ISSN 2354-0575

TENSILE PROPERTIES OF MONOCRYSTALLINE GOLD FILM USING MOLECULAR DYNAMICS SIMULATION

The-Van Tran, Anh-Son Tran
Hung Yen University of Technology and Education

Received: 21/01/2019
Revised: 15/02/2019
Accepted for publication: 05/03/2019

Abstract:

In this paper, the tensile properties of the monocrystalline gold film are studied by using molecular dynamics simulation. The stress-strain relation, crack growth behavior and effects of different temperature are considered. The results show that the stress concentration is obviously distributed in the middle and corners of the specimen, leading to the cracks are formed and propagated in these positions. Under the tensile process, the transformation from the face-centered cubic (FCC) into hexagonal closest packed (HCP) structures occurred. From the stress-strain diagram, the tensile strength and Young's modulus values decreased with increasing temperature. The RDF is decreased with a higher temperature.

Keywords: *Molecular dynamics; tensile strength; monocrystalline gold.*

1. Introduction

In recent years, crystalline metals have attracted intensive attention because of their excellent mechanical properties. Many previous studies investigated the mechanical properties of crystalline metals by experimental methods. However, as the size of the material decreases to the nanoscale, the use of experimental methods is not easy. With the rapid development of computer technology, molecular dynamics (MD) simulations have become more suitable than empirical methods for studying the properties of nanomaterials. Numerous processes have been investigated using MD simulations, including nanoindentation [1], nanoscratch formation [2], nanotension [3], and nanowelding [4]. Among various test processes, nanotension is commonly used to analyze the deformation and mechanical properties of nanocrystalline materials.

Crystalline gold is widely applied in electronic industries, for instance, the fabrication of semiconductor, superconductor are used in electronic, optical, and magnetic applications. Therefore, the understanding of the mechanical properties of crystalline gold is very important and necessary for fabrication processes.

In this paper, the author prepared monocrystalline gold film and focused to investigate the stress-strain relationship, deformation behaviors and crack nucleation of monocrystalline gold film at room temperature. Besides, the effects of different temperatures on the mechanical properties and the radial distribution function (RDF) of monocrystalline gold are also considered.

2. Methodology

In this study, the effects of nanotension on monocrystalline gold film are studied by using MD simulations. Fig. 1 shows the physical sample of monocrystalline gold film used for the tensile simulation. The crystalline unit of the face-centered cubic (FCC) Au substrate comprises x, y, and z-axes are directed along [100], [010], and [001], respectively. The geometric dimensions are approximately 2.04 nm (width) × 48 nm (length) × 35 nm (height). The two-dimensional (2-D) nanocrystalline nanomaterials are simulated in this study. In a real situation, 2-D nanomaterials can be patterned with different features at various scales. These 2-D patterns have different geometries from three-dimensional (3-D) bulk nanomaterials. The 2-D model has been selected because it is simple and nanofilms can be patterned. 2-D numerical models can be used with good accuracy instead of 3-D models if the in-plane stresses are primarily of interest. It is expected to adequate for a qualitative investigation of the nanocrystalline films. The fixed layers at the left and right sides of the sample along the y-axis direction are set to a fixed thickness of 6 Å. The lattice constant of gold is 4.08 Å, the total numbers of atoms of the substrates are approximate: 194,520. The periodic boundary condition is considered along the x-axis, while the free-boundary condition is assigned to the z-axis. The tensile speed of the fixed layer in the y-axis is fixed given unilaterally at 10 m/s until the set of steps is completed. The movement is integrated by the velocity–Verlet algorithm with a time step of 2 fs.

