Transactions of the Materials Research Society of Japan 29 [8] 3795-3797 (2004)

Two-dimensional molecular dynamics simulation of the nano-void influence on the elastic modulus of metals

H. A. Wu and X. X. Wang
Department of Mechanics and Mechanical Engineering, University of Science and Technology of China, Hefei, Anhui, China 230027

A two-dimensional triangular atomic lattice model is used to simulate three-dimensional face-center cubic (fcc) atomic lattice of single crystalline Ag to predict the mechanical properties of materials with nanoscale voids. The modified N-body Sutton-Chen potential developed for fcc metals was adopted to represent the interatomic interactions. Velocity Verlet scheme is implemented for time integration algorithm. Simulation temperature is kept constant by using Nosé-Hoover method. Two-dimensional simulation has great advantage of computing cost while maintains main physical mechanisms. It is found from the numerical results that the existence of nano-holes results in a decrease in the elastic modulus of single crystalline materials. The decrease of the modulus of materials with circle hole is approximately linearly related to the squared radius of the hole. With the same total area, a big hole causes more serious reduction of the modulus than small holes. It is also found that a flat ellipse hole reduces the modulus more significantly than circle holes of the same area. For materials with flat ellipse holes, the modulus is reduced much more in the direction of short axis than in the direction of long axis.
Key words: molecular dynamics simulation, elastic modulus, void, mechanical property, two-dimensional

1. INTRODUCTION

The approach of molecular dynamics (MD) simulation is one of the most promising methods for investigating the mechanical behavior of structures and materials at nano-scale [1]. In spite of rapid development in the application of quantum-mechanical techniques based on first principal [2], the use of empirical potentials for modeling materials at atomistic level is still necessary. Up to now, a variety of interatomic potentials has been used in the MD simulations of materials. These potentials include the Lennard-Jones (LJ) potential [3], the embedded atom potential (EAM) [4] and the Finnis-Sinclair (FS) potential [5]. Pair potentials, such as the well-known LJ potential, are not very suitable for metals but they have the advantage of being simple and less expensive computationally compared with the N-body potentials. However, this does not imply that all the N-body potentials are complicated and computationally expensive. For example the N-body FS type potential developed by Sutton and Chen [6] is relatively simple and not much more expensive in computations than the pair potentials.

The Sutton and Chen (SC) potential consists of a pairwise repulsive part and an N-body attractive part. The potential can be written as

$$E_{tot} = \varepsilon\left[\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}V(r_{ij}) - c\sum_{i=1}^{N}\sqrt{\rho_i}\right]$$

$$V(r) = (a/r)^n$$
$$\rho_i = \sum_{j\neq i}\left(\frac{a}{r_{ij}}\right)^m \qquad (1)$$

where r_{ij} is the distance between atoms i and atoms j, a is the fcc lattice parameter, ε is an energy parameter, and

$$c = n\sum_{j\neq i}\left(\frac{a}{r_{ij}}\right)^n \Bigg/ \left\{m\left[\sum_{j\neq i}\left(\frac{a}{r_{ij}}\right)^m\right]^{1/2}\right\} \qquad (2)$$

The material parameters for Ag are $n=6$, $m=12$, $\varepsilon = 2.5415\times10^{-3} ev$, $a = 0.409nm$, $c = 144.41$. The S-C potential combines the van der Waals attractive interaction at long range with the many-body cohesive interaction at short range and has been shown to predict the properties of a range of fcc metals quite well [6].

In continuum mechanics, two-dimensional models, such as plane stress, plane strain, and axis-symmetry, are employed to model some realistic three-dimensional problems, in order to make problems simple. These models can grasp the main physical mechanisms with less cost. In the present work, we intend to investigate the nano-void influence on the elastic property of Ag by molecular dynamics simulation. In order to increase the model size and reduce the simulation time, a two-dimensional (2D) Ag lattice is studied. Two-dimensional molecular dynamics [7] can simulate the models of bigger length size and longer timescale, while not neglecting the main physical mechanisms. It is a simplified modeling technique, which does not represent realistic atomistic configuration. For fcc metals, the crystal lattice will be triangle, as shown in Fig. 1.

In our present work, a two-dimensional triangular atomic lattice model is used to investigate the nano-void

influence on the elastic property of single crystalline. The size, shape and distribution of voids are discussed.

