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Applicability Analysis of Molecular Statics Simulation for Nano-materials

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Abstract

Molecular statics can simulate the process without time limitation, while molecular dynamics can only study the motion of system in small time range. Therefore, it's necessary to give attention and research on the application of molecular statics in engineering materials field. In order to investigate the applicability analysis of molecular statics simulation in nanomaterials scientific research, taking 3D copper monocrystal as the research object,the corresponding molecular statics model was established, the stress-strain data and Young's modulus at the absolute-zero temperature is got. Comparing the result of molecular static simulation with molecular dynamics simulation and the known experimental data, the results show that the model established by molecular statics can explain the mechanical properties of copper monocrystal subjected to tensile loading.

Keywords*: molecular statics, nanomaterials, copper monocrystal, mechanical properties*

1. Introduction

Nanoelectromechanical systems are evolving, with new scientific studies and technical applications emerging [1]. So, the research about the mechanical properties of nanomaterial becomes more and more crucial. The computer simulation is an important means of studies for metal material's microstructure properties [2-4]. Most of the simulations of metal nanomaterial are accomplished by molecular dynamics (MD), which could not only get the details of the movement of atoms, but also observe the microscopic details that cannot be obtained in many practical experiments, which makes MD very popular in the research field of the physical, chemical and materials science [5-8].

However, the limitation of the MD method is due to the small time step needed while solving Newton's equations [9]. The overall simulation time in MD is measured in nanoseconds, which is quite short to investigate many phenomena in materials science, such as crack initiation, plasticity, etc., even using parallel supercomputing.

Molecular Statics (MS) is less used in the applicable study of the mechanical properties of metal nanomaterial, but MS doesn't involve the mathematical integral method and can be simulated without the computer time constraints associated with the time step in molecular dynamics, which attracted the attention of many experts home and abroad. In 2006, Oleg Vinogradov proposed a new method of molecular statics based on individual displacements of atoms converging to an equilibrium state, the method is illustrated on a simple 2D crystal structure [10]. In 2010, A perfect 3D BCC crystal is subjected to tensile deformation, using a molecular statics approach, in order to investigate the reliability of the plastic part of the stress-strain data [11].

Given the advantages of molecular statics, this paper investigates the applicability analysis of molecular statics was established, the stress-strain data and Young's modulus at the absolute-zero temperature is got. Comparing the result of molecular static simulation with molecular dynamics simulation and the known experimental data, the results show that the model established by molecular statics can explain the mechanical properties of copper monocrystal subjected to tensile loading.

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2. Research Method-The Theory of Molecular Statics Simulation

In molecular statics the absolute zero temperature is assumed, i.e. the kinetic energy of atoms is zero and only the potential energy, defined by the corresponding interatomic potentials. Traditionally, molecular statics (MS) methods are based on various iterative energy minimization algorithms, such as first-order steepest descents or conjugate gradient and second-order Newton-Raphson or Quasi-Newton's. Atoms move to a lower energy state continuously from the initial position, which cannot overcome the potential barrier associated with dislocation formation corresponding to a discontinous atoms motion without any artificial trigger. For this reason, Kohlhoff use the MS method to dislocation nucleation and then the MD to find the equilibrium state during dislocation nucleation [12]. In [10], this drawback of the classical MS was overcome by displacing atoms independently in a manner analogous to MD. According to this advanced molecular statics, tension process of a 3D nano-single crystal copper was analyzed in this paper.

2.1. Potential Function

In the following, we used the Morse function to describe the pair-wise interaction potential. The Morse function is given by the following equation:

$$\Phi(r) = D[e^{2\alpha(r_0 - r_{ij})} - 2e^{\alpha(r_0 - r_{ij})}] \quad (1)$$

where α represents the width of the potential curve, while D represents its depth, both α and D are constants with dimensions of reciprocal distance and energy, respectively; r_0 is the equilibrium distance of the two atoms at zero temperature, while r_{ij} represents a variable distance between two atoms.When the distance between two atoms equals to r_0 ,the minimum of the potential $\Phi(r)_{\min} = -D$.

The interatomic force, as the derivative of the potential,is given in this case by:

$$F_{ij}(r) = 2\alpha D[e^{\alpha(r_0 - r_{ij})} - e^{2\alpha(r_0 - r_{ij})}] \quad (2)$$

Morse potential curve and force curve between atoms are shown in Figure 1. The blue line represents potential energy, while red dotted line represents an interatomic force. The inter-atomic force exceeding cut-off distance will be ignored, in order to reduce the interaction of atomic number and improve the computational efficiency.

