

SELF-ADAPTIVE MOLECULE/CLUSTER STATISTICAL THERMODYNAMICS METHOD FOR QUASI-STATIC DEFORMATION AT FINITE TEMPERATURE**

Hao Tan^{1,2} Haiying Wang^{1*} Mengfen Xia³ Fujiu Ke⁴ Yilong Bai¹

⁽¹⁾ State Key Laboratory of Nonlinear Mechanics (LNM), Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China)

⁽²⁾ Graduate University of Chinese Academy of Sciences, Beijing 100871, China)

⁽³⁾ Physics School of Peking University, Beijing 100871, China)

⁽⁴⁾ School of Physics and Nuclear Energy Engineering, Beijing University of Aeronautics and Astronautics, Beijing 100191, China)

Received 20 September 2010, revision received 29 January 2011

ABSTRACT Hybrid molecule/cluster statistical thermodynamics (HMCST) method is an efficient tool to simulate nano-scale systems under quasi-static loading at finite temperature. In this paper, a self-adaptive algorithm is developed for this method. Explicit refinement criterion based on the gradient of slip shear deformation and a switching criterion based on generalized Einstein approximation is proposed respectively. Results show that this self-adaptive method can accurately find clusters to be refined or transferred to molecules, and efficiently refine or transfer the clusters. Furthermore, compared with fully atomistic simulation, the high computational efficiency of the self-adaptive method appears very attractive.

KEY WORDS self-adaptive, slip shear deformation, particle method approximation, refinement criterion, switching criterion

I. INTRODUCTION

The advent of nanotechnology has necessitated a better understanding of how microstructural changes at the atomic level would affect the macroscopic properties of materials. However, our ability to model the material performance is quite limited. On nanometer scale, the most direct and popular simulation approach is the molecular dynamics (MD) method^[1]. An appealing feature of MD is that it follows the actual dynamical evolution of all atoms, but, for realistic systems, it is practically impossible to track all atoms by solving the equations of motion^[1]. More importantly, to resolve individual motion of atoms requires a time step of approximately femtoseconds, so that even on the most advanced massively paralleled computers, to simulate a process lasting microseconds is very difficult. Although a number of multi-scale methods have been proposed to link MD to meso- or macro-scale simulation approaches^[2-9], the inherent short time scale limitation of MD remains a stubborn problem.

* Corresponding author. Email: why@lnm.imech.ac.cn

** Project supported by the National Natural Science Foundation of China (Nos. 10932011, 10772181, 10732090, 10772012 and 11021262) and the National Basic Research Program of China (No. 2007CB814803).

Motivated by these facts, Tadmor et al.^[10,11] and Shenoy et al.^[12,13] proposed the quasi-continuum (QC) method to simulate the quasi-static deformation at 0K. The key idea of QC is kinematic slavery in which by virtue of finite element method(FEM), the positions of the majority of atoms are entirely constrained and determined only by the displacements of those nodes (repatoms or representative atoms) tied to the element that includes the atoms. The positions of all nodes at 0 K can be obtained by minimizing the coarse-grained potential energy of the system. They also applied the idea of kinematic slavery to MD simulation at finite temperature and proposed finite-temperature quasi-continuum method^[7]. It is shown that although the simulation can be considerably sped up at finite temperature, the total simulation time is usually limited to nanoseconds.

On the other hand, based on the statistical thermodynamics formulation of Helmholtz free energy of molecules and its minimization, Hu et al.^[14] and Wang et al.^[14,15] proposed a group of statistical thermodynamics methods, that is, molecule statistical thermodynamics (MST) method, cluster statistical thermodynamics (CST) method; and the hybrid molecule/cluster statistical (HMCST) method. The basic idea of these methods is that each molecule of a system is considered as oscillator and particle simultaneously based on statistical thermodynamics theory^[16]. Due to their ‘seamlessness’ or consistency in the underlying atomistic models in all regions of molecules and clusters, these methods can avoid the ghost force in the simulation. In addition, compared with conventional MD simulations, their high computational efficiency appears very attractive. However, in the proposed method, the regions of molecules and clusters are partitioned prior to the simulation, which hinders the further improvement of computational efficiency.

In this paper, we develop a self-adaptive molecule/cluster statistical thermodynamics method for quasi-static deformation at finite temperature. With the self-adaptive method, a cluster can be automatically refined when the criterion exceeds a prescribed value. And finally, when the size of cluster gets smaller than the cut-off distance of molecular interaction, the cluster will be automatically changed into molecules. We prove the effectiveness and the efficiency of the self-adaptive scheme with the 2-dimensional simulation of one-axial compression.