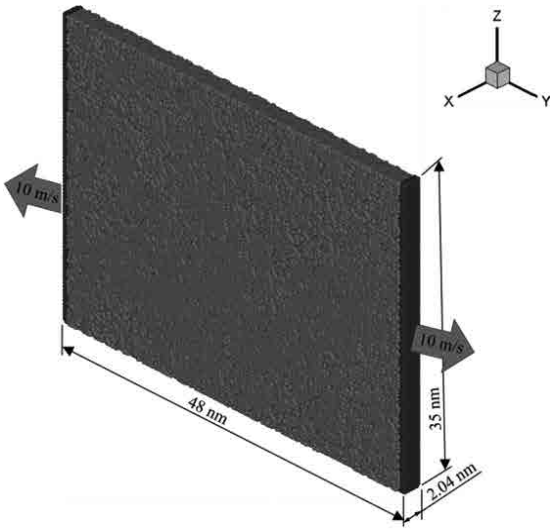

Figure. 1. *Physical model of monocrystalline gold film for the tensile simulation at room temperature*

The second–momentum approach of the many–body tight–binding (TB) potential [5] is used to express the Au–Au atomic interaction in the substrate. The TB potential is indicated as:

$$E_{TB} = \sum_i (E_R^i + E_B^i) \quad (1)$$

$$E_R^i = \sum_j A e^{-p[r_{ij}/r_0^{-1}]} \quad (2)$$

$$E_B^i = -\{\sum_j \xi^2 e^{-2q[r_{ij}/r_0^{-1}]}\}^{\frac{1}{2}} \quad (3)$$

where E_R^i is the repulsive energy, E_B^i is the attractive potential of atom i, r_{ij} is the distance between atoms i and j, and r_0 is the first-neighbor distance. The four parameters ξ, A, p, and q are determined from the cohesive energy experimental values, lattice parameter, bulk modulus, and elastic constants, respectively. The parameters for Au-Au interaction are A = 0.189 eV, ξ = 1.743 eV, p = 10.400, q = 3.867, and r_0 = 0.288 nm [6]. The used temperature is Kelvin temperature.

3. Results and discussion

3.1. Uniaxial stress-strain response and deformation behaviors of monocrystalline gold film at room temperature

Fig. 2 presents the stress-strain curve of the monocrystalline gold film under tensile test at 300 K. The phenomena can be roughly divided into three stages, namely the elastic stage, the plastic stage, and the strain hardening stage. In the elastic stages, the deformation of substrate can still be restored to the original shape. The second stage is the plastic stage, which cannot be restored to the original shape of the material at the beginning, and the material in the plastic zone. Finally, the strain hardening stage is more likely to cause obvious damage such as cracks and defects in the strain hardening zone.

It can be seen that the stress value rapidly rises to the maximum value of 2.75 GPa at a strain of 0.05. Then, the stress transmission is hindered due to the displacement and the slippage, lead to the decreasing of stress value. When the difference or the slip condition rise up to a certain degree, the stress value increases back to the relative value, and gradually become zero as the strain increases. The significant drop in stress value is due to the formation of gaps, slips or void defects in the specimen caused by the tensile process.

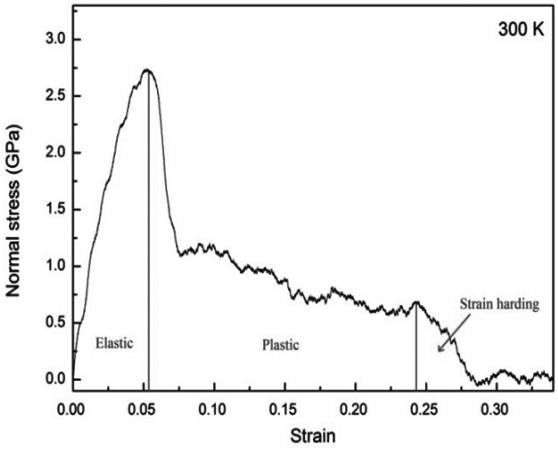

Figure 2. *Stress-strain diagram of monocrystalline gold film for the tensile simulation at 300K*