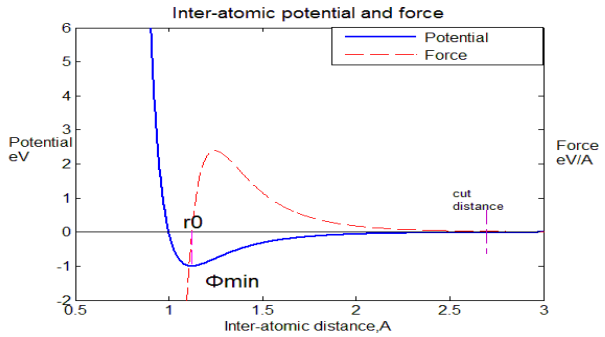

Figure 1. Interatomic Potential Energy and Force

Table 1. Morse Function Parameters of Cooper Monocrystal

Variable	magnitude
D	0.3429(eV)
α	1.3588(Å^{-1})
r_0	2.866(Å)

Morse function parameters of single crystal Cu [13], as shown in Table 1.

2.2. Iterative Process of Energy Minimization

The algorithm of energy minimization introduced in [14] is used. Accordingly, the iterative process is governed by the following function:

$$u_{k+1} = u_k + \beta_k p_k \quad (3)$$

Where k represents k-th iteration, and p_k is the unit vector defining the atom displacement from the position u_k to a new position u_{k+1} ,and β_k is the factor defining the magnitude of the displacement. The displacement takes place in the direction governed by the vector p_k ,which is the direction of the total unbalanced force acting on a given atom i from all other atoms within the cut-off distance. In the k-th the magnitude of the atomic displacement is expressed as:

$$\beta_{ij} = q(1 - e^{-c|F_{ij}|}) \quad (4)$$

Where *q* and *c* are constants and F_{ij} is the unbalanced force that can be calculate by Equation (2)

The smaller the *q* is, the higher the accuracy is, but the more numbers of iterations of finding the equilibrium state in the relaxation process. The constants *q* and *c* in Equation (4), found by numerical experiments based on the accuracy and efficiency , are equal to: *q* = 0.02 and *c*=1for the system used in this work.When the maximum force between the atoms is less than the convergence precision *ξ*, the atom gets the equilibrium position,and the iteration process ends.

2.3. Numerical Simulation

The Cu crystal structure analysis is shown in Figure 2, which is face-centered cubic lattice (FCC).

A pure 3D Copper crystal consisting of 8×4×4 fcc unit cells (see Figure 3) and comprising of 689 atoms was subjected to tensile loading. The unit lattice constant of Copper is 3.615 Å, and thus the corresponding length of the crystal is 28.92 Å in the X-direction while its width is equal to 14.46 Å.The surfaces of the crystal in the Y- and Z-directions were free. The tensile loading was achieved by extending simultaneously these two boundaries in the opposite directions along the x-axis. The crystal was defined as comprising of three parts: two boundaries and the atoms between them. Both boundaries comprised of layers of atoms within the cut-off distance. In Figure 3 the boundaries are shown in blue colors while the relaxing atoms in red.

Before loading, an ideal crystal was generated and then subjected to a relaxation procedure. Single step of the simulation process increases strain 0.5%.Convergence criteria (maximum allowable interatomic force)for *ξ*=5×10^{-6}eV/ Å. The cut-off distance is $r_{cut} = 10$ Å.

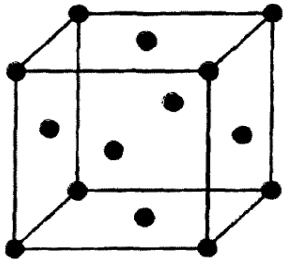

Figure 2. The Crystal Lattice of Cu

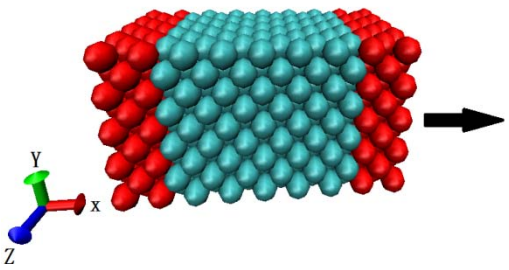

Figure 3. A 3D Ideal Cu Crystal, left and right boundaries are shown in red, arrow points the loading direction (the figure is done by molecular visualization program - VMD)

3. Results and Discussion

3.1. The Model Shape During the Elastic Deformation And the Plastic Deformation

Shown in Figure 4, at the strain ε=7.5%(during the elastic deformation), after enough relaxation processes, the model shape had nothing changed comparing to the original model, which is consistent with the macroscopic physical properties.