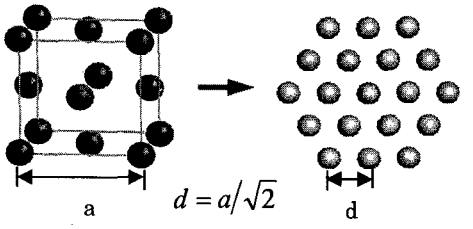


Fig.1 3D to 2D crystal lattice transformation

2. MODELING AND METHODOLOGY

The parameter in equation (2) has to be re-calculated for the 2D lattice, and it is 107.7. The cut-off distance for the calculation of potentials and forces is chosen to be 2.25 d , which is large enough to include the third-nearest neighbors. In the present atomistic simulation, the temperature is kept constant using Nosé-Hoover method [8]. The engine of a molecular dynamics program is its time integration algorithm, which is required to integrate the equation of motion of the interacting particles and track their trajectory. In molecular dynamics, the most commonly employed time integration algorithm is probably the so-called Verlet algorithm. Thus, the velocity Verlet scheme [3] is implemented in our program as follows:

$$\begin{aligned} \mathbf{r}(t+\Delta t) &= \mathbf{r}(t) + \mathbf{v}(t)\Delta t + \mathbf{a}(t)\Delta t^2/2 \\ \mathbf{v}(t+\Delta t/2) &= \mathbf{v}(t) + \mathbf{a}(t)\Delta t/2 \\ \mathbf{a}(t+\Delta t) &= -\nabla E(\mathbf{r}(t+\Delta t))/m \\ \mathbf{v}(t+\Delta t) &= \mathbf{v}(t+\Delta t/2) + \mathbf{a}(t+\Delta t)\Delta t/2 \end{aligned} \tag{3}$$

where the time-step Δt is set as 0.01ps.

We consider a rectangle of plate, with the size of 100200, i.e. 28.92nm50.09nm. In order to eliminate the surface effect, periodic boundary conditions are implemented. External tension force is uniformly distributed to the atoms of the top and bottom layer in Y direction, so the plate is in a unilateral extension state.

The initial configuration is created in accord with ideal geometrical lattice theory. In the beginning of the simulation process, the initial configuration is equilibrated at 0.01K for 50 ps, which is so called free relaxation. The extension loading will be applied in a step-by-step way. Since our objective is to study the quasi-static behavior of the material, equilibrium must be reached in each step before the next loading step is applied. From loading applied, we can compute stress, and from resulting deformation, we can compute strain. The mechanical properties of single crystalline are dependent on directions. In our present work, we only discuss the elastic modulus in [0 1] direction. The holes, as voids, are formed by removing some atoms.

3. RESULTS AND DISCUSSION

Using the methodology presented in Section 2, the elastic constitutive relation $\sigma_y = E \cdot \varepsilon_y$ can be computed. The stress-strain curve in the Y direction of plate without holes is illustrated in Fig. 2.

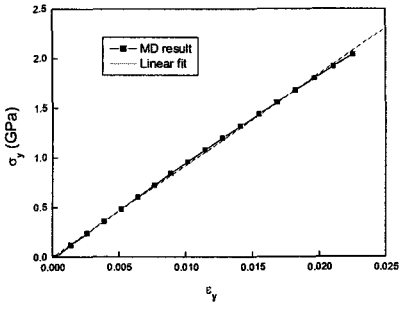


Fig.2 elastic stress-strain curve (no holes)

$$\sigma_y = 92.33\,\varepsilon_y$$

Now we insert a circle hole with the radius of 15 d , i.e. 4.3nm into the plate. The ratio of void to total area is 4.1%. The new stress-strain curve is illustrated in Fig.3. It is clearly demonstrated that the existence of nano-hole results in a decrease in the elastic modulus of single crystalline materials. We find that the stress-strain curve of the material even with hole is still linear and elastic when the strain is small enough (<0.02), which is in accord with our common knowledge in mechanics of materials.

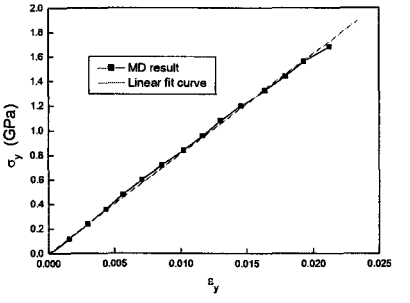


Fig.3 elastic stress-strain curve (with hole)

$$\sigma_y = 81.20\,\varepsilon_y$$

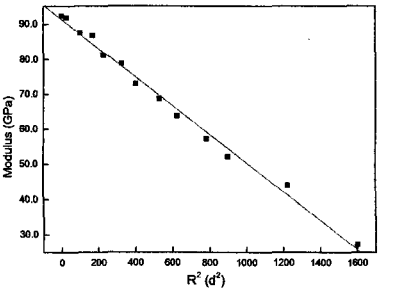
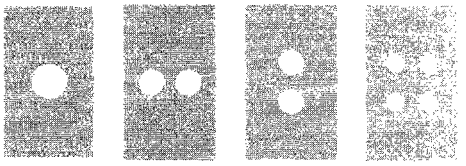


Fig.4 plot of elastic modulus as a function of square of radius of hole

We can further investigate the influence of the radius size of hole on modulus. We simulate another 11 similar models, with a hole of radius from 5d to 40d, i.e. from 1.4nm to 11.6nm. Together with two models simulated above, the curve of modulus varying with the radius of hole is plotted in Figure 4. It can be found that the decrease of the modulus of this material with circle hole is almost linearly related to the square of radius of the hole.

