Investigation of the Virial Stress Distribution and its Relation with the Macroscopic Properties of a Single Crystal Copper Plate with an Elliptical Void

Iman Ebrahimi, Mehrdad Farid

***Abstract*— In this paper different elliptical nano-void models in a single crystal copper are studied by using molecular dynamics method with the Embedded Atom potentials. By applying strain rate of 10^9 1⁄sec, we investigate distribution of virial stress per atom in the plate. Stress concentration factor is determined for different void shapes and crack lengths. By plotting stress-strain curves, it is shown that elastic modulus and maximum averaged stress (yield point) are more sensitive to the number of removed atoms than the sharpness of the void. Contrary to classical continuum mechanics, no infinite stress concentration is observed at the void tip when its curvature decreases to small values.**

***Index Terms*— Molecular dynamics, Embedded atom method, Single crystal copper, Virial stress**

I. Introduction

The The mechanical properties of materials are significantly influenced by the presence of flaws or imperfections. These imperfections lead to magnification of the local stresses and when the forces between atoms become so large that the chemical bonds are ruptured, failure occurs. The most widely used method to study material behavior in nano scales is molecular dynamics (MD) [1], [2]. MD is a numerical method of solving the classical equations of motion for multiparticle systems.

In nano-scale dimensions many parameters affect mechanical properties of materials. For example Tang et al. [3] investigated the effects of specimen size, loading strain rate and temperature on microscopic parameters. Huang and his coworkers [4] showed that the fracture process depends sensitively on the system size and loading method and they determined the Griffith crack length in silicon. Zhao et al. [5] modeled a nano-sized cylindrical hole subject to uniaxial tension in a copper plate. The effects of the cell size, the crystalline orientation, and the initial void volume fraction on the macroscopic stress–strain curve, incipient yield strength, and macroscopic effective Young's modulus were quantified. Behzadi and Rafii-Tabar [6] investigated the propagation of a Mode-I (edge) crack in a roughened two-dimensional (2D) (1 1 1) plane of an Ag lattice. Koh and his coworkers [7] used MD to determine elastic modulus of nano-crystal of copper and they studied the grain size effects on the elastic modulus. They investigated the crack growth in nano copper plates. Inamura et al. [8] studied wave propagation around a crack front for monocrystalline silicon. Yang [9] and his coworkers investigated the influences of structural parameters of a void and its neighboring atom distribution on the effective elastic modulus and atomic stress concentration. Potirniche [10] and his coworkers simulated a nano size nickel plate with cylindrical void. The void volume fraction evolution and the corresponding stress–strain responses were monitored as the void grew under the increasing applied tractions. Buehler et al. [11] analyzed one-billion-atom simulation of ductile materials failure and dislocation motion and work hardening in nano-scales were studied. Seppala and his coworkers [12] studied the effect of stress triaxiality on the growth of a void in a three-dimensional single-crystal face-centered-cubic lattice.

In the present work we model a single crystal copper plate with an elliptical void in the middle. By applying uniaxial load, we investigate the distribution of the virial stress per atom, the stress concentration and the stress-strain curves of the plate.

II. Calculation method

Molecular dynamics simulation is a numerical implementation to solve the equations of motion of a system of atoms or molecules. It was first used to model the thermodynamical behavior of gases and liquids. In the early 1980s, the first publication of using molecular dynamics in mechanical behavior of solids released [2].

The classical dynamic equations of motion are valid for particles with their velocity much less than the speed of light and masses much bigger than electron mass. The potential energy is considered as a function of the system spatial configuration and is described by interatomic potentials. A special form of multibodypotential is embedded atom method (EAM) for metallic systems. The embedded atom method has been successfully applied to study defects and fractures, grain boundaries in alloys and metals. An EAM potential energy U is in the form of

$$U_i = \sum_{j=1}^{N_i} \phi(r_{ij}) + f(\rho_i) \quad (1)$$

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where φ is the pair potential interaction, f is the embedding function, and ρ_i is the local electron density as a function of the distant between a host atom j and the embedded atom i. In this article we use a formulation developed by Daw (1993).

