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macroscale mechanical loads**

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A multiscale molecular dynamics allowing macroscale mechanical loads

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Abstract – We proposed a novel multiscale molecular-dynamics model in order to apply macroscale boundary conditions to microscale molecular systems, which is difficult for classical molecular dynamics. Unlike in statistical mechanics, in which macroscale quantities such as temperature and pressure are collected from molecular information, the proposed approach is a reversed procedure to find optimal molecular states when macroscale conditions such as traction are enforced. The model is originated from Parrinello-Rahman molecular dynamics but extends it to solve finite-size, inhomogeneous molecular-dynamics problems by generalizing the representative volume element to a “material point” in continuum mechanics. An example of compressing a nickel nanowire is presented to demonstrate the capacity of the method to simulate localized phase transition in a finite-size molecular system, which validates the effectiveness of the method.

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Introduction. – Due to the fast development of computer and computational technology, molecular dynamics (MD) today has ability to trace the evolution of an atomistic system across vast spatiotemporal domains. Typically, millions of atoms and microsecond time scale are considered as routine [1]. In the predictable future, we will be empowered to develop engineering models by using molecular dynamics with incomparable precision at the atomistic level. For instance, we may use molecular dynamics to simulate the mechanical performance of a smart phone, design a future automobile, or even simulate an aircraft under extreme conditions.

However, even with unlimited computing power, it is questionable how to apply realistic macroscale boundary conditions such as traction in classical molecular dynamics. Based on our understanding, mechanical loads are applied on boundary particles in classical molecular dynamics [2,3]. But that is not realistic because most experiments or engineering models are implemented in macroscopic environments. In realistic cases with macroscopic definition, constraints on specific particles are strong since forces and displacements defined in macroscale are actually in statistical or average senses in the whole boundary domain. We term macroscopic boundary condition as “weak” condition. Thus applying

“weak” conditions in molecular system is a cross-scale manipulation. Typically, the communication between macroscopic scale and atomistic scale include bottom-up and top-down styles considering the direction of message passing. The bottom-up approach to interpret fundamental physics is in the category of statistical mechanics [4]. In this approach, the macroscopic quantities such as temperature and pressure are derived from lower scale atomistic positions and velocities in a statistical manner, *e.g.* [5,6]. However, the reversed top-down procedure to apply “weak” condition is not thoroughly described on what the molecular state should be under specific macroscopic conditions like traction, and it is an up-coming challenging field. Much effort has been made on multiscale simulation [7–10] to build connection between microscale with atomistic resolution and macroscale with continuum behavior. Those works mainly put emphasis on computational efficiency, while left the physical issues behind. In this work, we are attempting to keep track of the response of the particle system and to seek optimal molecular states when “weak” conditions are enforced.

Early attempts were reported in the literature in the 1980s. Andersen [11] first proposed an isoenthalpic-isobaric ensemble molecular dynamics allowing the volume of a cubic lattice cell to vary. Subsequently, Parrinello

and Rahman [12,13] extended Andersen’s formalism to anisotropic cases allowing both the volume and the shape of a molecular-dynamics cell to vary. Since then, the Parrinello-Rahman molecular dynamics (PR-MD) has become the standard MD method to apply constant stress in a static ensemble. Their approach for including macroscale stress in molecular-dynamical simulation is insightful. However, PR-MD is essentially based on a representative volume element (RVE) with periodic boundary condition, which is restricted to analyzing homogenous systems in an equilibrium ensemble. It is inherently incapable of studying inhomogeneous and non-equilibrium molecular-dynamics systems that have defects, stress concentration and localized phase transformation, etc.

In this paper, we propose a novel multiscale molecular-dynamics model in order to involve macroscale quantities into atomistic scale. In principle, this approach enables us to apply “weak” (macro) boundary conditions in a molecular system. The proposed multiscale molecular dynamics is influenced by the philosophy of PR-MD, but it extends the PR-MD formalism to accommodate non-periodical boundary conditions, inhomogeneous systems and dynamic process. As a demonstration, we implement the theory in simulating the dynamic behavior and phase transition of a nickel nanowire under constant traction.