II. HYBRID MOLECULE/CLUSTER THERMODYNAMICS METHOD

The hybrid molecule/cluster thermodynamics method is a combination of molecule statistical method (MST) and cluster statistical method (CST). At nonzero temperature, the atoms in a solid merely oscillate about their equilibrium positions when no external load is applied. If an external load is applied, the equilibrium positions of atoms will alter, resulting in the deformation of the solid. In MST method, each atom is considered as oscillator and particle simultaneously, that is, when we investigate the detail of lattice deformation, the atom is treated as particle with determined equilibrium position; when we examine the contribution of thermal oscillation to the mechanical deformation of the atomic lattice; the atom is regarded as oscillator with various frequencies. In addition, three important assumptions are adopted in MST method: (1) the oscillations of atoms in a solid are harmonic^[17]; (2) classical limit is satisfied; (3) the coupling of oscillations of different atoms is negligible (local harmonic approximation)^[18]. Hence, the Helmholtz free energy of system is

$$A = \Phi_0 + 3kT \ln \left[\left(\frac{\hbar}{kT} \right)^N |\mathbf{D}|^{1/6} \right] \quad (1)$$

where A is Helmholtz free energy of system, and Φ_0 is sum of inter-atomic potential energies, k is Boltzmann’s constant, T is the temperature, \hbar is Planck’s constant, and \mathbf{D} is the local dynamical matrix of all the atoms in the system, which can be expressed as

$$D_{ij}^{\xi\eta} = \frac{1}{\sqrt{m_i m_j}} \frac{\partial^2 \Phi}{\partial x_{i\xi} \partial x_{j\eta}} \quad (2)$$

where m_i is the mass of atom i , $x_{i\xi}$ is the ξ th coordinate of atom i .

In case of large system, the MST method still has the limitation of data storage requirement since too many atoms need to be dealt with. In order to reduce the degrees of freedom, we develop a coarse-grained MST method, which is cluster statistical thermodynamics method (CST). In CST method, the system

is partitioned into several atomic clusters and each cluster is treated by statistical thermodynamics as subsystem of finite atoms. The Helmholtz free energy A of the whole system is supposed as the summation of the free energy A_α of cluster α , i.e.

$$A = \sum_{\alpha}^{N_c} A_{\alpha} \quad (3)$$

where N_c is the total number of clusters. In addition, according to the generalized Einstein approximation^[18], we assume that all atoms in the cluster have the same oscillating frequencies and contribute equally to the cluster. The Helmholtz free energy A_α of cluster α is expressed as

$$A_{\alpha} = \Phi_{\alpha} + 3N_{\alpha}kT \ln \left(\frac{\hbar |\mathbf{D}_{\alpha h}|^{1/6}}{kT} \right) \quad (4)$$

where Φ_{α} is the total inter-atomic potential of the cluster, N_{α} is the number of atoms within the cluster, and $|\mathbf{D}_{\alpha h}|$ is the determinant of the local dynamical matrix of atom h . Since the equilibrium position of atom in cluster is determined by the corresponding nodes of cluster, the degrees of freedom of the system are significantly reduced to the total number of nodes. However, CST method is unable to resolve atomic details of deformation.

Obviously, both MST and CST have intrinsic limits in simulation. It is reasonable to couple MST and CST, that is, MST method is used in regions with heterogeneous deformation, while CST is used in regions that deform uniformly. We named this multi-scale simulation technology as hybrid molecule/cluster statistical thermodynamic (HMCST) method.

In HMCST method, we divide the whole region into three parts: local region, non-local region, hand-shaking region, as shown in Fig.1. In non-local region, the MST method is applied, each molecule in this domain is treated as nodes (namely, non-local node). In local region, CST method is applied, and the nodes within is named as local node. We assume that local nodes only interact with molecules in clusters. In the region between local nodes and non-local nodes, the node will interact with molecules in both non-local and local domains; hence, we name this region as hand-shaking region, and the node in this region is either local or non-local node. Hence, the free energy of the system in HMCST can be formulated as

