A Three-Dimensional Atomic-Scale Finite Element Model for A Copper Nano Thin Film Subject to Uniaxial Tension

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Abstract - A three-dimensional atomic-scale finite element model was developed in this paper for simulation of a nano-scale uniaxial tension. First, the Morse's potential function was used to simulate the forces acting among particles. Furthermore, a non-linear spring and dashpot element with a lumped mass was used to establish an atomic model. The elongation of the spring at fracture was used to simulate the radius of fracture of the atomic link. This method was applied to investigate the proportional tension test of an idealized FCC single crystal copper film along the x direction. The study includes the stress-strain curve, the effect of five categories of atomic distances on the stress-strain curve; and the effect of strain-rate on the stress-strain curve. The results showed that (1)the simulated maximum stress for copper is very close to 30.0GPa, which is also the value of maximum equivalent stress obtained by Lin and Hwang [6], verifying the validity of the calculation of this paper. In the tension test of copper, necking develops gradually and eventually leads to fracture. The simulated deformed material element during each stage of deformation was similar to that simulated by Komanduri et al.[2](2)the influence of $r_{ij} = 6.2608 \overset{0}{A}$ on the five categories of atomic distance considered was limited and it may be neglected to save computation time,(3)when the strain-rate was large, the resistance to deformation was also large, leading to an increase in the yield stress and fracture stress.

Keywords - nano-scale uniaxial tension, Morse's potential function, three-dimensional atomic-scale finite element model.

I. INTRODUCTION

Several micro-manufacturing processes are currently being rapidly developed. These developments have resulted in precise components approaching the micro(10^{-6} *m*) and even the nano(10^{-9} *m*) scale [1]. Therefore studies of mechanical behaviors of nano-scale materials under micro- and nano-manufacturing processes become important. Special fabrication processes produce the structural elements made of these materials such that they are almost devoid of defects. These ideal materials (with no or very few defects and strength close to their theoretical values) are going to be the norm rather than the exception for nano components in MEMS and MOEMS. Thus, to understand the mechanical properties of nano-scale materials and its feature phenomenon is intrinsically important and nano technology has become the key technology of the twenty-first century.

Generally, the material properties of the nano components are determined using nano-indentation tests with extremely light loads in the range of nano Newtons [2]. While tensile testing is the most common way to determine the mechanical properties at a macro level; such tests at the nano-scale are extremely difficult, if not impossible to conduct. Even if this is possible, the costs involved in performing nano-regime tensile tests would be significant due to the inherent complexity of the equipment [3].

The substance is formed by discontinuous molecular or atomic granules when the components reach the nano scale. To study these tiny components, continuum mechanics is insufficient to explain the deformation mechanism of the discrete structure in nano-scale size. To understand the mechanical properties of nano-scale materials and their phenomenon more deeply, it is more reasonable to focus on the individual behavior of atoms or molecules. It is necessary to take the theoretical analysis and study it in order to understand the characteristics of nano components. The theoretical analysis and modeling of the problem is primarily based on molecular dynamics, using a finite element method based on a spring element atomic model or a model of nonlinear spring and dashpot.

Irving and Kirkwood [4] introduced molecular dynamics in the 1950's. In this approach, a potential is used to determine the interaction forces among molecules. The molecules follow Newton's law of motion and the integration of the equations of motion leads to the trajectory of molecular motion, which further leads to the corresponding physical properties under dynamic loading. Subsequent investigations show that molecular dynamics could effectively model the microscopic dynamic tensile test, but it is computationally expensive [2][5-6].

In order to reduce the computation time, some researchers used the finite element method based on an atomic model instead of using molecular dynamics. Jeng and Tang [7] used a finite element method based on a two dimensional atomic model to investigate the micro-phenomenon of a nano film subject to uniaxial tension. Since this was a quasi-static test, the computation time was greatly reduced. The result showed that the extension of the specimen increased non-linearly with increasing load and it also showed that the stiffness of the membrane decreased with a decreasing film thickness, indicating the size effect on the nano scale. Chou et al. [8] used the finite element method to model the BCC atomic structure of Li using spring elements. They investigated Poisson's ratio and modulus of elasticity at the nano scale and found that there was a compressive prestress applied to the atom at the center of the lattice, when a tensile prestress was applied to the atoms at the corners of the lattice, and the modulus of

elasticity was by far larger than that of the bulk material, indicating a very significant scale effect.