Multiscale model. – As shown in fig. 1, we divide a system occupying domain Ω into several subsystems (supercells) Ω_α , where α is the index of supercells. The shape of each supercell is not necessary to be regular, and thus it can be made adaptive to fit the domain of the system. Consider a representing atomistic position \mathbf{r}_i in the α -th supercell by the following decomposition:

$$\mathbf{r}_i(t) = \mathbf{r}_\alpha(t) + \phi_\alpha(t) \cdot \mathbf{s}_i(t), \quad (1)$$

where \mathbf{r}_α is the center of mass of the α -th cell, ϕ_α is the deformation gradient of the α -th cell which is uniform for each cell and i is the index of atoms. The deformation gradient ϕ_α is a continuum mechanics concept that is used to describe the deformable state of a “material point”, which is a supercell in the molecular model. Each individual supercell is subjected to rotation and stretch under ϕ_α as the “material point” in continuum mechanics. However, continuity among supercells is not required because there might be gaps and overlaps in atomistic resolution when material defects are involved. Breaking the continuity ensures the independency of each cell. \mathbf{s}_i is the independent local coordinate of the i -th atom inside the supercell as internal degrees of freedom which control the pattern of atomistic distribution but do not influence ϕ_α which is the shape or contour of the cell. The product $\phi_\alpha \cdot \mathbf{s}_i$ is interpreted as the relative position to the center of mass. In continuum mechanics, the motion of a “material point” consists of rigid body translation, rotation and stretch, which are described by the deformation gradient. However, in the proposed multiscale molecular model, to capture atomistic motions, we require an independent variable $\mathbf{s}_i(t)$ that is a

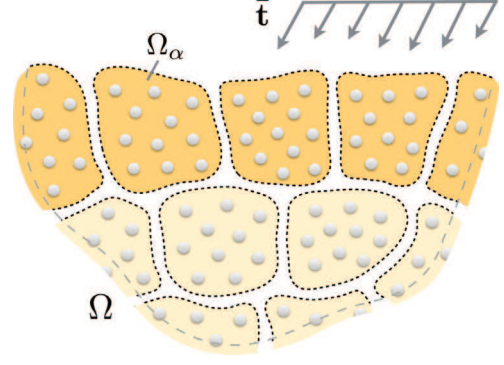


Fig. 1: (Color online) A molecular system is divided into several supercells. Each supercell is a material point standing on the level of continuum mechanics. The decomposition $\mathbf{r}_i = \mathbf{r}_\alpha + \phi_\alpha \cdot \mathbf{s}_i$ gives the atomic positions inside each cell. Boundary cells exposed to surface traction are marked in dark color, while the light color is used for interior cells.

function of time. Owing to the independence of each particle in the supercell, the decomposition (1) is equivalent to the full-scale atomistic representation. Thus, we establish a complete multiscale structure for a molecular system that span from continuum macroscale to atomistic scale. The multiscale kinematics structure offers convenience to study the statistical behavior of a molecular system. The Lagrangian of the α -th supercell is proposed as

$$\begin{aligned} \mathcal{L}_\alpha = & \frac{1}{2} M_\alpha \dot{\mathbf{r}}_\alpha \cdot \dot{\mathbf{r}}_\alpha + \frac{1}{2} \mathbf{J}_\alpha : (\dot{\phi}_\alpha^T \dot{\phi}_\alpha) \\ & + \frac{1}{2} \sum_{i \in \alpha} m_i \dot{\mathbf{s}}_i \cdot \mathbf{C}_\alpha \cdot \dot{\mathbf{s}}_i - V_\alpha^{int} - V_\alpha^{ext}, \quad (2) \end{aligned}$$