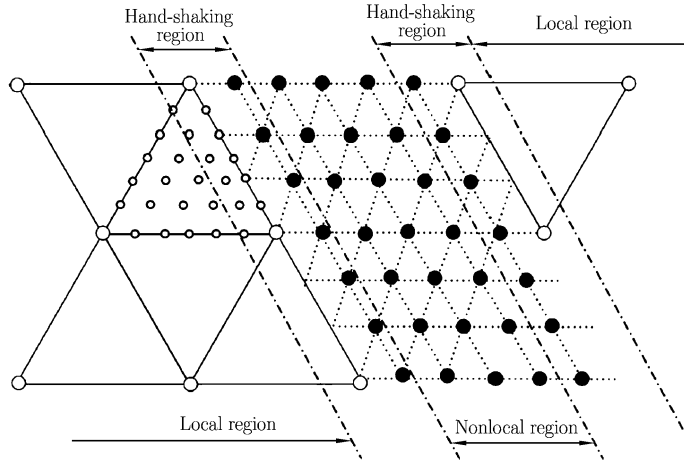


Fig. 1 Schematic figure of local, non-local, handshaking regions and nodes partition. The small hollow circles represent atoms, while the big solid and hollow circles are non-local and local nodes respectively^[15].

$$A^{\text{tot}} = A^{\text{LC}}(\{\mathbf{x}^{\text{LC}}\}) + A^{\text{NL}}(\{\mathbf{x}^{\text{NL}}\}) + A^{\text{SH}}(\{\mathbf{x}^{\text{SH}}\}) \quad (5)$$

where A^{tot} is the total free energy of the whole system, and A^{LC} , A^{NL} and A^{SH} the free energy in local region, non-local region and hand-shaking region, respectively. Simulation in Ref.[15] demonstrates that the ghost force can be avoided in the HMCST method due to the unified formulation of Helmholtz free energy in local, nonlocal and hand-shaking regions.

III. SELF-ADAPTIVE ALGORITHM

The key issue in a self-adaptive algorithm is the refinement criterion, i.e., a standard to judge whether a cluster should be refined or not. As we know, dislocation is the most common defect in crystalline solids. The details of dislocation structures, mechanism of their nucleation and motion can profoundly

affect the macroscopic response of the material. Hence, the refinement criterion we propose in this paper is designed for this kind of defects.

A crystalline material, which is supposed with no defect in initial configuration, consists of a regular array of atoms, forming crystal lattice. When extra force is applied, the lattices will undergo deformation. If the deformation is small, the response is elastic absolutely. However, when the deformation exceeds a certain level, a dislocation appears, distorting nearby planes of atoms. During this process, shear deformation of lattice is an important factor that results in dislocation. Therefore, properly characterizing the shear deformation of lattice is the first step in the construction of refinement criterion.

Now, we use a two-dimensional example to illustrate how to characterize shear deformation of lattice in CST simulation. In CST method, the crystal is partitioned into clusters represented by nodes at vertices of each cluster. Let's consider a particular node, whose position before deformation is \mathbf{x} , and after deformation \mathbf{x}' . The displacement of the node is given by the displacement vector $\mathbf{u} = \mathbf{x}' - \mathbf{x}$. The local deformation of cluster is characterized as the gradient of the displacement, which is a two-order tensor defined as

$$\mathbf{T} = \nabla \mathbf{u} \quad (6)$$

We assume the initial configuration is a perfect crystal and atomic slips only occur along the most closely packed direction in the crystal. For a particular slip system α , a local coordinate system is established by setting the slip direction $\mathbf{s}^{(\alpha)}$ and the normal of the slip plane $\mathbf{m}^{(\alpha)}$ as the base vectors. Hence, the displacement gradient can be represented in term of their components and coordinates as

$$\mathbf{T} = \frac{\partial u_s}{\partial x_s} \mathbf{s} \otimes \mathbf{s} + \frac{\partial u_m}{\partial x_m} \mathbf{m} \otimes \mathbf{m} + \frac{\partial u_s}{\partial x_m} \mathbf{s} \otimes \mathbf{m} + \frac{\partial u_m}{\partial x_s} \mathbf{m} \otimes \mathbf{s} \quad (7)$$

In Eq.(7), the items $\frac{\partial u_m}{\partial x_s}$ represent the simple shear deformation in the slip direction, and $\theta = \tan^{-1} \left(\frac{\partial u_m}{\partial x_s} \right)$, as shown in Fig.2. We define the components $\frac{\partial u_m}{\partial x_s}$ as 'slip shear deformation' and label it 'K', which is a key quantity representing the magnitude of simple shear deformation that occurs in slip direction.