In both of these cases, the molecular dynamics could effectively be used to model the interactive forces among molecules and their motions in order to perform analyses of the micro-dynamic processes; but, in the case of uniaxial tension, the time-step could either be too large or too small. In the former case, the speed of extension could become too large, not compatible to the actual physical phenomenon, and lead either to numerical instability or inaccurate results. In the latter case, a very large amount of computational time is required. The finite element method based on the spring element atomic model is a quasi-static approach. In this approach, the position of the next atom is calculated based on the concept that the atom moves to the minimum energy position when forces among the atoms are equilibrated. The procedure reduces the calculation time but can not perform the microscopic transient state analysis. In the finite element analysis using an atomic model of a non-linear spring and dashpot, a dashpot is included in this paper to damp out the excessive vibrations so that the atoms achieve equilibrium swiftly. This is a three dimensional model and it can effectively perform the microscopic transient analysis. Based on this method, a two dimensional model has also been developed to investigate the uniaxial tension of a copper film micro-structure. This is an explicit method using the finite difference method (FDM) for time and finite element method (FEM) for space. The stiffness matrix does not have to be inverted and no simultaneous equations need to be solved. Furthermore, it can avoid numerical divergence due to a step-by-step calculation of a non-linear problem and it saves computation time. The present model is used in this paper to investigate the effects of atomic distance and the strain rate on the deformation and the stress-strain relation.

II. THEORETICAL FUNDAMENTALS

A. Physical Model

Due to many difficulties encountered during tension test of nano-film, the physical model of this experiment is designed to perform a proportional tension test along the *[100]* direction of a copper nano film, see Fig.1. The advantages of the proportional tension test are allowing for larger strain rate, saving computer time, and obtaining more uniform deformation in the specimen.

During the proportional tension test, the displacement of each atom is given by the following equation:

$$x_i(t + \Delta t) = x_i(t) + \frac{x_i(t)}{L} \times \Delta L \qquad (1)$$

where x_i is the displacement of the ith atom along the *x* direction; ΔL is increment of displacement along the *x* direction; and L is the total length of the copper nano-film along the *x* direction.

Fig.2 shows the initial structure of the copper nano film. Since the material is a nano film, it is on the nano scale along the *x* direction. The dimensions of the copper nano-film structure are $14a_0 \times 6a_0 \times 6a_0$, in which a_0 is a lattice constant.

In this paper, the atoms of the idealized FCC single crystal copper are viewed as particles. The total count of particles for the whole structure is *2016* and the temperature

of the system is *293K*. The parameters of the physical model are given in Table 1.

B. Morse's Potential Function

For a microscopic system, the kinematic trajectory of particles depends upon the interactive forces between particles. A suitable choice of potential energy function is paramount for accurate simulation results. Three different potential functions (L-J, Morse's and EAM) have been used by Holian etc. [9] to simulate plastic deformation caused by impact while a two dimensional ball collides against a wall. Morse's and EAM (i.e. embedded atom method) potential energy functions are commonly used among researchers. According to previous papers, EAM is often more precise than Morse's and is widely used to simulate metal bonding. However, the EAM potential energy function is more complex than Morse's one.

Morse's potential energy function is used to model the interactive forces between atoms *i* and *j* in this paper and it is defined as

$$\Phi(r_{ij}) = D\{e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}\} \qquad (2)$$

where $\Phi(r_{ij})$ is the Morse's potential energy function, r_{ij} is the distance between atoms *i* and *j*, D is the binding energy, α is a material parameter and r_0 is the equilibrium distance. The aforementioned parameters are listed in Table 2.