where M_α is the total mass of the supercell; m_i is the mass of the i -th atom; $\mathbf{J}_\alpha = \sum_i m_i \mathbf{s}_i(t) \otimes \mathbf{s}_i(t) \approx \sum_i m_i \mathbf{s}_i(t_0) \otimes \mathbf{s}_i(t_0)$ is the Euler inertia tensor of the α -th cell, which is approximately invariant in time [14]; $\mathbf{C}_\alpha = \phi_\alpha^T \phi_\alpha$; $V_\alpha^{int} = \frac{1}{2} \sum_{i \neq j} \varphi(r_{ij})$ is the internal potential energy given by pair interaction φ with r_{ij} the distance between i -th and j -th atoms inside the α -th cell, and V_α^{ext} is the external potential. Note that the kinetic energy in the Lagrangian is decoupled to the three terms which represent rigid body translation, cell motion and internal motion, respectively. The mix kinetic energy with cross-terms is negligible comparing with other terms. This simplification is suggested by Parrinello and Rahman [12,13], and it is explained in [15].

The essential part of the proposed Lagrangian is the external potential V_α^{ext} . Several sources may contribute to this term. The first contribution is from the interaction of particles surrounding the α -th cell, which gives

$$V_\alpha^{atom} = \sum_{i \in \alpha, j \neq \alpha} \varphi(r_{ij}). \quad (3)$$

Besides interatomic force, a supercell is sometimes exposed to external loads applied at remote distance. Loads in this

circumstance are macroscale forces, and they are usually in the form of surface traction $\bar{\mathbf{t}}_\alpha$ and body force $\bar{\mathbf{b}}_\alpha$ categorized in continuum mechanics. External potential energy of this kind can be expressed as

$$V_\alpha^{surface} = -S_\alpha^0 \bar{\mathbf{t}}_\alpha \cdot \mathbf{r}_\alpha, \text{ and } V_\alpha^{body} = -\Omega_\alpha^0 \bar{\mathbf{b}}_\alpha \cdot \mathbf{r}_\alpha, \quad (4)$$

where S_α^0 is the surface area exposed to $\bar{\mathbf{t}}_\alpha$ in the referential configuration, and Ω_α^0 is the referential volume of the α -th supercell. In eq. (4), we apply forces at the center of mass by assuming that higher-order terms such as rotation are negligible. The total external potential for the α -th supercell reads as

$$V_\alpha^{ext} = V_\alpha^{atom} + V_\alpha^{surface} + V_\alpha^{body}. \quad (5)$$

There is one more case worth noting in which a supercell may also have a prescribed stress state. In this case, the external potential energy should be the work conjugation of stress and strain. As an example, we prescribed the first Piola-Kirchhoff (PK-I) stress $\bar{\mathcal{P}}_\alpha^{ext}$ [16] at the traction boundary, and the external potential energy is

$$V_\alpha^{stress} = -\bar{\mathcal{P}}_\alpha^{ext} : \phi_\alpha \Omega_\alpha^0. \quad (6)$$

Stress is an overall effect of thermodynamical states of the particle ensemble, so that we can replace V_α^{ext} by V_α^{stress} in eq. (5) depending on the problem of interest.

The Lagrange equations of motion based on variables \mathbf{r}_α , ϕ_α and \mathbf{s}_i are derived through standard procedure, and they are written as

$$M_\alpha \ddot{\mathbf{r}}_\alpha = \sum_{i \in \alpha, j \neq \alpha} \mathbf{f}_{ij} + S_\alpha^0 \bar{\mathbf{t}}_\alpha + \Omega_\alpha^0 \bar{\mathbf{b}}_\alpha, \quad (7)$$

$$\ddot{\phi}_\alpha \cdot \mathbf{J}_\alpha = \left(\mathcal{P}_\alpha^{ext} - \mathcal{P}_\alpha^{int} \right) \Omega_\alpha^0, \quad (8)$$

