ISSN 2354-0575

EFFECTS OF ATOMICS GROWING ORIENTATION TO MECHANICAL PROPERTIES OF Cu/Ta BILAYER USING MOLECULAR DYNAMICS SIMULATION

Anh-Tuan Do, Anh-Son Tran
Hung Yen University of Technology and Education

Received: 10/01/2019
Revised: 15/01/2019
Accepted for publication: 26/02/2019

Abstract:

In this article, the effects of different atomics growing orientations to mechanical properties of Cu/Ta nanofilms with a circle void defect under tension process are studied using molecular dynamics simulation. The stress-strain relationship, structural phase transformations, dislocation mechanism, and local stress concentration are examined. The results show that the Cu[100]/Ta[111] nanofilm exhibited the most excellent mechanical properties. The FCC structures are mainly transformed into HCP structures, and <112>, <110> dislocations occurred in Cu sections. The local stress concentrations are focused around the intersection regions between void defect and Cu/Ta interface.

Keywords: *Molecular dynamics; Cu/Ta nanofilms; Hirth dislocations; Thompson tetrahedron.*

1. Introduction

Recently, metallic nanofilms are widely studied because of their excellent mechanical properties as follows: good toughness, high strength, and great hardness, etc [1]. Besides, metallic nanofilms are very easy in fabrication and adjustment corresponding to different specific conditions [2]. There are many factors that affect the mechanical properties of metallic nanofilms, however, atomics growing orientation directly influence on the deformation mechanisms and mechanical responses of metallic nanofilms under testing processes. Therefore, in order to analyze the changes in the structures of metallic nanofilms, a careful and systematic study of the deformation mechanisms and mechanical properties of nanofilms in different atomics growing orientations conditions is required.

Cu/Ta nanofilms is one of the most metallic nanofilms commonly used in aerospace, electronic, optical, and magnetic industries. Therefore, studying the mechanical properties of Cu/Ta is a very urgent requirement. However, it is very difficult to establish a Cu/Ta nanofilm with different atomics growing orientations by the experiment. With the strong development of computer technology, molecular dynamics (MD) simulation is a very accurate and reasonable choice to investigate the properties of materials at nanoscale [3-6].

In this study, the stress-strain relationship, structural phase transformations, dislocation mechanism, and local stress concentration of Cu/Ta nanofilms are studied by MD simulation under tension process. The Cu/Ta specimens are constructed with different atomics growing orientations. The results obtained provide a deeper insight on the deformation and mechanical properties of Cu/Ta nanofilms.

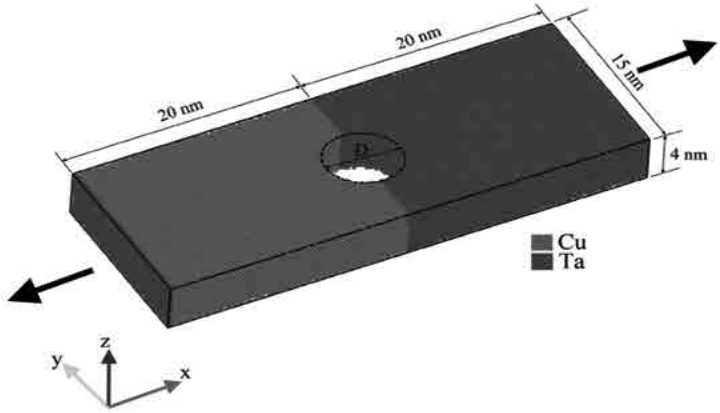

Fig. 1. *The simulation Cu/Ta nanofilm specimen under tension process*

2. Methodology

Fig. 1 shows the simulation models of Cu/Ta nanofilms under tension process. The sizes of the simulation specimen are 40 nm (length) × 15 nm (height) × 4 nm (thickness) corresponding to the x-, y-, and z-axes. Many previous studies have performed simulations with samples of approximately sizes [7,8]. The thickness is enough to out the size effect. The essential difference is at the boundaries: the bulk Cu and Ta systems with periodic boundaries have no locations for dislocation initiation. The diameter (D) of void defect is 3 nm. The different atomics growing orientations along x direction of the Cu/Ta nanofilms are [100]/[100], [100]/[110], [100]/[111], [111]/[100], [111]/[110], [111]/[111]. Periodic boundary conditions are determined in y- and z-axes, and the axial tension is specified along the x-axis.

The testing conditions of the simulations are at room temperature, a strain rate of 10^8 s^{-1}, and a time step of 2 fs. 10^5 time steps have been run in each simulation.