Next, we need to calculate the gradient of slip shear deformation. In CST simulation, the displacements of atoms in cluster are linearly interpolated by those of the nodes at vertices of cluster. As a result, the deformation field is approximately uniform in each cluster, but discontinuous between adjacent clusters. Hence, the computation of slip shear deformation gradient can not be obtained directly from the derivative of the discontinuous slip shear deformation field. In our scheme, we employ the particle method approximation^[19] to generate a local continuous field for derivation.

The particle method approximation is a method of constructing local approximation field within the range of a discrete set of known data points. As illustrated in Fig.3, the triangle with solid lines is the cluster in CST

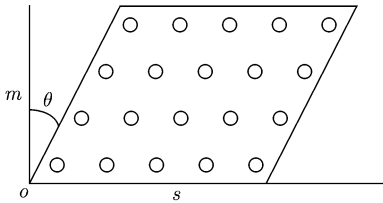


Fig. 2. Idealized simple shear deformation that occurs in the slip direction. This shear deformation may result in atomistic slip in crystal.

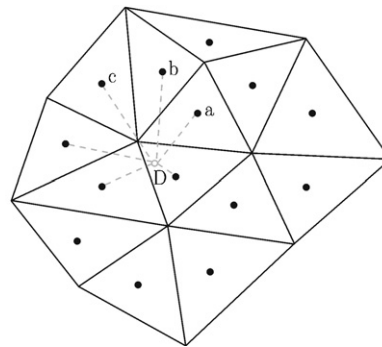


Fig. 3. The triangle with solid lines is the cluster in CST formulation, and the black solid dots, like a, b and c, is the central of these clusters. The slip shear deformation of point a, b, and c can be obtained from Eq.(7). The gray hollow dot named D is an arbitrary point in the region, whose value of slip shear deformation is determined by the neighboring discrete black dots a, b and c.

the cluster in CST method; and the solid black dots are known data points at the centre of cluster. The slip shear deformation of a known point is the cluster's value calculated from Eq.(7). The hollow circle noted as D is an arbitrary point in computational region, and its slip shear deformation is unknown and to be determined by those of known data points.

In particle method approximation, the slip shear deformation field can be approximated by

$$K^h(\mathbf{x}) = \sum_{I=1}^{N_c} W(\mathbf{x} - \mathbf{x}_I, h) K(\mathbf{x}_I) S_I \quad (8)$$

$$\sum_{I=1}^{N_c} W(\mathbf{x} - \mathbf{x}_I) S_I = 1 \quad (9)$$

where $K^h(\mathbf{x})$ is the approximated local slip shear deformation field of point with coordinate \mathbf{x} , $W(\mathbf{x} - \mathbf{x}_I, h)$ is the kernel function (h is the smoothing length), $K(\mathbf{x}_I)$ is the value of slip shear deformation at the point of the central of cluster I , S_I is the area of cluster I , and N_c is the number of clusters in the simulation. In this paper, the Gaussian function is chosen as kernel function

$$W(\mathbf{x}, h) = \frac{1}{(\pi h^2)^{n/2}} \exp\left(-\frac{\mathbf{x}^2}{h^2}\right) \quad (1 \leq n \leq 3) \quad (10)$$

where n is the dimension of the computation. It should be noted that the kernel function attenuates quickly over distance. Therefore, the field of slip shear deformation in a cluster is mainly affected by the deformation of adjacent clusters. In addition, the selection of kernel function is just a smoothing technology, which has little effect on the computational result. Actually, we tried different kernel functions in our simulation such as cubic spline, Gaussian function, and obtained the same results.

The gradient of slip shear deformation between two arbitrary points A and B, with coordinates \mathbf{x}_A and \mathbf{x}_B respectively, can be represented in the form of finite difference as

$$G^{(s)} = \frac{K^h(\mathbf{x}_A) - K^h(\mathbf{x}_B)}{r_{AB}} \quad (11)$$

where $G^{(s)}$ is the gradient of slip shear deformation, $K^h(\mathbf{x}_A)$ and $K^h(\mathbf{x}_B)$ are the slip shear deformation calculated in Eqs.(8) and (9) at point A and B, respectively.