The interactive force between atoms *i* and *j* is derived from eq.(2) and is expressed as:

$$F(r_{ij}) = \frac{\partial \Phi(r_{ij})}{\partial r_{ij}} = -D\{-2\alpha e^{-2\alpha(r_{ij}-r_0)} + 2\alpha e^{-\alpha(r_{ij}-r_0)}\} \qquad (3)$$

where $F(r_{ij})$ is the interactive force.

The interactive force is composed of two terms, one is the repulsive force and the other is the attractive force as shown in Fig.3. Note that the equilibrium distance, r_0 is the location of minimum potential energy, and also the location of zero interactive force. Atoms will repel to each other when their distance is shorter than r_0, and will attract otherwise. The attractive force decreases to zero rapidly and can therefore be ignored, so the Morse's cut-off potential energy function is defined as:

$$\Phi_c(r_{ij}) = \begin{cases} \Phi(r_{ij}), r_{ij} \le r_c \\ 0, r_{ij} > r_c \end{cases} \qquad (4)$$

where $\Phi_c(r_{ij})$ is the Morse's cut-off potential energy and r_c is the cut-off radius.

In order to simplify calculation and analysis when incorporating these potentials in finite element method, the interactive force in eq.(3) will be re-expressed in a dimensionless form.

III. FINITE ELEMENT MODEL

A. Formulations

The finite element atomic model with non-linear spring and dashpot is shown in Fig.4, where the *ith* atom and *jth* atom are located at a node. The mass of the atom is lumped at the node and the interactive forces acting between atoms are modelled by the non-linear spring and dashpot. If one of the atoms is fixed, then the equation of equilibrium for this, single degree of freedom, non-linear spring-dashpot system can be expressed using d'Alembert's principle as:

$$m\ddot{r}_{ij} + c\dot{r}_{ij} + f_{int}(r_{ij}) = f_{ext} \qquad (5)$$

where m is the mass of atom located at the center of node; c is the coefficient of viscosity; $f_{int}(r_{ij})$ is the interactive force between atoms, which is related to the distance r_{ij} between atoms; and f_{ext} is the external force acting on the node.

The interactive force between atom i and atom j, $f_{int}(r_{ij})$, expressed in terms of non-linear spring and dashpot, is a function of the distance between atoms and given by:

$$f_{int}(r_{ij}) = \begin{cases} \dfrac{\partial \Phi(r_{ij})}{\partial r_{ij}}, r_{ij} \le r_c \\ 0, r_{ij} > r_c \end{cases} \qquad (6)$$

From the above equation, the spring constant of the non-linear spring can be determined. It can completely define the attractive force between atoms; it can determine the fracture strain under compression and tension, which is the fracture criterion for the material; and it can be used to model the cut-off radius between atoms that appears in eq.(4).

The damping force is introduced in eq.(5) to avoid excessive vibrations of the atoms so that equilibrium can be quickly achieved. At critical damping, the coefficient of viscosity c can be expressed as:

$$c = 2m\omega\xi \qquad (7)$$

where ω is the natural frequency and ξ is the damping ratio.

The mass-spring-dashpot model may be formulated into a finite element formulation with the following governing equation and illustrated in Fig.5:

$$M\ddot{x} + C\dot{x} + F_{int}(x) = F_{ext} \qquad (8)$$

where M is the mass matrix; C is the viscosity matrix; $F_{int}(x)$ is the internal force referring to the global coordinate system; and F_{ext} is the external force. All of these parameters are with reference to the global coordinate system.

D0″Governing Equation and Solution Method

The governing equation of the non-linear finite element method is

$$M\ddot{x}(t) + F(x,\dot{x}) - P(x,t) = 0 \qquad (9)$$

The boundary conditions to be satisfied include the boundary condition for traction

$$\sigma_{ij} n_i = t_i(t) \qquad (10)$$

the boundary condition for displacement

$$x_i(X_\alpha, t) = D_i(t) \qquad (11)$$

and the boundary condition for contact

$$(\sigma_{ij}^+ - \sigma_{ij}^-) n_i = 0 \qquad (12)$$

where $F_e(x,\dot{x}) = \int_{V_e} B^t \sigma(\varepsilon,\dot{\varepsilon}) dV_e$ is the non-linear part, which is due to material and geometrical non-linearity; $x,\dot{x},\ddot{x}$ are respectively the displacement, velocity and acceleration; M is the mass matrix; σ_{ij} is the Cauchy stress; n_i is the unit normal vector on the boundary; $\varepsilon,\dot{\varepsilon}$ are respectively the strain and the strain rate; and $P(x,t)$ is a non-linear term induced by external forces.

