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A local Quantum–Atomistic–Continuum model for mechanical behaviors at micro-nano scale

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ABSTRACT

To study non-linear mechanical properties of materials from electronic structure information, we present a physics-based sequential model in this paper. We formulate the ground state strain energy functional to extract continuum description of mechanical quantities from quantum scale. For the large-scale Kohn–Sham density functional calculation, we use linear combination of small-scale interactions to approximate the initial many-body interaction. The expansion is taken to an even-order to keep both the precision and the surface effect. In our deformation framework, the low-frequency deformation part of total displacement is decoupled from the high-frequency thermal vibration. Basic elements are determined based on complex Bravais lattice. Continuum mechanical tensors, such as the Cauchy stress and the elastic constant, are explicitly derived from discrete atomistic system. To confirm the validation of our model, we simulate 3-dimensional single copper nanowires under external tension and bending, along with comparisons against other experimental results.

1. Introduction

Computational simulations are valuable tools for studying materials properties. Generally, atomistic-to-continuum (AtC) models are widely established and used as the properties are known to be majorly associated with 0-dimensional (points), 1-dimensional (lines) and 2-dimensional (faces) defects in 3-dimensional crystals [18]. Investigations of these models provided rigorous theoretical supports and effective computational techniques in the context of multi-mechanism researches.

In order to accurately describe the details of materials responses to external loads, proper initial parameters and boundary conditions are particularly needed. Thus extracting continuum quantities from discrete systems is a core task in current AtC models. Coarse-graining procedures are often required when micro-nano mechanical quantities are accepted by continuum equations. In line with Hardy's formulation [10], Delph [8] built general expressions for local stress tensors with multibody interatomic potentials. Combined with atomistic and continuum features, Chandraseker and Mukherjee [4] calculated elastic moduli and loading curves of single-walled carbon nanotubes (SWCNT). Cheng and Ngan [5] revealed the crystal structural transition process and the plasticity mechanism of the sintered nanoparticles. Based on the maximum plastic dissipation principle, Xu et al. [26] presented a finite hyperelastic–plastic constitutive model.

In most current AtC models, mechanical quantities are determined only by empirical functionals of distances between different structures. However, since material responses are investigated at micro-nano scale, the empirical functionals between particles and grains, which neglect quantum mechanics effects to some extent, are no longer accurate enough for multi-element system. Meanwhile, Kohn–Sham density functional theory (DFT) [12,15] was coded and applied to complex systems. Physical and chemical quantities obtained by first-principles calculations are confirmed by research findings [7, e.g.]. DFT models improved the precision without spurious physical assumptions. For further insights in materials properties, high efficient DFT computable models are still urgent to be developed for numerous atoms non-periodic systems.

Since the boundary conditions under different scales are generally incompatible, many models need special regions, overlapping regions in most cases, to link atom regions to continuum regions towards numerical convergence. It should be noted that the overlapping regions are not easy to be determined in real-time simulations, thus seamless method, such as Iyer et al. [13], is particularly required. For the same reason, the Atomic-Continuum-Coupled (ACC) model were developed by Xiang [25] and Li et al. [16].

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By considering the local quantum mechanics effects, we present a local Quantum–Atomistic–Continuum (QAC) model to study the physical nature of micro-nano mechanism in this paper. The "local quantum effects" means that calculations of total energy and atom energy actually reflect quantum interactions between nuclei and electrons. In what follows, our model suggests some new ideas to the current physics-based AtC models.

- The total quantum strain energy functional governs the coupling of different scales. Continuum descriptions of mechanical tensors are obtained by taking derivatives of the strain energy functional. The key steps involved are smearing functions for the position vector and coarse-graining procedures for the energy function from quantum scale. Thus atom region and continuum region can be linked consistently without overlapping areas.
- We employ a linear expansion method and truncate high-order terms to solve the huge task of Kohn–Sham DFT calculations. With this approximation, it becomes possible to simulate large-scale atomistic system. Besides, by performing traditional full DFT calculation, one can only get the ground state total energy instead of the energy of each atom, since the atom energy is equally regarded as E_{total}/N_{atom}. So one can only calculate the homogenized mechanical quantities. However, by our methods, we can get the anisotropic quantities, such as the elastic constants. The constitutive relation is also naturally involved.
- Most of micro-nano devices have particular structural topologies. Physical properties of these systems are known to be extremely sensitive to the variation of intrinsic structures. Dislocations and defects occur when micro-structures are disordered. Instead of using traditional finite element triangulations, we present two methods based on complex Bravais lattice to construct basic deformation elements.

The outline of this paper is as follows. In Section 2, a quick review of the ACC model is given. In Section 3, the quantum strain energy distribution of atomistic system is described. In Section 4, we introduce basic deformation elements and formulate continuum descriptions of strain, stress and other mechanical tensors explicitly. In Section 5, 3-dimensional numerical examples of single copper nanowires under external tension and bending are preformed to confirm our model, along with comparisons against other commonly used results. Conclusions are drawn in Section 6. The detailed derivations of equations in Section 4 are provided in Appendix A.

