

# Efficiency and fidelity of molecular simulations relevant to dislocation evolutions



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## ABSTRACT

The comparative simulations of dislocation evolution in nanoindentation are carried out in terms of both molecular dynamics (MD) and energy minimization (EM) methods, to explore what really govern the computational efficiency and fidelity in molecular simulations relevant to dislocation evolutions. It is found that although all simulations can present similar relationship between indentation force and depth, there still might be some significant differences in the simulated dislocation patterns and computational efficiency. Firstly, the EM simulations show more complicated dislocations. Secondly, the necessary computational effort of EM increases nonlinearly with indentation depth, compared to the linear dependence in MD simulations, namely EM shows higher efficiency than MD in shallow indentation, but vice versa in deeper ones. More importantly, it is revealed that the time consumption of the minimization iteration is strongly dependent on the moving of dislocation loops and increases greatly when dislocation loops move long distances. Whereas MD simulations of complicated dislocations patterns may need less time cost but present immature dislocation evolutions, since the relaxation steps in MD simulations are fixed beforehand, regardless of the dislocation loops moving to equilibrium state or not.

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## 1. Introduction

Dislocation evolution is key microscopic event for understanding plasticity, damage and failure of crystal materials and structures. It is a long pursuit to gain both high efficiency and high fidelity in large scale molecular simulations of dislocation evolutions. Molecular dynamics (MD) and energy minimization (EM) methods are two of the commonly used approaches [1–5]. MD, based on Newton's second law of motion for atoms, has been widely used to describe dynamic behavior of dislocations in nanoscale materials [1,2,6]. However, the time scale of MD is limited to several nanoseconds with loading strain rate usually higher than  $10^8 \text{ s}^{-1}$  [7]. EM, on the other hand, based on minimization of a given system's energy, is usually used to investigate dislocation evolutions at quasi-static conditions [3,4].

Molecular statics (MS) is a typical EM method with potential energy as the objective of minimization. It has been applied to structural optimization of biomacromolecules [8] and quasi-static simulation of solid atomistic systems [3,4]. Kang and Huang have successfully used MS to investigate dislocation evolution in copper

nanowires under tensile, rotating and shear deformations [9]. However, temperature of the system simulated using MS is limited to 0 K. EM can be extended to handle systems at finite temperature if free energy is used as objective of minimization. For example, the molecular statistical thermodynamics (MST) method proposed by Hu et al. uses the statistical thermodynamics formulation of Helmholtz free energy of molecular system [10]. Applications of MST indicate that it is an effective approach for simulating dislocation evolution in nanostructures under quasi-static deformation at finite temperature [11,12].

In order to simulate dislocation evolution in large scale molecular systems, multi-scale methods based on EM have also been proposed in the last few decades. In multi-scale simulations, atomistic representation is used in regions under inhomogeneous deformation dominated by dislocation evolutions to capture atomistic details, while quasi-continuum representation is used in regions under homogeneous deformation without dislocation to reduce computational costs. One of the typical multi-scale methods is the quasi-continuum method (QC) which solves the positions of representative atoms by minimize the coarse-grained potential energy of the system at temperature 0 K [13]. Based on the framework of EM, some other multi-scale methods such as coupling of length scales method [14], bridging domain method

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[15], bridging scale method [16], composite grid atomistic continuum method [17] and multi-resolution molecular statics [18] have also been proposed and applied for studies of dislocation evolution in large scale systems [19]. Based on MST, Wang et al. proposed the hybrid molecule/cluster statistical method [10] which is a multi-scale approach for simulating dislocation evolution in nanostructures at finite temperature. Chen and Ming [20,21] proposed a constrained Cauchy-Born elasticity accelerated multigrid method and reduced considerable computational costs in nanoindentation with simple dislocations. Although so many multi-scale methods have been proposed in the past years, few of them have been widely used. One of the main reasons is that efficiency improvement of some EM-based multi-scale methods against MD in practice is not remarkable. Therefore, what really governs the computational efficiency and how to improve it should be further investigated.

Although both MD and EM-based simulations have been performed to investigate dislocation evolution in molecular systems at different conditions, the computational efficiency and fidelity of the two methods is rarely studied systematically. A deep investigation of the problem will provide useful information for simulations relevant to dislocation evolutions in large scale molecular systems regarding (i) making choice between MD and EM-based methods for a specific problem, (ii) modifying related settings in MD and EM-based methods in order to obtain reasonable results, (iii) understanding bottle-neck of computational efficiency in EM-based multi-scale methods and, (iv) developing new algorithms to accelerate the simulation relevant to dislocation evolutions. In this work, the comparative simulations of dislocation evolution in nanoindentation were carried out in terms of both MD and MS, to explore what really govern the computational efficiency and fidelity in molecular simulations of dislocation evolutions.

## 2. Computational framework

The MD and MS simulations are performed on a nanoindentation system consisting of a substrate material indented by a conical diamond tip, as illustrated in Fig. 1. Nanoindentation is a flexible characterization technique in mechanical analysis of nanostructures. Simulation of nanoindentation has been commonly used as a benchmark to examine new multi-scale methods because [22,23], (i) it provides dislocation evolution details for understanding mechanical behavior of materials at nanoscale; (ii) complex dislocation nucleation and evolution can be triggered by indentation

tip easily and new methods are examined whether they could capture these changes and; (iii) relation of indentation force and depth obtained from experiments and large scale simulations can be compared directly.