$$m_i \mathbf{C}_\alpha \cdot \ddot{\mathbf{s}}_i = \sum_{j \neq i} \mathbf{f}_{ij} \cdot \phi_\alpha - m_i \dot{\mathbf{C}}_\alpha \cdot \dot{\mathbf{s}}_i, \quad (9)$$

where $\mathbf{f}_{ij} = \varphi'(r_{ij}) \hat{\mathbf{r}}_{ij}$ is the pair force with $\hat{\mathbf{r}}_{ij}$ being the unit vector point from the i -th atom to the j -th atom, and

$$\mathcal{P}_\alpha^{int} = \frac{1}{\Omega_\alpha^0} \sum_{i \in \alpha} \left(-\phi_\alpha m_i \dot{\mathbf{s}}_i \otimes \dot{\mathbf{s}}_i + \frac{1}{2} \sum_{j \in \alpha} \mathbf{f}_{ij} \otimes \mathbf{s}_{ij} \right), \quad (10)$$

$$\mathcal{P}_\alpha^{ext} = \frac{1}{\Omega_\alpha^0} \sum_{i \in \alpha, j \neq \alpha} \mathbf{f}_{ij} \otimes \mathbf{s}_i \quad (11)$$

define the internal and external first Piola-Kirchhoff stresses, respectively. Note that the applied external PK-I stress is a dead load, which is independent of the surface traction $\bar{\mathbf{t}}_\alpha$ and surface body force $\bar{\mathbf{b}}_\alpha$. The above equations are derived for the case in eq. (5). However, if the case of eq. (6) is considered, we simply replace \mathcal{P}_α^{ext} by a prescribed value.

Equations (7)–(9) are essential but incomplete for the proposed multiscale MD model. Note that the decomposition in eq. (1) is not unique. For example, at a given

time t , atomistic position can be

$$\begin{aligned} \mathbf{r}_i(t) &= \mathbf{r}_\alpha(t) + \phi_\alpha(t) \cdot \mathbf{s}_i(t) \\ &= \mathbf{r}_\alpha^*(t) + \phi_\alpha^*(t) \cdot \mathbf{s}_i^*(t) \end{aligned} \quad (12)$$

for different sets of \mathbf{r}_α , ϕ_α and \mathbf{s}_i . However, as discussed before, physical interpretations of \mathbf{r}_α and ϕ_α must be hold, namely, ϕ_α and \mathbf{r}_α should represent the deformation gradient and the center of mass, respectively. Recall that \mathbf{s}_i only changes the internal pattern of atomistic distribution (the microstate). After the decomposition, the motion in \mathbf{s}_i space should be constrained so that it will not introduce macroscale deformation or rigid body motion of the supercell (the macrostate). With these considerations, we need to impose constraints to enforce these conditions. In practice, we may recalculate \mathbf{r}_α after a fixed number time steps by using

$$\mathbf{r}_\alpha = \sum_i m_i \mathbf{r}_i / \sum_i m_i. \quad (13)$$

Considering that the deformation gradient may be non-unique, we may use the following map to pull ϕ_α^* back to ϕ_α :

$$\phi_\alpha \cdot \mathbf{s}_i = \phi_\alpha^* \cdot \psi_\alpha \cdot \psi_\alpha^{-1} \cdot \mathbf{s}_i^*. \quad (14)$$

This manipulation can ensure the uniqueness of ϕ_α , if we can find a proper ψ_α . The detailed technique on how to construct ψ_α will be reported in a separate paper.

Moreover, as mentioned before, there is no requirement on the initial cell shape, so that it can be anything that fits the boundary geometry. However, during evolution, we describe the deformation by a uniform ϕ_α in each cell. Thus, the shape change must be homogeneous, or piecewise constant. From this consideration, the cell size cannot be too big. Note that the homogeneous deformation has nothing to do with the internal pattern \mathbf{s}_i . It is about the contour of the cell at the macroscopic level. On the other hand, the cell size cannot be too small. This is because a minimum number of particles is required, so that it guarantees the average quantities of each cell being statistically meaningful.