To integrate the equations of motion, isobaric-isothermal ensemble (NPT) is used and Parrinello-Rahman algorithm is chosen. In this method, the desired temperature is adjustable and by changing the cell size of the simulated system the pressured is adjusted.

In atomic systems the stress tensor is only defined where atoms are located. In the present work we use virial stress to calculate the stress per atom in an atomic system. For a pair potential, the virial stress is defined as [2]

$$\sigma_{ij} = \frac{1}{V}\left(\sum_{\alpha,\beta,\alpha\neq\beta}\left(\frac{\partial\phi(r)}{\partial r}\frac{r_i}{r}r_j\right)\right) \quad , \quad r = r_{\alpha\beta} \qquad (2)$$

where r_i is the projection of the interatomic distant vector r along coordinate i and α, β are the atom numbers used in the calculation. We only consider the force part, excluding the part containing the effect of velocity of the atoms (the kinetic part).

The pressure P is calculated by [2]

$$P = NK_BT - \frac{1}{3}\frac{1}{V}\sum_{i=1}^{N}\sum_{j=1,j<i}^{N}\langle r_{ij}\frac{d\phi}{dr_{ij}}\rangle \qquad (3)$$

where N is the number of atoms in the system, K_B is the Boltzmann constant, T is the temperature and V is the volume. The first term stems from the kinetic contributions of particles hitting the wall of the container, and the second term stems from the interatomic forces.

III. Simulation Method

To investigate the effects of a nanovoid in a copper plate, several simulations are performed by subjecting the model to uniaxial tension. The initial cell is a face center cubic single crystal copper plate with the dimensions of $46a_0 \times 40a_0 \times 5a_0$, where a_0 is the lattice constant. Total number of atoms are 36800 and x, y, z axes are in [1 0 0] , [0 1 0] , [0 0 1] directions. Periodic boundaries are chosen for y and z directions. After generating the void by removing atoms in an elliptic region in the middle of the plate, the model is equilibrated with no external load by 3000 timesteps and then by using the conjugate gradient method, energy of the system is minimized (energy minimization corresponds to the physical situation of cooling down a material to absolute zero point). To subject the system to uniaxial tension, six atom layers of both edge sides of the plate are chosen to move in x direction by constant velocity. Previous works showed that strain rate has important effects on the stress-strain curves. In this study, 10^9 1/sec is used in all simulations for the strain rate. To integrate the equations of motion and to insure uniaxial stress state, NPT ensemble is used and timestep of 0.001psec is chosen and all simulations are performed at 0K.

IV. Results and Discussion

A. Effect of void sharpness

To study the effects of void sharpness in nano-scales, five specimens with different elliptic voids are employed. As shown in Fig.1 by fixing a and changing b value, different curvatures are gained.

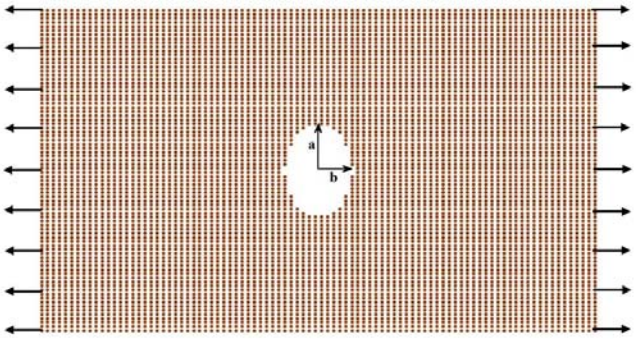

Fig. 1. By changing b different curvatures is gained.

Virial stress distribution per atom for a plate containing an elliptical void is illustrated in Fig.2. Maximum stress is occurred at the top and bottom of the void while minimum stress is occurred on the left and right sides of the void. This minimum stress is very close to zero that we can say these atoms do not feel any tension. Stress concentration factor is defined as $k_t = \sigma_{max}/\sigma$, where σ_{max} is the maximum stress and σ is the virial stress per atom while there is no void in the plate.