In CST method, if we select points A and B as the intersection points of the circum-circle of the cluster and the line through the mass center (point O) perpendicular to slip direction (as shown in Fig.4), we obtain the gradient of slip shear deformation between A and B from Eq.(11). If $G^{(s)}$ is small, it implies that the deformation in the local region is not very heterogeneous and the current partition of cluster can meet the accuracy requirement in this region, and thus no refinement is needed. However, cluster in which $G^{(s)}$ is greater than some prescribed tolerance is targeted for refinement. Refinement then proceeds by adding three new nodes at the mid-side of the targeted cluster.

This refinement may continuously reduce the size of clusters. However, to ensure the validity of the generalized Einstein approximation employed in the Helmholtz energy calculation for clusters, the size of cluster cannot be too small^[15]. For two-dimensional simulation, the radius of inscribed circle of cluster would be larger than the truncated distance of inter-atomic potential energy, which physically implies that the deformation of the central atom of cluster is not affected by the atoms in other clusters. Hence, the cluster size is restricted to larger than the truncated distance. If the size of cluster gets

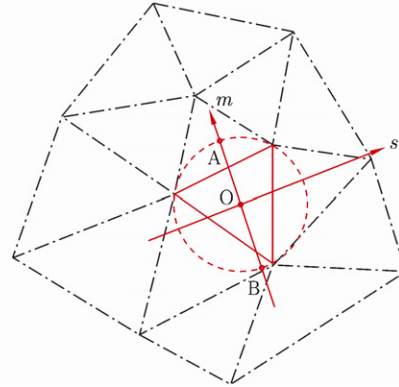


Fig. 4 The triangle with solid lines is the cluster to be investigated. Point O is the mass center of the triangle. The circle with dashed lines is the circum-circle of this triangle. Line s is in the direction of slip, and line m is perpendicular to it. Both line s and line m run through point O. A and B are the intersection points of the circum-circle and line m .

smaller than the truncated distance, the cluster will be transferred into molecules completely.

To sum up, the self-adaptive algorithm includes the following steps:

1. Calculate the slip shear deformation of every cluster.
2. Calculate the gradient of slip shear deformation $G^{(s)}$ of every cluster by particle method approximation.
3. Refine clusters whose $G^{(s)}$ is greater than prescribed tolerance by adding mid-side nodes.
4. After refinement, if the size of new cluster is smaller than the truncated distance, the cluster will be eliminated and this region is transferred into MST.

IV. EXAMPLE

In this section, we will validate the proposed adaptive algorithm by simulating a uniaxial compression process and comparing the results obtained from self-adaptive molecule/cluster statistical thermodynamics (SMCST), MST and CST methods respectively. For a two-dimensional single hexagonally packed lattice of Cu, we implement a uniaxial quasi-static compressive loading at 300 K, as shown in Fig.5. The initial dimensions of the sample are 67.3 nm×32.7 nm, containing 38077 atoms. Figure 6 shows the initial cluster partition in SMCST and CST simulation, and the total number of cluster and node are 120 and 72, respectively. All these clusters are equilateral triangles containing 318 atoms. For all the three simulations, the left end is held fixed, free boundary conditions are use in two horizontal boundaries, and right end of the sample moves 0.2 nm in each loading step. Lennard-Jones potential

$$e(r) = 4\varepsilon_p \left[\left(\frac{r_0}{r} \right)^{12} - \left(\frac{r_0}{r} \right)^6 \right] \quad (12)$$

is adopted to idealize the interaction between atoms in our calculation where $r_0 = 2.3276 \text{ \AA}$ and $\varepsilon_p = 0.4912 \text{ eV}$ are parameters, and the truncated distance $r_c = 7.8379 \text{ \AA}$ ^[20].

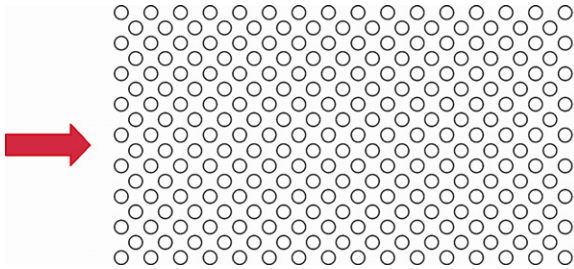


Fig. 5. Schematic of initial atomic configuration of a two-dimensional hexagonally packed lattice under uniaxial compression. For all the simulations, the atoms on the left end are held while those on the right end move.