Example. – We have studied dynamical responses and phase transition of a nickel nanowire under constant traction with the proposed multiscale model. Mechanical behaviors of bulk Ni such as stress-strain relations [17], phase transition [13], etc. were extensively studied. Finite diameter nanowire, which is different from bulk metal, has mechanical properties largely depending on the surface-volume ratio, surface energy, crystallographic orientation, etc., and it has attracted much attention in the past decade, see *e.g.* [18–21]. Equations (7)–(9) enable us to describe the behavior of a nanowire when the macroscale traction is applied to the end boundary of the nickel nanowire, as shall be discussed subsequently. The example is for demonstration purpose rather than solving a realistic large scale problem.

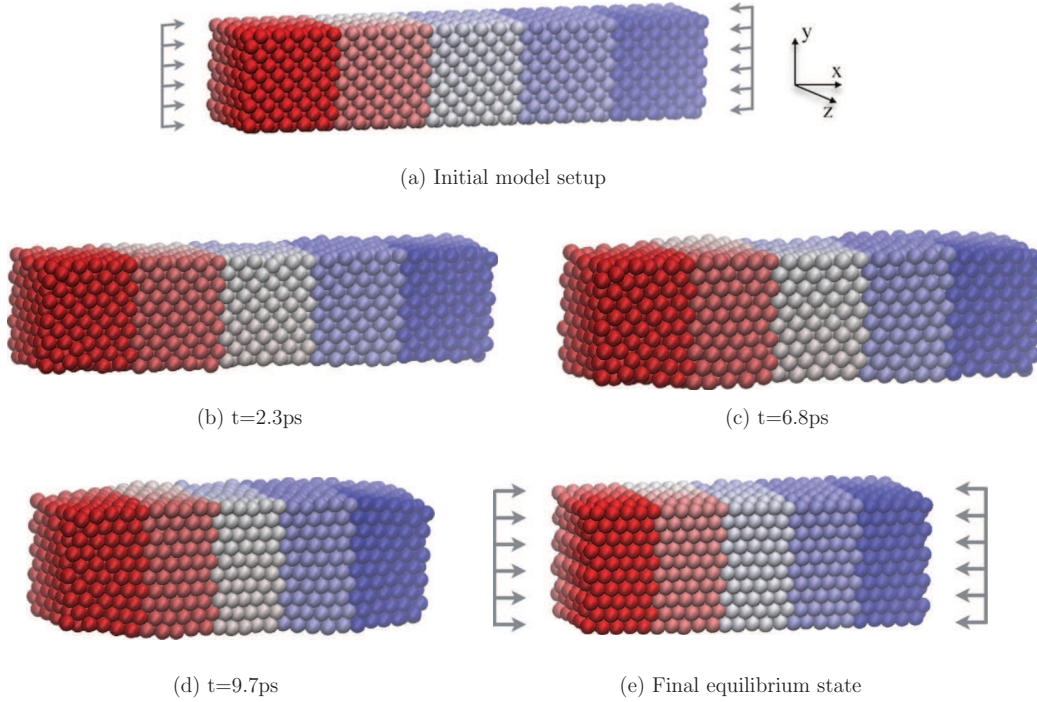


Fig. 2: (Color online) Initial (a), final (e) configuration of the nanowire when a constant surface traction of $\bar{t} = 1.66$ GPa is symmetrically applied on its both ends, and snapshots (b)–(d) of the propagation of phase transition. Gradient colors are used to distinguish cells.