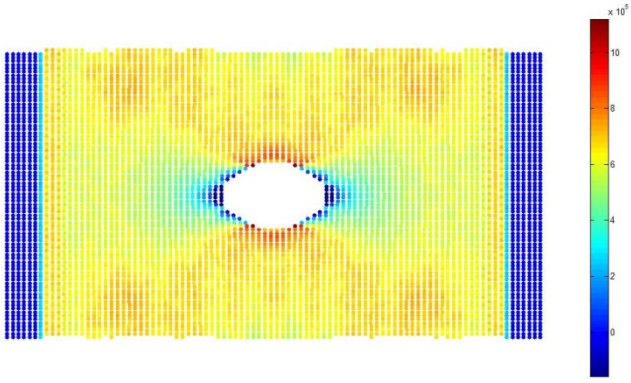

Fig. 2. Virial stress per atom distribution in a plate with a cylindrical void.

Fig.3 shows changes in k_t with different void curvatures. As predicted, by decreasing the curvature k_t will increase to a finite value. In classical continuum mechanics by decreasing curvature, stress concentration factor goes to infinity. This difference can be because of the discrete geometry of material atoms in nano-scale dimensions preventing sharp void edges.

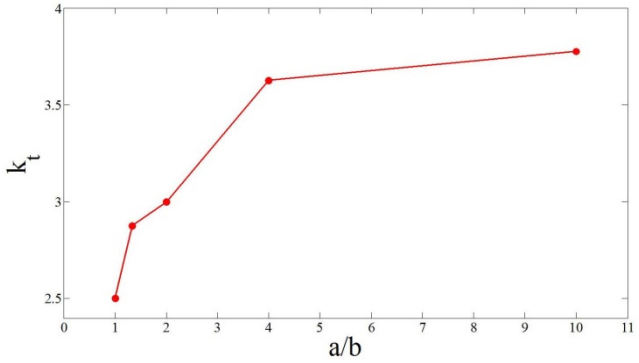

Fig. 3. Stress concentration factor at the crack tip for different curvatures.

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Fig.4 shows stress-strain curves for different curvatures. By decreasing the curvature, yield point increases even the stress concentration increases.

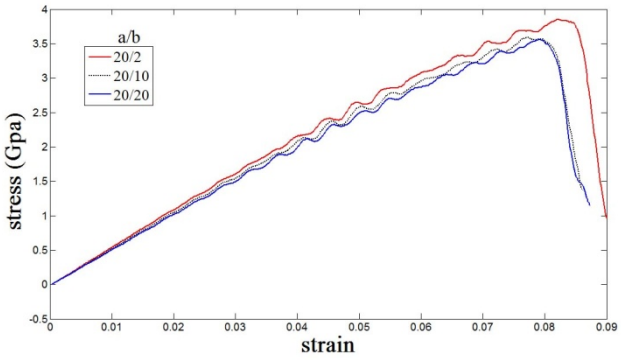

Fig. 4. Stress-strain curves for different elliptical void curvatures.

While curvature is being decreased, the total number of atoms does not remain the same, this leads to affect the total potential energy of the system. Increasing the number of removed atoms to decrease the sharpness is the reason of decreasing the yield point. To gain higher curvatures we remove atoms of the right and left sides of the void. These atoms _as shown before_ feel almost no stress, but their removal leads to a decrease in the yield point. Removing these atoms or any atoms in the specimen changes potential energy and this will cause the system failure. So it seems that the yield point is more sensitive to the total number of removed atoms than the stress concentration of the sample.

Fig.5 shows the changes in σ_{xx} in the void section. Maximum stress is in the edge atom of the void. By getting away of this atom, stress will decrease to its minimum, but it will not reach σ (stress per atom in the plate with no void). With decreasing the curvature, the changes in σ_{xx} near the void increases that makes stress concentration smaller in a specific distant (Fig.5).