2. Review of the ACC model

The deformation assumption adopted in the ACC model [16] is the finite deformation. In the continuum framework, consider a one-to-one mapping φ from the reference configuration Ω_0 to the current configuration Ω_r. Suppose that the deformation environment of point X at continuum scale is uniform with that of a representative volume element (RVE) Λ_r centered at X at atomistic scale. Then for any point $X \in \Omega_0, x = \varphi(X) \in \Omega_r$. The deformation gradient tensor is defined as

$$F = \frac{\partial x}{\partial X} = \frac{\partial \varphi(X)}{\partial X}. \tag{1}$$

In order to derive continuum description from discrete system, we use a single value function

$$g(s) = \varphi(X + s(Y - X)) = \varphi(X + sR_{XY}). \tag{2}$$

In the current configuration, the distance between any two points x and y at continuum scale is

$$r_{xy} = y - x = \varphi(Y) - \varphi(X) = \int_0^1 \frac{\partial g}{\partial s} ds = \int_0^1 F(X - sR_{XY}) R_{XY} ds. \tag{3}$$

Furthermore, the right Cauchy strain tensor is

$$E = F^T F. \tag{4}$$

Consider a local atomistic system with M atoms. The interatomic potential function of the system can be expressed as

$$U(q_1, \cdots, q_M) = \sum_I V_1(q_I) + \frac{1}{2}\sum_{I,J} V_2(q_I, q_J) + \frac{1}{6}\sum_{I,J,K} V_3(q_I, q_J, q_K) + \cdots = \sum_I U_I, \tag{5}$$

where q_I is the position of atom I, V_1 is the external potential, V_2 is the pair potential, and V_n is the n-body potential. U_I is regarded as the potential energy of atom I. For metallic systems, the EAM potential is a common technique in current simulations

$$U_I = e\left(\sum_{J \neq I} \rho(r_{IJ})\right) + \frac{1}{2}\sum_{J \neq I} V_2(r_{IJ}). \tag{6}$$

Here e represents an embedding function accounting for effects of the free electrons in metals, and $\rho(r)$ is the electron density.

If we choose $\Lambda_{r'}$ larger than the union of Λ_r and cut-off radius of the EAM potential, interactions between atoms inside Λ_r and atoms outside $\Lambda_{r'}$ are 0. Then the strain energy density of Λ_r is

$$w_r = \frac{1}{V}\sum_{I \in \Lambda_r} U_I(x) = \frac{1}{V}\sum_{I \in \Lambda_r}\left\{ e\left(\sum_{J \in \Lambda_{r'}} \rho(r_{IJ})\right) + \frac{1}{2}\sum_{J \in \Lambda_{r'}} V_2(r_{IJ})\right\}, \tag{7}$$

where V is the reference RVE volume, and $I \in \Lambda_r$ means summing over all atoms in Λ_r. The first PK stress tensor and the Cauchy stress tensor can be derived sequentially by

$$P_{hK}(X) = \frac{\partial w_r}{\partial F_{hK}} = \frac{1}{V}\sum_{I \in \Lambda_r}\left\{ \frac{\partial e}{\partial \rho}\left(\sum_{J \in \Lambda_{r'}} \rho(r_{IJ})\right) \sum_{J \in \Lambda_{r'}} \int_0^1 \left[\left(\frac{\partial \rho(r')}{\partial r}\right)^h R_{IJ}^K\right] ds + \frac{1}{2}\sum_{J \in \Lambda_{r'}} \int_0^1 \left[\left(\frac{\partial V_2(r')}{\partial r}\right)^h R_{IJ}^K\right] ds \right\}, \tag{8}$$

$$\sigma = \frac{1}{\det(F)} P F^T = \frac{1}{2\det(F)}\left(P F^T + F P^T\right), \tag{9}$$

where the superscript $(\cdot)^i$ is the i-th coordinate component, and

$$r' = \int_0^1 F\left(X + (s' - s)R_{IJ}\right)\, ds' R_{IJ}. \tag{10}$$

For more details and essential concepts of the ACC model, see Li et al. [16]. This model extracts continuum descriptions of mechanical quantities from atomistic scale. However, the quantum mechanics effects are partly neglected in this model. In the next section, the quantum strain energy density functional will be introduced into the ACC model, and the numerical implementation for general cases will be discussed.

3. Quantum energy density of atomistic system

Let us consider a local atomistic system which is composed of N_{nucl} nuclei and n_{elec} electrons. In this section, uppercase variables are used for quantities of nuclei and lowercase variables are used for electrons. The Hartree atomic units are adopted so that the four fundamental physical constants are dimensionless, i.e. $m_e = e = 4\pi\varepsilon_0 = \hbar = 1$.