The simulation model of the nickel nanowire is divided into $5 \times 1 \times 1$ supercells, and each supercell has $5 \times 5 \times 5$ unit cells. As is shown in fig. 2(a), different colors were used to distinguish the five supercells. The nanowire consists of 2500 atoms in total. Atomic positions were generated as face-center-cubic (F.C.C.) structure according to metal crystallography. The lattice constant $a = 0.352$ nm which makes the length of the Ni nanowire 8.8 nm, and the cross section of the nanowire is 1.58×1.58 nm². The axial orientation of the wire is $\langle 100 \rangle$ along the $x_1(x)$ -coordinate, and lateral directions $\langle 010 \rangle$ and $\langle 001 \rangle$ correspond to $x_2(y)$ and $x_3(z)$ coordinates. The Ni lattice is modeled using the pairwise Morse potential [22] with the parameters fitting to the lattice constant and elastic constants. During the entire procedure, the temperature is controlled around 350 K by the standard thermostat technique in molecular dynamics. The equation of motion, eq. (7), is integrated by using the Velocity Verlet method [23], and eqs. (8), (9) are solved by using a sixth-order predictor-corrector algorithm [24]. The integration time steps used in simulation are 0.0015 ps, 0.0012 ps and 0.00015 ps for each scale.

At the beginning of the calculation, the nanowire is relaxed in a stress free state for 5000 steps in order to reach a minimum energy configuration. The change of wire length and the change of the cross-section area are less than 1% comparing to the initial configuration. We then apply compressive traction $\bar{t} = 1.66$ GPa on both ends of the nanowire as shown in fig. 2(a). The traction remains constant throughout the simulation in the $\langle 100 \rangle$ direction.

Figures 2(b)–(d) show a series of snapshots of the loading history. At the beginning, when $t < 3$ ps, an elastic wave propagates through the nanowire, and the entire structure is in a state of linear elastic deformation with non-uniform stretches along the wire as observed in fig. 2(b). However, during this stage, the entire nanowire almost stays in the F.C.C. phase. Subsequently, phase transformation initiates at both ends, and it quickly propagates to the center, as shown in fig. 2(c), (d). After $t = 10$ ps, the entire nanowire turns into the hexagonal-close-packed (H.C.P.) phase. Based on the morphology of the final equilibrium configuration shown in fig. 2(e), the original $\{001\}$ planes in F.C.C. switches to $\{0001\}$ closely packed planes in the H.C.P. phase. The phase transformation results in lattice constant changes, and the new lattice constants $a = 0.249$ nm and $c = 0.41$ nm indicate the formation of a H.C.P. structure. To this end, the length of the nanowire changes to 6.25 nm that is 0.71 times the original length. Note that these values are averaged throughout the entire nanowire.

We have recorded the evolution history of the nanowire length in time under the surface traction of different magnitudes. We plot the curves of the stretch (L/L_0) for several compressive loads \bar{t}_x in fig. 3. For $\bar{t}_x = 0.33$ GPa and $\bar{t}_x = 0.67$ GPa, the stretch oscillates for about 50 ps then gradually reaches an equilibrium state around 1. The periods of vibration are about 11 ps and 12 ps, respectively. Since the length does not change significantly, the lattice structure is still F.C.C. with some sort of elastic

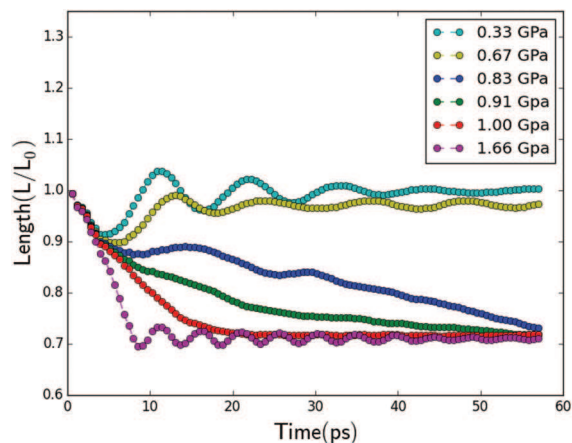


Fig. 3: (Color online) Convergence of normalized length (L/L_0) with time. For small traction, *i.e.* $\bar{t}_x = 0.33$ GPa and $\bar{t}_x = 0.67$ GPa, the nanowire went through oscillation but still in the elastic limit of F.C.C. for bigger traction from $\bar{t}_x = 0.83$ GPa to $\bar{t}_x = 1.0$ GPa, the normalized length gradually converged to about 0.7 and rest in that new H.C.P. configuration. For even bigger traction, the nanowire experienced long oscillation as for small traction after a rapid phase transition.