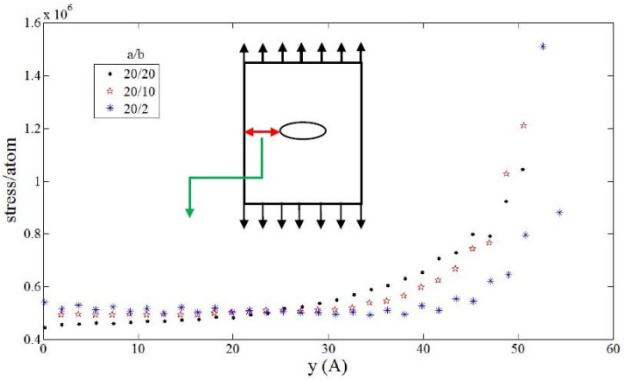

Fig. 5. Distribution of σ_{xx} between the edge of the plate and the void.

B. *Crack length effects*

To simulate a crack, we use an elliptic void with large ratio of major to minor radius. The Major axis is perpendicular to loading direction. Fig.6 shows the virial stress distribution per atom in a plate with a crack in the middle.

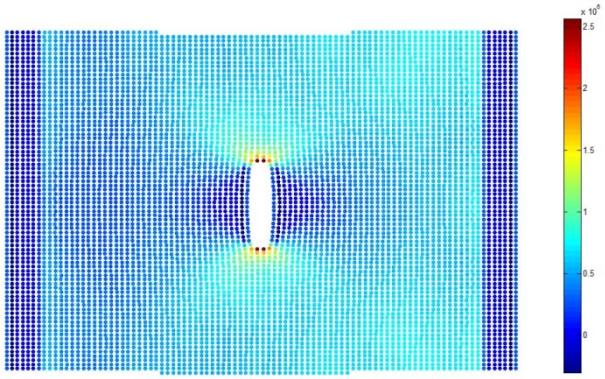

Fig. 6. Distribution of virial stress (σ_{xx}) per atom in the plate with a crack in the middle.

Maximum stress is occurred on the top and bottom of the crack and the minimum stress occurred in the left and right sides of the crack, while these atoms have little contribution in stress distribution, their presence _as discussed earlier_ has important effects on the elasticity modulus and the yield point of the plate.

As shown in Fig.7 by increasing the crack length, the stress concentration increases.

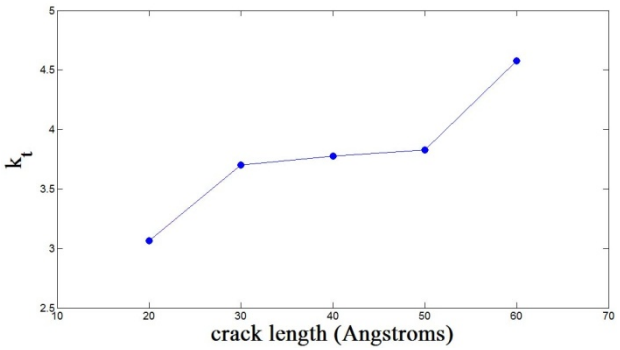

Fig. 7. Stress concentration factor at the crack tip for different crack lengths.

Fig.8 shows the stress-strain curves for different crack lengths. By increasing the crack length and subsequently the stress concentration, both yield point and elastic modulus decrease.

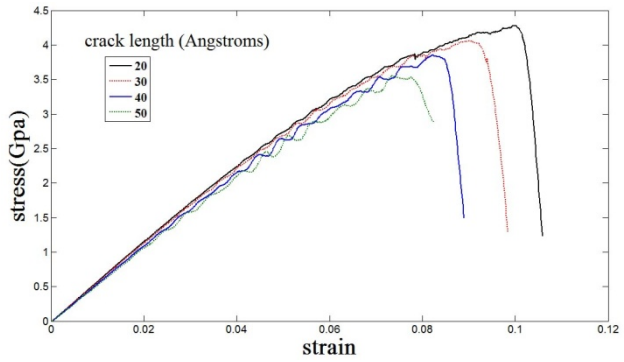

Fig. 8. Stress-strain curves for different crack lengths.