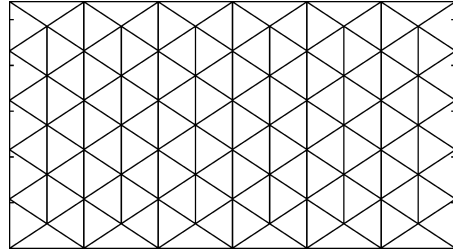


Fig. 6. Initial partition of clusters in SMCST and CST simulations. There are 120 clusters with 72 nodes. Both size and shape of these clusters are uniform.

In order to facilitate the comparison of the results, the stress is defined as the derivative of Helmholtz free energy with respect to the displacement of the moving boundary, that is

$$\sigma = -\frac{1}{L_0} \frac{\partial A}{\partial L} \quad (13)$$

where L_0 is the initial width in vertical direction and L is the current length.

We first study the stress-strain curves obtained from different simulations, as shown in Fig.7. Prior to point D in the SMCST curve, the response is completely elastic and these curves are found to be in excellent agreement with each other, indicating that all these methods can accurately simulate elastic deformation in the initial phase.

The atomic configuration at points E and G are shown in Fig.8, which show dislocation slip from point D to E, and point F to G, respectively. Hence, the stress drops in the curves of SMCST method and MST simulation correspond to the sliding of dislocation. However, the CST method does not reproduce this mechanical behavior at all. This is not surprising, because CST simulation eliminates the atomic level

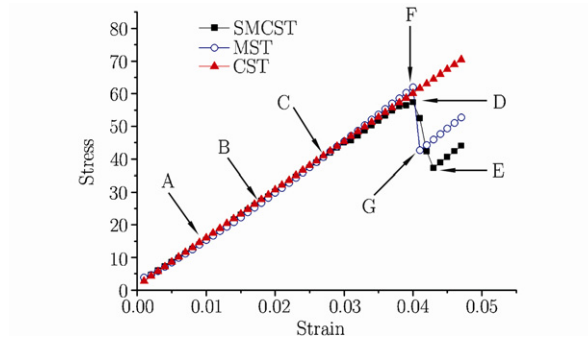


Fig. 7. Stress-strain curve obtained CST, MST, and SMCST simulation respectively.

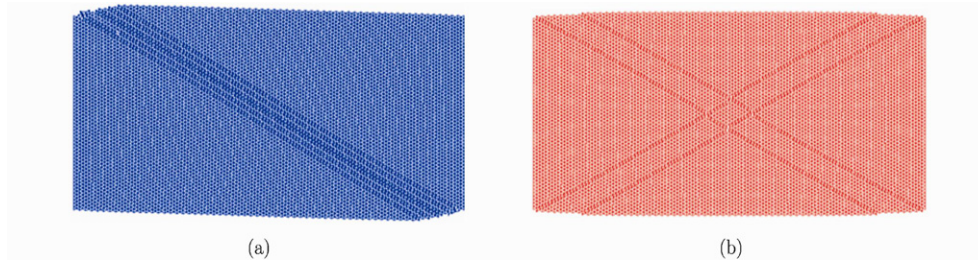


Fig. 8. Atomic configurations of SMCST (a) and MST (b) simulations after the first slip at point E and G, respectively.

deformation details and suppresses localized deformation completely. More importantly, both MST and SMCST demonstrate the slipping of atoms along the most closely packed direction as theoretical analysis. Figure 8 shows the atomic configurations from MST and SMCST after their first slips, respectively. The slip zones predicted by MST are symmetrical in both the most closely packed direction, while the SMCST loses the symmetry. The reason is that SMCST predicted more slips in one direction compared with MST because of interface between MST and CST. Thus it inhibited the emergence of slip in the other direction.