A discrete governing equation is

$$Ma^n + Cv^n + Kd^n = F^{ext} \qquad (13)$$

where M is the mass matrix; C is the viscosity matrix; K is the stiffness matrix; F^{ext} is the external force; a^n, v^n, d^n are respectively the acceleration, velocity, and displacement of time step n.

Eq.(13) is solved explicitly and the procedures of solution are:

The governing equation (13) may be rewritten as

$$Ma^n = P^n - F^n + H^n \qquad (14)$$

where M is a diagonal mass matrix; P^n is external force and body force; F^n is a stress divergence vector; and H^n is the hourglass resistance.

The central difference method is used for the time step t^{n+1}. The difference equations are:

$$a^n = M^{-1}(P^n - F^n + H^n) \qquad (15)$$

$$v^{n+\frac{1}{2}} = v^{n-\frac{1}{2}} + a^n \Delta t^n \qquad (16)$$

$$u^{n+1} = u^n + v^{n+\frac{1}{2}} \Delta t^{n+\frac{1}{2}} \qquad (17)$$

where $\Delta t^{n+\frac{1}{2}} = \dfrac{(\Delta t^n + \Delta t^{n+1})}{2}$; v,u are respectively the node velocity and displacement vectors with reference to the global coordinate system.

Adding the increment of the displacement vector to the initial position vector, one obtains the geometric position of time step t^{n+1}:

$$x^{n+1} = x^0 + u^{n+1} \qquad (18)$$

Based on the position of the atom, the average length along the x direction of the copper nano-film may be calculated for each time step. Therefore, the strain may be expressed as:

$$\varepsilon_x = \frac{L(t) - L}{L} \qquad (19)$$

where L and $L(t)$ are respectively the initial length and the average length at time t of the copper nano film along the x direction. The tensile stress may be expressed as

$$\bar{\sigma} = \frac{F}{A} \qquad (20)$$

where F is the tensile force and A is the cross-sectional area when the atoms are at equilibrium.

IV. RESULTS AND DISCUSSION

A. Atomic Distance

This paper considers an FCC single crystal copper. According to the positions of the atoms in the unit cell, the atoms can be divided into face-centered atoms and cornered atoms. Their relations and distances to neighboring atoms are as follows:

Face-centered Atom: The relations between a face-centered atom i and its neighboring atoms and their distances are shown in Fig.6(a) and are given by:

$$r_{i-1} = \frac{\sqrt{2}}{2} \times a_0 = 2.5559 \overset{o}{A} \quad r_{i-2} = \frac{\sqrt{2}}{2} \times a_0 = 2.5559 \overset{o}{A}$$

$$r_{i-3} = a_0 = 3.6147 \overset{o}{A} \qquad r_{i-4} = \sqrt{\frac{3}{2}} \times a_0 = 4.4271 \overset{o}{A} \qquad (21)$$

where r_{i-1}, r_{i-2}, r_{i-3} and r_{i-4} denote the distances among atom i and its neighboring atoms *1, 2, 3* and *4*, respectively.

Cornered Atom: The relations between cornered atom i and its neighboring atoms and their distances are shown in Fig.6(b) and are given by:

3

$$r_{i-1} = \frac{\sqrt{2}}{2} \times a_0 = 2.5559 \overset{o}{A} \quad r_{i-2} = a_0 = 3.6147 \overset{o}{A}$$

$$r_{i-3} = \sqrt{\frac{3}{2}} \times a_0 = 4.4271 \overset{o}{A} \quad r_{i-4} = \sqrt{2} \times a_0 = 5.1120 \overset{o}{A}$$

$$r_{i-5} = \sqrt{3} \times a_0 = 6.2608 \overset{o}{A} \tag{22}$$

where r_{i-1}, r_{i-2}, r_{i-3}, r_{i-4} and r_{i-5} denote the distances among cornered atom i and its neighboring atoms *1, 2, 3, 4* and *5*, respectively.