The MD simulation package Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [6] is applied to simulate the tension processes. The interaction potential energies between the atoms in Cu/Ta nanofilms are evaluated by the embedded atom method (EAM) [9]. The OVITO software [10] is used to indicate the tension processing. In OVITO software, the common neighbor analysis (CNA) is used to classify atoms that are connected with particular phases and defects in crystalline systems. The dislocation extraction algorithm (DXA) [10] is applied to determine the dislocations in the Cu/Ta nanofilms structures during the process, and exports the representational line for each dislocation defect and also useful for identifying the Burgers vectors.

3. Results and discussion

In this section, the mechanical properties and deformation behaviors of Cu/Ta nanofilms are assessed in terms of tensile stress-strain responses, dislocations, distributions of stress, and structural transformations of Cu, Ta atomics.

3.1. Tensile stress-strain responses

The stress-strain response is the most characteristic element to evaluate the mechanical properties of materials.

Fig. 2 shows the stress-strain relationship of Cu/Ta nanofilms with different growing orientations under tension process at room temperature and a strain rate of 10^8 s^{-1}. The maximum stress values achieved is at about the corresponding strain in 0.012 – 0.020 range. Then, the plasticity stage is going on, which can be presented by the vibration of the stress-strain curves. The plasticity stage lasts due to the effects of circle void defect in the specimens. The plasticity deformation is dominated by nucleation of dislocation at the surface of the void defect. The stress concentration is distributed and transferred around the void defect causes the prolongation of the plasticity stage. In the cases of Cu/Ta nanofilms with [111][100], [111][110], and [111][111] growing orientations, the stress values in plasticity stages are higher than these values in the cases of Cu/Ta nanofilms with growing orientations of [100][100], [100][110], and [100][111]. However, the opposite situation occurs with the tensile strength values. The tensile strength values are 2.51, 2.64, 2.83, 2.44, 2.47, and 2.05 Gpa corresponding to [100][100], [100][110], [100][111], [111][100], [111][110], and [111][111] growing orientations, respectively. The specimen with growing orientation of [100][111] exhibits the best tensile strength.

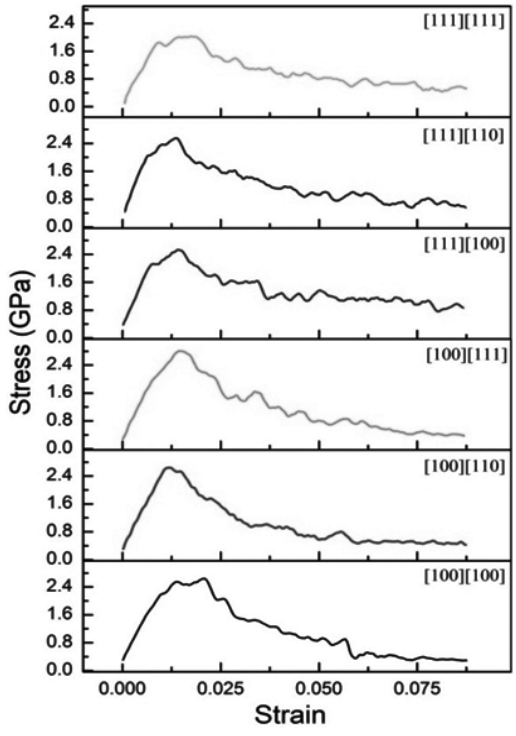

Fig. 2. *The stress-strain relationship of Cu/Ta nanofilms with different growing orientations under tension process at a temperature of 300 K, a strain rate of 10^8 s^{-1}*

3.2. Structural transformations and local stress distributions

The structural transformations and local stress distributions are very important factors to

investigate the deformation mechanism of Cu/Ta nanofilms under tension process. Fig. 3 presents the dynamic response of Cu/Ta nanofilms with different growing orientations under tension precess over the peak stress value at room temperature and strain rate of 10^8 s^{-1}. As we can see, the FCC structures are transformed into HCP structures in Cu element, while the BCC structures are changed into amorphous structures in Ta element. The dynamic responses of Cu/Ta specimens with growing orientations are [100][100], [100][110], and [100][111] are shown in Fig. 3(a). The oblique dislocations are obviously observed in Cu elements. However, the vertical and oblique dislocations occur together with growing orientations of Cu/Ta are [111][100], [111][110], and [111][111] in Fig. 3(b). Almost of these oblique dislocations are originated from the interface between Cu and Ta elements. Compare the dynamic responses of the Cu/Ta nanofilms under the tension process over the peak point, the Cu/Ta with growing orientations [100][111] exhibits the most stable in structural materials. That means the Cu/Ta [100] [111] exposes the best mechanical properties than other cases, which is consistent with the result in tensile strength of this specimen in section 3.1.

