1(q_\alpha) + \frac{1}{2}\sum_{\alpha,\beta} V_2(q_\alpha, q_\beta) \\ &\quad + \frac{1}{6}\sum_{\alpha,\beta,\gamma} V_3(q_\alpha, q_\beta, q_\gamma) + \cdots \\ &= \sum_\alpha U_\alpha, \end{aligned} \tag{1}$$

where q_α is the instantaneous position of atom α, V_1 the external potential, V_2 the pair potential between atoms, $V_n (n \geqslant 3)$ n-body potential. U_α is called site energy of atom α

$$U_\alpha = V_1(q_\alpha) + \frac{1}{2}\sum_\beta V_2(r_{\alpha\beta}) + \frac{1}{6}\sum_{\beta,\gamma} V_3(r_{\alpha\beta}, r_{\alpha\gamma}) + \cdots, \tag{2}$$

where $r_{\alpha\beta} = x_\alpha - x_\beta$ is the distance between atom α and β in current configuration. The interaction between atoms is completely determined by their relative positions.

Suppose that the interaction between atoms can be written as Eq. (2). There are also many different potential functions, such as LJ potential, EAM potential and Tersoff potential, all satisfy this requirement. However, some potential functions obtained by quantum mechanics cannot be expressed as Eq. (2) directly which need to be processed, and they will not be under consideration in this paper.

2.3. Representative volume element

The microstructure of solid materials can be characterized by atomic cluster Λ_r, as shown in Fig. 1, which is comprised of all the atoms belonging to the domain Ω_r. Ω_r is called representative volume element (RVE), and is also considered as a part of continuum. It is the basic element to study local mechanical behavior of materials by ACC model.

For the sake of calculating the total potential energy of atomic cluster Λ_r, the interaction between the atoms inside Λ_r and their neighboring atoms outside Λ_r cannot be ignored, and then mark the atoms set, which interact with the atoms inside Λ_r, as Λ_N. And the occupied domain Ω_N is called extended RVE.

In solid physics, the potential energy of Ω_r can be expressed as:

$$U_r = \sum_{\alpha\in\Lambda_r} \eta_\alpha U_\alpha, \tag{3}$$

where η_α is occupation coefficient of atom α inside RVE Ω_r in current configuration, and U_α the site energy of atom α. Occupation coefficient η_α is defined as

$$\eta_\alpha = \frac{|C_\alpha \cap \Omega_r|}{|C_\alpha|}, \tag{4}$$

where C_α is *Voronoi* cell of atom α inside Λ_N. It is defined strictly as

$$C_\alpha = \{X \in \Omega_N \mid |X - X_\alpha| \leqslant |X - X_\beta|,\ \forall\beta \in \Lambda_N \text{ and } \alpha \neq \beta\},$$

and $|C_\alpha|$ is the volume of C_α. It is not difficult to see that, actually, η_α indicates the energy contribution rate of atom α to RVE.

2.4. Consistent hypothesis of deformation environment

Deformation gradient in continuum mechanics is defined as:

$$F(X) = \frac{\partial x}{\partial X}. \tag{5}$$

The local mechanical behavior of material is characterized by atomic clusters. In order to connect discrete system with continua,

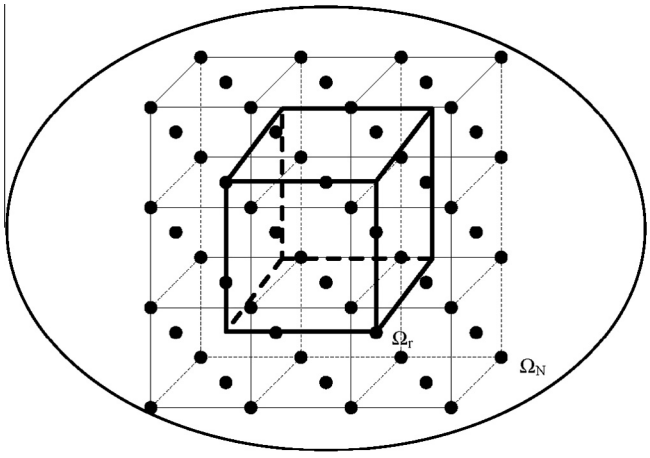

Fig. 1. RVE Ω_r and extended RVE Ω_N.