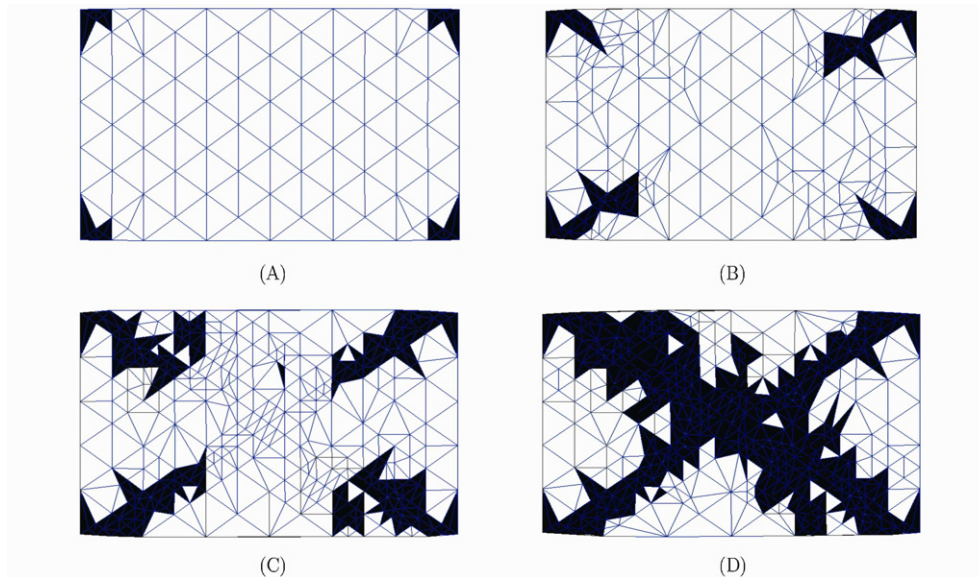


Fig. 9. Nonlocal (MST) and local (CST) region at the points A, B, C and D in the strain-stress curve of SMCST . The black zone is the nonlocal (MST) region while the white is local (CST) region. The triangles in the local region are the clusters in simulation.

Figures 9(A)-(D) show the region partition at points A, B, C, D in stress-strain curves, respectively. The black zone is the nonlocal (MST) region while the white zone is the local (CST) region. The triangles in the local region are the clusters in the simulation. Obviously, some clusters have been refined adaptively and some even have been transferred into atoms entirely for capturing atomic level configuration details. In addition, the nonlocal (MST) region gradually expands as the deformation of compression increases. Finally, the MST zone forms two strips, which is slip band essentially. The directions of the two strips make an angle of about 30 degree with the horizontal axis, which is the most closely packed direction for the lattice. Figure 9 proves that the above-mentioned self-adaptive algorithm can effectively find clusters to be refined and transferred to molecular simulation, and the refinement and transferring techniques works well in the simulation.

Finally, let us compare the computing efficiency with the same PC. Figure 10 shows the computation time consumed in MST and SMCST method, respectively. For the same simulation, the calculation for each loading state takes about 9.78 minutes in average for SMCST, while about 130.38 minutes for MST. Thus, the adaptive method has very high computing efficiency compared with MST by at least 13 times.

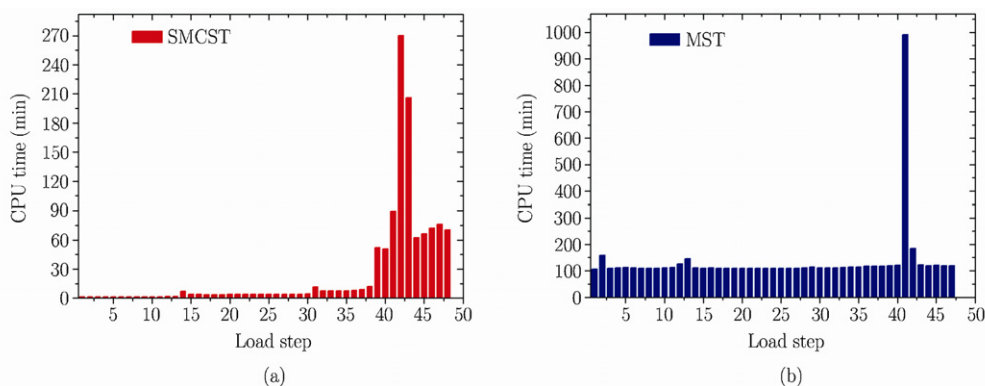


Fig. 10. CPU time consumed in the simulation of uniaxial quasi-static compression with SMCST (a) and MST (b) method, respectively.

V. CONCLUDING REMARKS

The rapid evolution of nanotechnology necessitates novel, sophisticated, and physically based approaches to bridge the gaps between different length and time scales. In this paper, a self-adaptive molecular/cluster statistical thermodynamics (SMCST) method for the simulation of quasi-static deformation at finite temperature is developed and verified. The SMCST method is based on MST and CST methods, which couple different spatial and temporal scales in a unified framework by treating atoms as oscillators and particles simultaneously, as well as clusters. In the self-adaptive algorithm, the gradient of slip shear deformation is calculated and used as the criterion for cluster refinement. In addition, the cluster is to be transferred to molecular when its size gets smaller than a critical value. The simulation of a quasi-static uniaxial compression at 300 K proves that the self-adaptive algorithm can accurately find the clusters to be refined or transferred to molecular, and efficiently refine or transfer the clusters. The SMCST method has also been demonstrated to be significantly faster than the MST method.