Fig. 3 shows the stress distributions of the monocrystalline gold film under different strains at 300 K. By comparison with Fig. 2, it can be found that the deformation behavior of specimen in Fig. 3(a) at ε = 0.059 is within the elastic stage range. The slight necking has occurred in the four corners of the material, where the stress is obviously observed. Transfer behavior is shown in Fig. 3(b). The strain value in the plastic stage, the twin crystal phenomenon appears on the left side of the specimen. Similar to Fig. 3(a), the stress is concentrated in the four corners. In addition, the stress is segmented at the boundary of the 45° dotted line in the middle of the specimen. In Fig. 3(c), the strain value is in the stage of strain hardening, and the stress concentration position is formed by the extension of the boundary line appearing in Fig. 3(b). The cracking occurs due to stretching, and the stress is continuously concentrated in the four corners of the specimen. The strain value is also on the strain hardening stage, however, the

cracking damages from the corner and middle of the specimen are formed due to the very high value of intermediate stress concentration at these positions, as shown in Fig. 3(d). Due to the high local stress concentration in the corners and middle of specimens, the link between atoms is weakened. Therefore, the link breakdown occurs, leading to the cracks are formed. Slippage also occurs in the middle and it is a cause of cracking specimen. In addition, near the fixed layer end on the left side of the material, the twinning phenomenon is continued until the end during the tensile process.

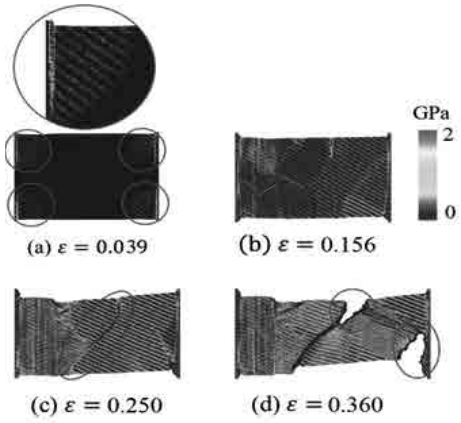

Figure 3. *The stress distributions of the monocrystalline gold film under tensile process at 300 K*

Fig. 4 shows the common neighbor analysis (CNA) diagrams of the monocrystalline gold film under the tensile process at 300 K. Fig. 4(a) shows that the position of the slip is the same as the position of the stress distribution, which is formed from the four corners of the specimen. At a strain of 0.156 in Fig. 4(b), a boundary is produced along the 45° line in the middle of the material (position B), which could not be easily judged in the stress map, the stress transmission is less obvious. The twin dislocation is evidently observed on the left side of the specimen (position A), which causes the different direction of the slippage, leading to the obvious change can be seen in the stress transmission. While the 45° boundary in the middle of the specimen only cuts off the original difference, there is no change the directionality, no obvious change in stress transmission. The twin dislocations are transferred into the vertical dislocations at a strain of 0.250 in Fig. 4(c). However, the stress transmission is still in the original direction and did not change following the shift of the row slip. In addition, the 45° boundary line can be clearly seen in the middle of the specimen. The stress is significantly concentrated on this line.

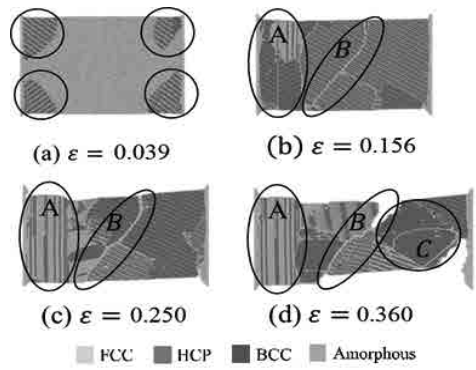

Figure 4. *CNA diagrams of the monocrystalline gold film under the tensile process at room temperature*

Fig. 4(d) presents the interesting phenomena. When the strain is 0.360, the FCC structures are extremely changed into HCP structures (position C) due to the slip and steering caused by the intense tensile strain. The stresses are very high and concentrated in this area. In addition, the material is fractured from the intersection of the 45° boundary line in the middle and the right fixed layer from the corner. The vertical dislocations still exist on the left side of the specimen (position A).