From above, the distances among atoms may be summarized into five categories. They are

$$r_{ij} = 2.5559 \overset{o}{A}, \quad 3.6147 \overset{o}{A}, \quad 4.4271 \overset{o}{A}, \quad 5.1120 \overset{o}{A}, \quad 6.2608 \overset{o}{A} \tag{23}$$

where r_{ij} is the distance between two neighboring atoms i and *j*.

B. Verification of Model

It is seen from Fig.3 that the force between copper atoms diminishes quickly with increasing distance between the atoms. The force is minimal when the distance is greater than *2.5* times the equilibrium distance (r_0) of the atoms. Therefore, in this section, the cut-off radius r_c is taken as *2.5* times r_0 (=6.565 $\overset{o}{A}$) and, when the distance exceeds this amount, the calculation stops. It is shown from eq.(23) that five atomic distances among neighboring atoms are all smaller than r_c, and therefore they all need to be considered in the simulation.

Flow stress-strain curve: This paper considers a proportional extension along the x direction of a copper nano-film. The strain rate used is $1 \times 10^{10} s^{-1}$ which is same as that used by Lin and Hwang [6]. Fig.7 shows the flow stress-strain curve of the copper nano-film calculated by use of the new three dimensional atomic finite element model proposed in this paper. It is seen from the figure that the maximum stress in the copper material is about 30.0GPa which is very close to the value of the maximum equivalent stress obtained in the tensile test by Lin and Hwang [6]. Thus, the calculated value in this paper is quite reasonable.

Deformation diagram: Fig.8 shows different deformation stages of the copper nano film subject to uniaxial proportional tension, calculated by use of the three dimensional atomic level finite element model proposed in this paper. After the model has achieved equilibrium, tension is applied along the x direction and the shape of the copper nano-film not only extends along the x direction but also gradually shows necking in the y and z directions. When ε_x exceeds *0.275* and the atomic distance is greater than r_c for the middle portion of the atoms, interactive forces among the atoms become very small and negligible. Therefore, the stress decreases gradually which leads finally to fracture. This result is very similar to the simulated deformation process during material extension obtained by Komanduri et al. [2].

C. Effect of Atomic Distance

To investigate the effect of atomic distance, the relationship between a face-centered atom or a cornered atom as described in Fig.6 to another atom at the same distance is considered according to eq.(23) and divided into five categories. The relationships and the corresponding atoms are shown in Fig.9 and Table 3.

From eq.(3), the distance while the maximum interactive force between atoms i and j occurs can be derived as follows:

$$\frac{\partial F(r_{ij})}{\partial r_{ij}} = -D\{4\alpha^2 e^{-2\alpha(r_{ij}-r_0)} - 2\alpha^2 e^{-\alpha(r_{ij}-r_0)}\} = 0$$

$$4\alpha^2 e^{-2\alpha(r_{ij}-r_0)} - 2\alpha^2 e^{-\alpha(r_{ij}-r_0)} = 0$$

$$2e^{-2\alpha(r_{ij}-r_0)} - e^{-\alpha(r_{ij}-r_0)} = 0$$

$$2e^{-\alpha(r_{ij}-r_0)} = 1$$

$$\alpha(r_{ij} - r_0) = -\ln 0.5$$

$$r_{ij\,max} = \frac{-\ln 0.5}{\alpha} + r_0 = 0.51 \overset{o}{A} + 2.626 \overset{o}{A} = 3.136 \overset{o}{A} \tag{24}$$

where $r_{ij\,max}$ is the distance while the maximum interactive force between atoms i and j occurs.