deformation, and the vibration of the curve reflects the elastic wave propagation. We also observe that when $\bar{t}_x = 1.66$ GPa, the curve has a similar dynamic response of vibration with a period about 5 ps. But the final stretch of the nanowire in static state is around 0.7. Compared to the result discussed above, this is the stretch ratio between H.C.P. and F.C.C. lattices. Before the elastic vibration in the new H.C.P. configuration, the stretch approaches quickly to the value about 0.7 within 10 ps. This is the time frame for phase transition. If we examine fig. 2, the loading history shown is in the range of 0–10 ps. The curves at $\bar{t}_x = 0.83$ GPa, $\bar{t}_x = 0.91$ GPa and $\bar{t}_x = 1.0$ GPa reveal a critical gradual damping process. When the stretch reaches 0.7, the nanowire simply stops vibration. The speed of convergence increases as the traction increases. The range around the above tractions is the critical domain that can activate the phase transition.

We have also calculated the traction-stretch relation for the nanowire, and we plot the result in fig. 4. As the compressive surface traction increases, the stretch (normalized length) decreases following the curve in Path I, until a critical value is reached at about 0.8 GPa. The structure then jumps to another curve which is marked as Path II. These two paths reflect the linear elastic deformations of the two distinct structures of F.C.C. and H.C.P. within their own ranges, and they are separated at a critical point. As we unload the traction gradually from the new H.C.P. structure (Path II), we find that the curve goes straight up (Path III) without turning back to the original F.C.C. structure. Apparently the new structure is stable under further loading/unloading. Note that all the data are obtained from the final equilibrium states.

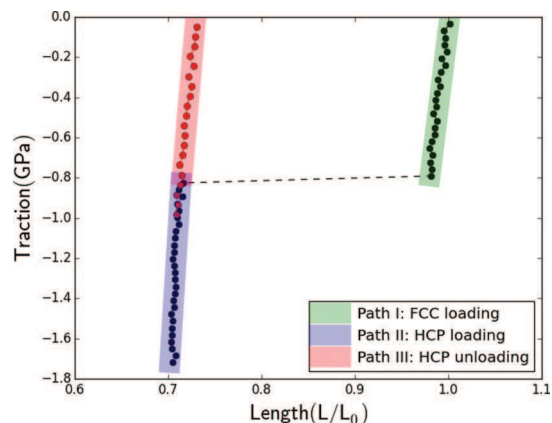


Fig. 4: (Color online) Traction-length relation for the nanowire in equilibrium state. The loading and unloading directions are all along the axial direction of the nanowire.

Summary. — In conclusion, the proposed multiscale molecular dynamics can seamlessly incorporate macroscale quantities into molecular systems, so that we can apply macroscopic boundary conditions such as traction in molecular simulations. Moreover, the proposed method generalizes PR-MD to solve realistic problems without the restriction of periodic boundary condition, while all salient features of PR-MD are preserved. In other words, the proposed multiscale MD can solve finite-size, inhomogeneous, dynamic problems. As an example, we use the method to calculate the dynamic evolution and phase transition of a nanowire to illustrate the capability of the theory of handling traction boundary condition. We showed that original F.C.C. nickel nanowire transits to H.C.P. configuration when the compressive load exceeds a critical value. The surface traction also leads to dynamic vibration either in elastic range of F.C.C. or in new phase of H.C.P. except in the critical transition domain. The loading-unloading process further examined the material property before and after the transformation. The results demonstrate that this new multiscale molecular-dynamics method is promising, and it has some potential applications that may not be achievable by conventional molecular dynamics.

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