Finally, the transformation from the FCC into HCP structures is mainly exhibited, the cracks occurred in the middle and corner areas of the specimen with the increasing of strain under tensile process.

3.2. Temperature effects

Temperature is a factor that greatly influences the deformation mechanism of the material. Therefore, to obviously analyze the different transitions in deformation mechanisms with increasing temperature, the substrate temperatures are respectively determined of 300, 500, 700, 900 and 1000 K in this study.

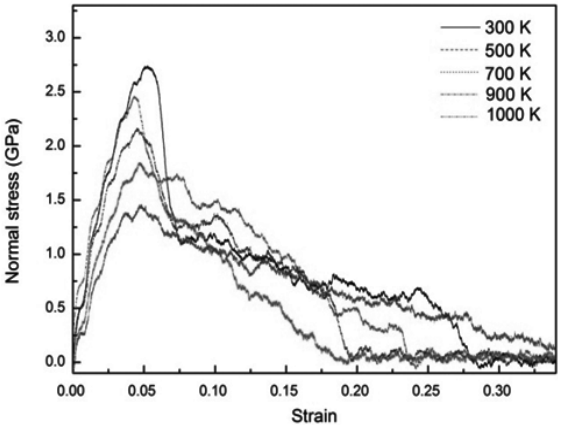

Figure 5. *Stress-strain diagram of monocrystalline gold films at different temperatures*

Fig. 5 illustrates the tensile stress-strain diagram of monocrystalline gold films at different temperatures. When the strain is at about 0.04 - 0.06 range, the corresponding stress is maximized. Then, the stress is vibrated by the tensile alteration, resulting in the dislocation is distributed in the sample. On the other hand, Fig. 5 shows that the temperature is increased, the slope is decreased. That means Young's modulus is greater with the lower temperature. This phenomenon can be interpreted by a larger amplitude of atoms fluctuating around its balance position at a higher temperature, which leads to that atomic bond is easier to be broken under applied load than lower temperature. In addition, the mobilization of preexisting dislocation generated in diffusion bonding at high temperature also contributes to the lower yielding stress. The similar results are found in a previous simulation study [7]. Atomic activity is more intensely enhanced and the material is softer as increasing temperature, lead to the tensile strength decreases. The tensile strengths are 2.75, 2.48, 2.20, 1.8 and 1.46 GPa at 300, 500, 700, 900 and 1000 K, respectively.

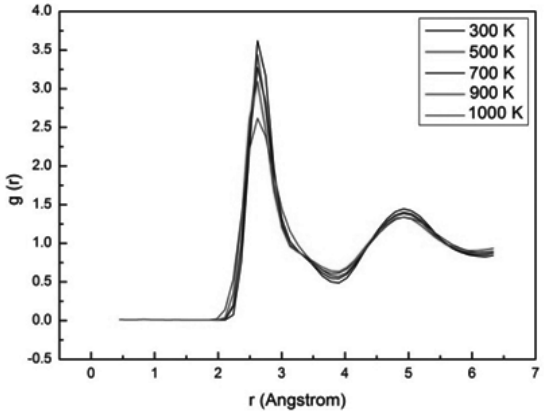

Figure. 6. *The radial distribution function of monocrystalline gold at different temperatures*

The RDF is calculated to give valuable information about the structural disorder of the material to organize the structural analysis. The RDF diagram of monocrystalline gold films at different temperatures is shown in Fig. 6. Each individual RDF curve shows a complete loss of the structural order of the material. The peak value of RDF decreased with the increasing temperature, which means that the structural stability of the material increases with the decreasing temperature. It can also be presented that the material at lower temperatures is relatively more stable due to the motions of the atoms are weaker. This result is a good agreement with a previous study by Hussain *et al.* [9]

4. Conclusion

The tensile properties and deformation behaviors of monocrystalline gold films are investigated by using MD simulations. The conclusions of this study are listed as follows:

(1) The stress concentration is obviously distributed in the middle and the corners of the specimen, leading to the cracks are formed and propagated in these positions.