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V. Conclusion

By using molecular dynamics simulation we investigated the effects of existence of an elliptical void in a single crystal copper plate. By applying uniaxial load on the plate, the virial stress per atom, the stress-strain curves and the stress concentration factors were obtained and the following results were gained:

1. In a plate that has an elliptical void perpendicular to the loading direction, by decreasing the curvature, the stress concentration increases but there is no significant change in it. Especially when $a/b > 4$ this increment will be insignificant. In classical continuum mechanics by decreasing the curvature, the stress concentration factor increases rapidly in such a way that it reaches infinity in low curvatures. In nano scales because of discrete atom positions in the plate, it does not show high sensitivity to sharp voids.
2. By decreasing the sharpness, it seems that the elastic modulus and the yield point should increase, but contrarily they decrease. To gain higher curvatures we have to remove atoms in right and left sides of the void. The removing of atoms causes potential energy to decrease and leads to lower elastic modulus and yield point.

References

[1] Liu, W. K., Karpov, E. G., & Park, H. S. (2006). Nano Mechanics and Materials. West Sussex: John Wiley & Sons.
[2] Buehler, M. J. (2008). Atomistic Modeling of Materials Failure. Springer. pp.
[3] Tang T et al. Molecular dynamics simulations of void growth and coalescence in single crystal magnesium. Acta Mater (2010), doi:10.1016/j.actamat.2010.05.011.
[4] Huang, S., Zhang, S., Belytschko, T., Terdalkar, S. S., & Zhu, T. (2009). Mechanics of nanocrack : Fracture, dislocation emission, and amorphization. Journal of the Mechanics and Physics of Solids, Vol. 57, 840-850.
[5] Zhao, K., Chen, C., Shen, Y., & Lu, T. (2009). Molecular dynamics study on the nano-void growth in face-centered cubic single crystal copper. Computational Materials Science, Vol. 46 , 749-754.
[6] RafiiTabar, H., & Behzadi, S. (2008). Atomistic modelling of crack propagation in a randomly rough nanoscale metallic surface. Journal of Molecular Graphics and Modelling , Vol. 27, 356-363.
[7] Koh, S., Tummala, R., Saxena, A., & Selvam, P. (2008). A Numerical Analysis of Crack Growth and Morphology Evolution in Chip-to-Packages Nano-Interconnections. Electronic Components and Technology Conference (pp. 1625-1629). IEEE.
[8] Inamura, T., Takezawa, N., Shibuya, K., & Yamada, K. (2007). Dynamic Phenomena at Mode-I Crack Front in Silicon Simulated by Extended Molecular Dynamics. Annals of the CIRP, Vol.56 , 561-564.
[9] Yang, X., Zhou, T., & Chen, C. (2006). Effective elastic modulus and atomic stress concentration of single crystal nano-plate with void. Computational Materials Science, Vol. 40 , 51-56.
[10] Potirniche, G., Horstemeyer, M., Wagner, G., & Gullett, P. (2005). A molecular dynamics study of void growth and coalescence in single crystal nickel. International Journal of Plasticity, Vol. 22 , 257-278.
[11] Buehler, M. J., Hartmaier, A., Gao, H., Duchaineau, M., & Abraham, F. F. (2004). Atomic plasticity: description and analysis of a one-billion atom simulation of ductile materials failure. Computer Methods in Applied Mechanics and Engineering, Vol. 193, 5257–5282.
[12] Seppala, E. T., Belak, J., & Rudd, R. E. (2004). Effect of stress triaxiality on void growth in dynamic fracture of metals: A molecular dynamics study. PHYSICAL REVIEW, Vol. 69, 134101.1-134101.19.
[13] Schijve, J. (2003). Fatigue of Structures and Materials. Delft: Springer.
[14] Buehler, M. J., Gao, H., & Huang, Y. (2003). Atomistic and continuum studies of stress and strain fields near a rapidly propagating crack in a harmonic lattice. Theoretical and Applied Fracture Mechanics, Vol. 41, 21-42.
[15] Liu, W., Karpov, E., Zhang, S., & Park, H. (2004). An introduction to computational nanomechanics. Computer methods in applied mechanics and engineering, Vol. 193, 1529-1578.

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