The distribution of holes can also influence the elastic modulus of materials. Below shows four models that have the same ratio of void. The radius of hole in model (a) is $20\,d$. The radius of holes in model (b) and (c) is $14.14\,d$. The two holes arrange in extension direction in model (c), while in perpendicular direction in model (b). The radius of holes in model (d) is 10. The resulting modulus is listed in Table I.



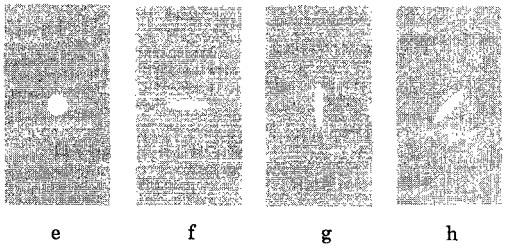
a b c d

Fig.5 models of different distribution of holes

Table I Elastic modulus of model (a, b, c, d)

Model	a	b	c	d
Modulus(GPa)	73.00	71.92	78.93	76.84

Compare model (b) with model (c), the former causes more decrease of modulus than the latter, which results from that its holes are arranged in the perpendicular direction of extension, i.e. its valid area of withdrawing extension loading is smaller. Compare model (a) with model (b), the same mechanism causes model (b) has lower modulus. Compare model (a) with model (d), the total area and direction parameter are the same, but modulus of (a) is lower than (d), from which we can infer a general conclusion that a big hole causes more significant reduction in the modulus than small holes with same total area.



e f g h

Fig.6 models with ellipse holes

We consider now ellipse holes. As illustrated in Figure 6, four models have the same void ratio. The radius of the circle hole is 9.54d; the lengths of the long and short axes are 20d and 4.5d respectively. The resulting modulus is listed in Table II.

Table II Elastic modulus of model (e, f, g, h)

Model	e	f	g	h
Modulus(GPa)	88.02	77.80	90.96	84.63

We find that the influences on the modulus of same size ellipse holes with different direction are quite different. The modulus of (f) is smaller than (e), while the modulus of (g) is lager than (e), which can be understand with the valid area theory. We can conclude that the existence of ellipse hole reduces the modulus of materials mainly in the direction of short axes. For model (h), we can expect that its modulus in X and Y direction are reduced in the same way. Compare (h) with (e), the modulus of former is smaller. From this fact, we can deduce another general conclusion that flat ellipse holes reduce the modulus more seriously than circle holes with same void area.

4 CONCLUSION

The S-C N-body potential, which was developed for fcc metals, has been used to carry out the molecular dynamics simulation of 2D lattices of a simple metal Ag. Our intention is to predict the mechanical properties of materials from atomistic scale. Scientists owe the reduction of some property parameters of realistic materials, compared with prediction from lattice theory, to the existence of various kinds of defects.

In this paper, the influence of nano-hole on the elastic modulus is simulated. The existence of holes results in the decrease of the elastic modulus of single crystalline materials. The decrease in the modulus of materials with circle hole is almost linearly related to the squared radius of the hole. With same total area, a big hole causes more serious reduction of the modulus than small holes. Flat ellipse holes reduce the modulus more seriously than circle holes. For materials with flat ellipse holes, the modulus is reduced much more in the normal direction of long axis than in the normal direction of short axis.

References

[1] H. Rafii-Tabar, *Physics Reports*, 325, 240-310 (2000)
[2] R. Car, *Quantitative Structure-Activity Relationships*, 21, 97-104 (2002)
[3] M. P. Allen, D. J. Tildesley, "Computer simulation of liquids", Clarendon Press, Oxford (1987)
[4] M. S. Daw and M. I. Bakes, *Physical Review B*, 29, 6443-6453 (1984)
[5] M. W. Finnis and J. E. Sinclair, *Philosophical Magazine A*, 50, 45-55 (1984)
[6] A. P. Sutton and J. Chen, *Philosophical Magazine Letters*, 61, 139-147 (1990)
[7] L. Hua, H. Rafii-Tabar and M. Cross, *Philosophical Magazine Letters*, 75, 237-244 (1997)
[8] W. G. Hoover, *Physical Review A*, 31, 1695-1697 (1985)

(Received October 13, 2003; Accepted April 24, 2004)