(2) The transformation from the FCC into HCP structures occurred under the tensile process.

(3) The tensile strength and Young's modulus values decreased with increasing temperature.

(4) The RDF decreased with the higher temperature.

References

[1]. Díez-Pascual, A. M., Gómez-Fatou, M. A., Ania, F., & Flores, A. Nanoindentation in polymer nanocomposites. *Progress in Materials Science*, 2015, **67**, pp. 1-94.

[2]. J. Li, B. Liu, H. Luo, Q.H. Fang, Y.W. Liu, Y. Liu, A molecular dynamics investigation into plastic deformation mechanism of nanocrystalline copper for different nanoscratchingrates. *Computational Materials Science*, 2016, **118**, pp. 66-76.

[3]. Pogorelko, Viktor V., and Alexander E. Mayer. Influence of copper inclusions on the strength of aluminum matrix at high-rate tension. *Materials Science and Engineering: A*, 2015, **642**, pp. 351-359.

[4]. R. Cao, C. Deng, The ultra-small strongest grain size in nanocrystalline Ni nanowires. *Scriptamaterialia*, 2015, **94**, pp. 9-12.

[5]. F. Cleri, V. Rosato, Tight-binding potentials for transition metals and alloys. *Physical Review B*, 1993, **48**, pp. 22.

[6]. C.Goyhenex, Revised tight-binding second moment potential for transition metal surfaces. *Surface Science*, 2012, **606**, pp. 325-328.

[7]. A.B. Lebedev, Y.A. Burenkov, A.E. Romanov, V.I. Kopylov, V.P. Filonenko, V.G. Gryaznov, Softening of the elastic modulus in submicrocrystalline copper. *Materials Science and Engineering: A*, 1995, **203**, pp. 165-170.
[8]. Huang, S., Gao, Y., An, K., Zheng, L., Wu, W., Teng, Z., & Liaw, P. K. Deformation mechanisms in a precipitation-strengthened ferritic superalloy revealed by in situ neutron diffraction studies at elevated temperatures. *Acta Materialia*, 2015, **83**, pp. 137-148.
[9]. F. Hussain, M. Imran, M. Rashid, H. Ullah, A. Shakoor, E. Ahmad, S.A. Ahmad, Molecular dynamics simulation of mechanical characteristics of CuZr bulk metallic glasses using uni-axial tensile loading technique. *Physica Scripta*, 2014, **89**, 115701.

TÍNH CHẤT CHỊU KÉO CỦA MÀNG NANO VÀNG ĐƠN TINH THỂ SỬ DỤNG MÔ PHỎNG ĐỘNG LỰC HỌC PHÂN TỬ

Tóm tắt:

Trong bài báo này tính chất chịu kéo của màng nano vàng đơn tinh thể được nghiên cứu sử dụng mô phỏng động lực học phân tử. Mối quan hệ giữa sức căng và ứng suất, trạng thái mở rộng của vết nứt và những ảnh hưởng của nhiệt độ khác nhau được điều tra. Kết quả cho thấy ứng suất tập trung được phân bố chủ yếu ở giữa và tại các góc của mẫu, dẫn đến các vết nứt được hình thành và mở rộng tại các vị trí này. Dưới ảnh hưởng của quá trình kéo, sự chuyển đổi từ cấu trúc nguyên tử FCC thành cấu trúc HCP đã xảy ra. Từ biểu đồ sức căng và ứng suất, giá trị của độ bền kéo và mô đun đàn hồi giảm xuống khi nhiệt độ tăng lên. Chức năng phân phối xuyên tâm (RDF) của vật liệu cũng giảm dần với nhiệt độ cao hơn.

Từ khóa: *Động lực học phân tử; độ bền kéo; vàng đơn tinh thể.*