The substrate in Fig. 1 consists of facial cubic crystal (FCC) Cu with lattice constant of 3.615 Å. The dimensions of the substrate ( $L_x \times L_y \times L_z$ ) is  $43.4 \times 43.4 \times 21.7$  nm with 3,542,000 atoms. The free surface at the top is (0 0 1) crystal plane and the other two side surface are (1 0 0) and (0 1 0). Periodic boundary conditions are imposed against the side surfaces to approximate a nanofilm with infinite width. Atomistic layers with depth of 1.5 nm at the bottom are fixed to provide a support in  $z$  direction. The substrate is indented by a conical-shaped indenter tip consists of 149,683 C atoms of diamond lattice. In both MD and MS simulations, the tip moves against the top surface of the substrate with 0.01 nm for each loading step. The maximum indentation depth is 2.53 nm.

The embedded atom model (EAM) potential developed by Mishin et al. [24] is used for Cu atoms. The potential has been widely applied to simulate mechanical responses of FCC metals and reasonable results have been obtained in comparison with experimental measurements [25]. Interactions between C atoms in the tip and Cu atoms in the substrate are modeled by a Morse potential [12]

$$\Phi = D_0 [e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)}], \quad (1)$$

with parameters  $D_0 = 0.087$  eV,  $\alpha = 5.14 \text{ Å}^{-1}$ ,  $r_0 = 2.05 \text{ Å}$ . The indenter tip is assumed to be rigid during simulations, so interactions between C atoms is ignored.

In MS simulations, total potential energy of the system at each loading step is minimized using conjugate gradient (CG) algorithm. In CG algorithm [26], atomistic position vector ( $\mathbf{x}_k$ ) is updated according to the current conjugate direction ( $\mathbf{d}_k$ ) and step size ( $\alpha_k$ ):

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k, \quad (2)$$

where  $k$  indicates the iteration step of conjugate directions.  $\mathbf{d}_k$  is calculated from atomistic force vector ( $\mathbf{f}_k$ ) and searching direction. At each loading step, there will be different number of iteration steps ( $n_{iter}$ ) which is related to characteristics of energy profiles. At iteration step  $k$ ,  $\alpha_k$  is determined through line-searching methods in which the system's energy and atomistic force vector needs to be evaluated for several times ( $n_{line}^k$ ). Therefore, the total times of energy and force evaluation ( $n_{eval}$ ) at a loading step is

$$n_{eval} = \sum_{k=1}^{n_{iter}} n_{line}^k. \quad (3)$$

The system is assumed to reach an equilibrium state when the resolution criterion ( $\varepsilon$ ) of minimization is satisfied:

$$\max(e_{k+1}^i - e_k^i) < \varepsilon, \quad i = 1, 2, \dots, N \quad (4)$$

where  $N$  is the total of atoms,  $e_{k+1}^i$  and  $e_k^i$  are the per-atom potential energies at the  $k+1$  and  $k$  iteration step respectively. In this work,  $\varepsilon$  with values of  $1 \times 10^{-3}$ ,  $1 \times 10^{-4}$  and  $1 \times 10^{-5}$  eV is considered in order to investigate its effect on simulation results.

In experiments, nanoindentation is usually performed with loading velocity slower than  $1 \mu\text{m/s}$  which can be assumed quasi-static. The quasi-static process can be modeled effectively using MS; however it is hard to perform a quasi-static simulation with MD whose intrinsic time scale is about 1 fs. In practice, at each loading step, the system is relaxed with pre-specified number of MD time-steps ( $n_r$ ) to equivalent a quasi-static process. At each time-step, atomistic position vector  $\mathbf{x}_k$  is updated according to the current velocity and force vectors:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{v}_k \Delta t + \frac{\Delta t^2}{2m} \mathbf{f}_k \quad (5)$$

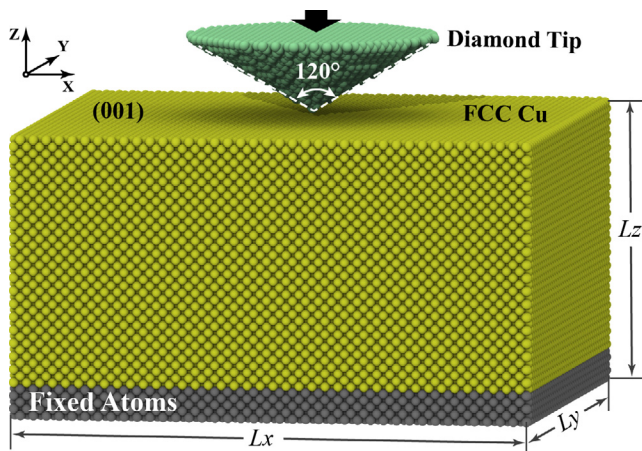


Fig. 1. Configuration of the nanoindentation system consisting of Cu substrate and diamond tip used in MD and MS simulations.

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