As strain increased,Copper crystal model reaches the elastic limit,whose deformation effect shown in Figure 5, the deformation is plastic deformation, even after the relaxation process of restitution.

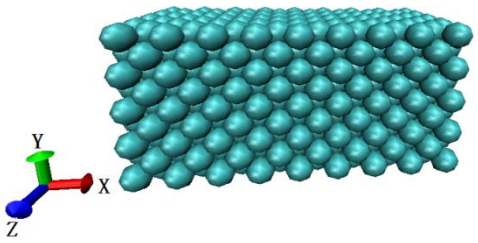

Figure 4. Strain ε=7.5%, the Model Shape During the Rlastic Deformation (after enough relaxation processes)

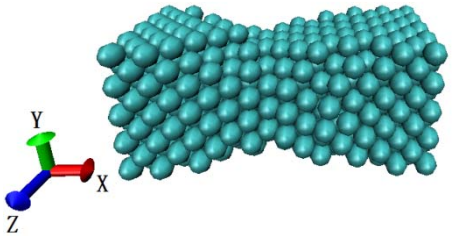

Figure 5. Strain ε=30.0%, the Model Shape During the Plastic Deformation

3.2. Stress-Strain Curves And Young's Modulus

The stress-strain curve of single copper crystal obtained by using molecular statics simulation is shown in Figure 6. When the strain ε=8.40%, the stress σ=9.97Gpa, reaching the yield limit, the elastic modulus E=118.72GPa; Applying the Ordinary-Least-Square (OLS) rule to obtain a more accurate value 106.6Gpa;

At temperature of -270 °C, i.e. T=3.15K,Young's modulus of Cu obtained by experiment is 139Gpa [15], which is bigger than our result, There are at least three reasons for this discrepancy: first, we tested numerically an ideal and pure crystal,while the experimental specimens may have various kinds of defects; second, the real materials are multigrain structures in which the grain boundaries affect the stress-strain data, and third, according to the Hall-Petch relationship, the grain size influences the yield stress.

The MD simulations of copper carried by Liang Haiyi [16], was shown in Fig.7, curve 2 and curve 3 are the stress-strain curve of the copper crystal film and copper crystal bulk. Curve 1 is the stress-strain curve of crystal copper got by MD which is similar to our model.When the strain ε=9.0%, the stress σ=11.17Gpa, reaching the yield limit, the elastic modulus E =124.11GPa，which is quite close to our molecular statics results：118.72Gpa，and the trend of stress-strain curve is also very close to our result.

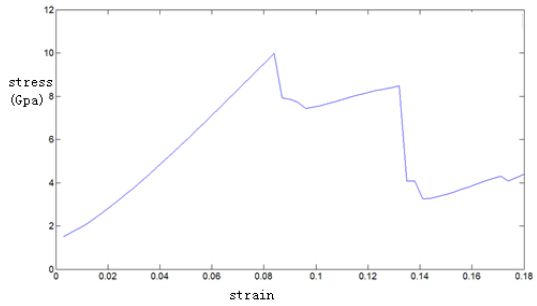

Figure 6. The Stress-Strain Curve of Crystal Copper during Tension Process by Molecular Statics Method

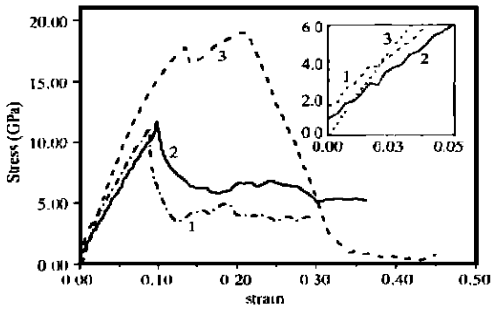

Figure 7. Stress-Strain Curve of Single Crystal Copper during Tension Process by Molecular Dynamic Method [13]

4. Conclusion

This paper investigated the mechanical properties of copper crystal subjected the tensile loading along the [1 0 0] direction by using molecular statics with Morse potential. Comparing MS results with MD results, we found that the trend of stress-strain curve is basically same, and the Young' modulus got by this two methodare very close, which validate our simulation results .However, MD involves the mathematical integral method, which can only study the motion of system in small time range.MS does not involve mathematical integration method, which overcome the shortcomings of MD. With the further development of MS method, it will play a more important role in the field of molecular simulation and materials science.

Acknowledgements

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