References

- [1] Leach, A.R., *Molecular Modeling Principles and Applications*, 2nd edition. New Jersey: Prentice Hall, 2001.
- [2] Kohlhoff, S., Gumbsch, P. and Fischmeister, H.F., Crack-propagation in BCC crystals studied with a combined finite-element and atomistic model. *Philosophical Magazine A*, 1991, 64(4): 851-878.
- [3] Tan, H.L. and Yang, W., Atomistic/continuum simulation of interfacial fracture. *Acta Mechanica Sinica*, 1994, 10(2): 151-161; 10(3): 237-249.
- [4] Wagner, G.J. and Liu, W.K., Coupling of atomistic and continuum simulations using a bridging scale decomposition. *Journal of Computational Physics*, 2003, 190(1): 249-274.

- [5] Broughton, J.Q., Abraham, F.F., Bernstein, N. and Kaxiras, E., Concurrent coupling of length scales: Methodology and application. *Physical Review B*, 1999, 60(4): 2391-2403.
- [6] Shilkrot, L.E., Miller, R.E., and Curtin, W.A., Coupled atomistic and discrete dislocation plasticity. *Physical Review Letters*, 2002, 89(2): 025501.
- [7] Dupuy, L.M., Tadmor, E.B., Miller, R.E. and Phillips, R., Finite-temperature quasi-continuum: Molecular dynamics without all the atoms. *Physical Review Letters*, 2005, 95(6): Art. 060202.
- [8] Rudd, R.E. and Broughton, J.Q., Coarse-grained molecular dynamics and the atomic limit of finite elements. *Physical Review B*, 1998, 58(10): 5893-5896.
- [9] Xiao, S.P. and Belytschko, T., A bridging domain method for coupling continua with molecular dynamics. *Computer Methods in Applied Mechanics and Engineering*, 2004, 193(17-20): 1645-1669.
- [10] Tadmor, E.B., Ortiz, M. and Phillips, R., Quasi-continuum analysis of defects in solids. *Philosophical Magazine A*, 1996, 73(6): 1529-1563.
- [11] Tadmor, E.B., Phillips, R. and Ortiz, M., Mixed atomistic and continuum models of deformation in solids. *Langmuir*, 1996, 12(19): 4529-4534.
- [12] Shenoy, V.B., Miller, R., Tadmor, E.B., Phillips, R. and Ortiz, M., Quasi-continuum models of interfacial structure and deformation. *Physics Review Letters*, 1998, 80(4): 742-745.
- [13] Shenoy, V.B., Miller, R., Tadmor, E.B., Rodney, D., Phillips, R. and Ortiz, M., An adaptive finite element approach to atomic-scale mechanics—the quasi-continuum methods. *Journal of the Mechanics and Physics of Solids*, 1999, 47(3): 611-642.
- [14] Hu, M., Wang, H.Y., Xia, M.F., Ke, F.J. and Bai, Y.L., Cluster statistical thermodynamics (CST) — to efficiently calculate quasi-static deformation at finite temperature based on molecular potentials. In: IUTAM Symposium on Mechanical Behavior and Micro-mechanics of Nanostructured Materials, Solid Mechanics and Its Applications, 2007, Volume 144, Part 5, 163-170.
- [15] Wang, H.Y., Hu, M., Xia, M.F., Ke, F.J. and Bai, Y.L., Molecular/cluster statistical thermodynamics methods to simulate quasi-static deformations at finite temperature. *International Journal of Solids and Structures*, 2008, 45(3): 3918-3933.
- [16] McQuarrie, *Statistical Mechanics*. New York: Harper & Row, 1976.
- [17] Born, M. and Huang, K., *Dynamical Theory of the Crystal Lattices*. Oxford: Oxford University Press, 1954.
- [18] LeSar, R., Najafabadi, R. and Srolovitz, D.J., Finite-temperature defect properties from free-energy minimization. *Physics Review Letters*, 1989, 63(6): 624-629.
- [19] Belytschko, T. and Xiao, S.P., Stability analysis of particle methods with corrected derivative. *Computers and Mathematics with Applications*, 2002, 43(3-5): 9-350.
- [20] Najafabadi, R. and Srolovitz, D.J., Evaluation of the accuracy of the free-energy-minimization method. *Physical Review B*, 1995, 52(13): 9229-9241.