The effect of the five categories of atomic distance is discussed in this section. Among the five categories, the first two categories are closest to $r_{ij\,max}$. Therefore, in order to discuss the effect of the other three categories, four examples are considered in the simulation of tensile test. Case 1 considers only the first two categories with the shortest atomic distances; Case 2 considers only the first three categories of atomic distance; Case3 considers the first four categories of atomic distance; and Case4 considers all five categories. Table 4 lists the number of elements and CPU time for each case. Fig.10 shows the simulated results for all cases using strain rate= $1 \times 10^{10} s^{-1}$ and $r_c = 2.5 r_0$. It is seen that the results for cases 3 and 4 are very close. Therefore, to save computation time, it is suggested that the latter case be neglected.

D. Effect of Strain Rate

The strain-rate effect on tension test is studied here using strain rates of $1 \times 10^{10} s^{-1}$ and $5 \times 10^{10} s^{-1}$. Fig.11 shows that the stress-strain curve is definitely influenced by the strain-rate. At the condition of large strain rate, the material resistance to deformation increases, leading to an increase in the overall and fracture stresses.

V. CONCLUSIONS

In this paper, an atomic model is constructed using the idea of non-linear spring, dashpot and lump mass. Based on this model, a three dimensional atomic scale finite element model has been developed for use in the nano-scale tension test. The mass of the atom is lumped at the node; the non-linear spring is used to connect the nodes and the connection force between the nodes, either repulsive force or attractive force, can be calculated; and the elongation at fracture of the spring can be used to determine the cut-off radius of the atomic link. From the simulation and analysis, the following conclusions can be drawn:

(1) In the proportional tension test along the x direction of the copper nano film, the simulated copper material's maximum stress at a strain-rate of 10^{10} per second is very close to *30.0GPa*, which is also the value of maximum equivalent stress obtained by Lin and Hwang [6], verifying the validity of the calculations in this paper.

(2) In the tension test of copper, necking develops gradually and eventually leads to fracture. The simulated deformed material element during each stage of deformation is similar to that simulated by Komanduri et al. [2].

(3) The influence of $r_{ij} = 6.2608 \overset{o}{A}$ on the five categories of atomic distance considered is limited and may be neglected to save computation time.

(4) The stress-strain curve is influenced by the strain-rate. When the strain-rate is large, the resistance to deformation is also large, leading to an increase in the ultimate stress and fracture stress.

VI. REFERENCES

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Table 1 Parameters of the physical model

Material	Cu
Dimensions	$14a_0 \times 6a_0 \times 6a_0$
Lattice Constant(a_0)	$3.6147 \overset{o}{A}$
Potential Function	Morse Potential
Temperature	293K
Loading	Proportional uniaxial tension
Direction	[100]

Table 2 Parameters of Morse potential function

Parameters	D (J)	α ($\overset{o}{A}^{-1}$)	r_0 ($\overset{o}{A}$)
Cu	5.449×10^{-20}	1.3588	2.626

Table 3 Relations for five categories of atomic distances in a unit lattice and the corresponding number of atoms

Atomic Distance (r_{ij})	Atoms to each face-centered atom	Atoms to each cornered atom
$2.5559 \overset{o}{A}$	8	none
$3.6147 \overset{o}{A}$	1	3
$4.4271 \overset{o}{A}$	4	none
$5.1120 \overset{o}{A}$	none	3
$6.2608 \overset{o}{A}$	none	1

Table 4 Number of elements and CPU time for all cases

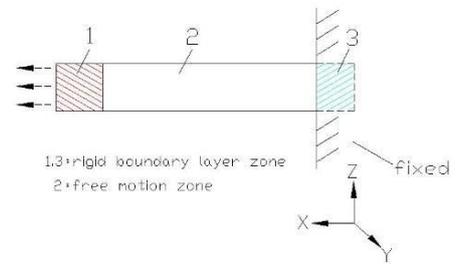| Case	No. of elements	CPU time(sec) using a Pentinum 4 3.0 GHz
1	19342	986
2	41902	1635
3	53136	2172
4	59672	2349

Fig.1 A physical model of proportional tension test
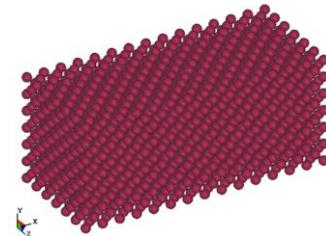

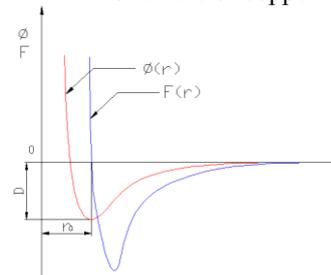Fig.2 The initial structure of copper nano film

Fig.3 Relation between Morse's potential function and force between molecules
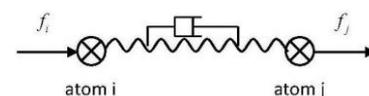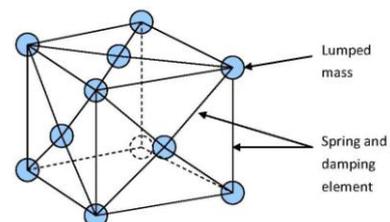

Fig.4 A single DOF mass-spring-dashpot element
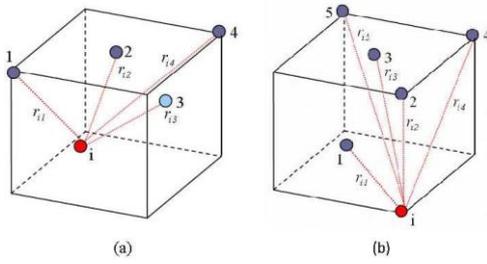
Fig.5 A schematic 3D model

Fig.9 Schematic diagrams for the five atomic distances

Fig.6 Relationship and distance for FCC crystal: (a) between face-centered atom and its neighboring atoms, (b) between cornered atom i and its neighboring atoms
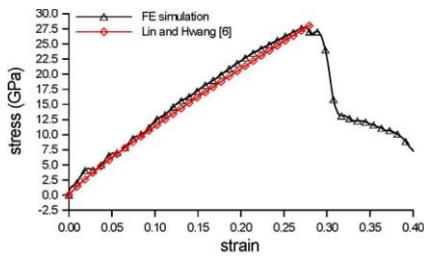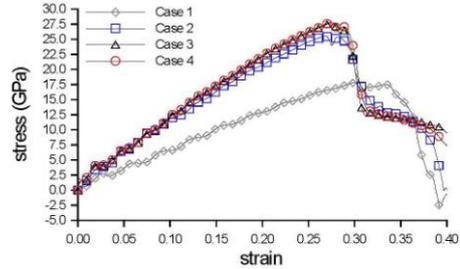

Fig.10 The simulated tensile stress-strain curves for different combinations of atomic distances

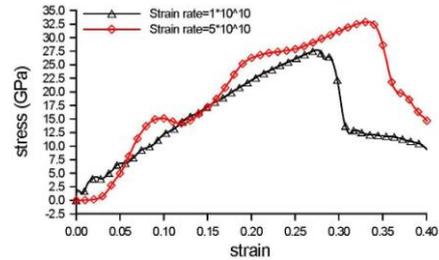Fig.7 Present solution compared with Lin and Hwang [6] for tensile test at $1\times10^{10}s^{-1}$

Fig.11 Stress-strain curves at strain rates of $1\times10^{10}s^{-1}$ and $5\times10^{10}s^{-1}$

(1) $\varepsilon_x = 0$ (2) $\varepsilon_x = 0.1$

(3) $\varepsilon_x = 0.2$ (4) $\varepsilon_x = 0.25$

(5) $\varepsilon_x = 0.3$ (6) $\varepsilon_x = 0.4$

Fig.8 Copper nano film at different deformation stages

(a) $r_{ij}=2.5559\overset{o}{A}$ (b) $r_{ij}=3.6147\overset{o}{A}$ (c) $r_{ij}=4.4271\overset{o}{A}$

(d) $r_{ij}=5.1120\overset{o}{A}$ (e) $r_{ij}=6.2608\overset{o}{A}$

6