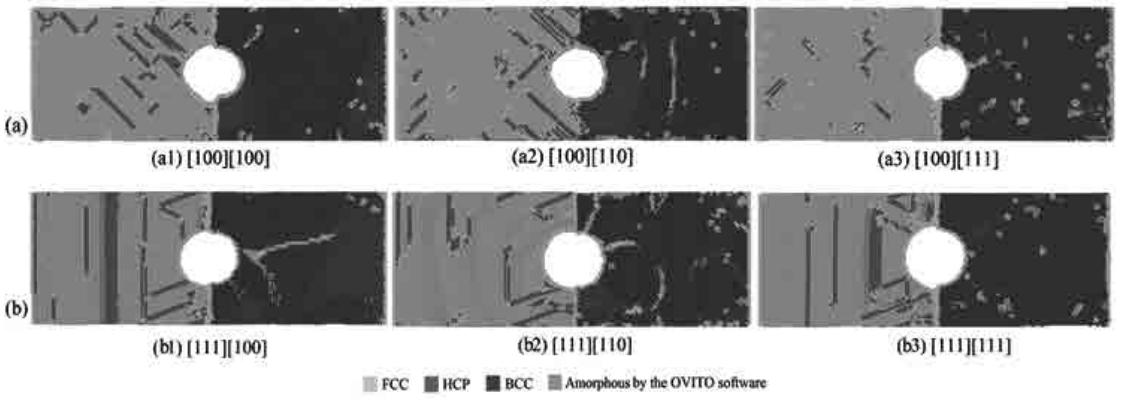

Fig. 3. *Dynamic response of Cu/Ta nanofilms with different growing orientations under tension process over the peak stress value at room temperature and strain rate of 10^8 s^{-1}. (a) The growing orientation of Cu is [100] and (b) The growing orientation of Cu is [111]*

Fig. 4 illustrates the local stress distributions of Cu/Ta nanofilms under the tension process over the peak stress at 300 K and strain rate of 10^8 s^{-1}. The larger stresses mainly concentrated on Cu elements due to the more intense deformation happened in Cu elements. The maximum stress concentrations focus around the circle voids, in particular, at the intersections between the circle voids and the interfaces of Cu/Ta elements, where the most severe deformations are observed. Atomic bonds in these areas are the weakest. All distortions originate from these locations, then spread to the surrounding areas causes the appearance of cracks.areas.

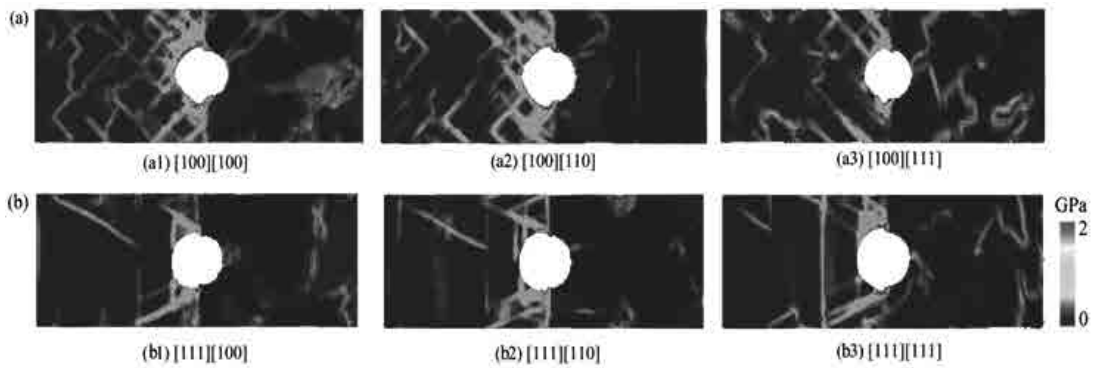

Fig. 4. *The local stress distributions of Cu/Ta nanofilms under the tension process over the peak stress at room temperature and strain rate of 10^8 s^{-1}. (a) The growing orientation of Cu is [100] and (b) The growing orientation of Cu is [111]*

3.3. Dislocations and fracture structures

In order to investigate the dislocations and fracture structures of Cu/Ta nanofilms under tension process, the Thompson tetrahedron used for indexing Burgers vectors and slip planes of Cu crystal (FCC) is presented in Fig. 5.

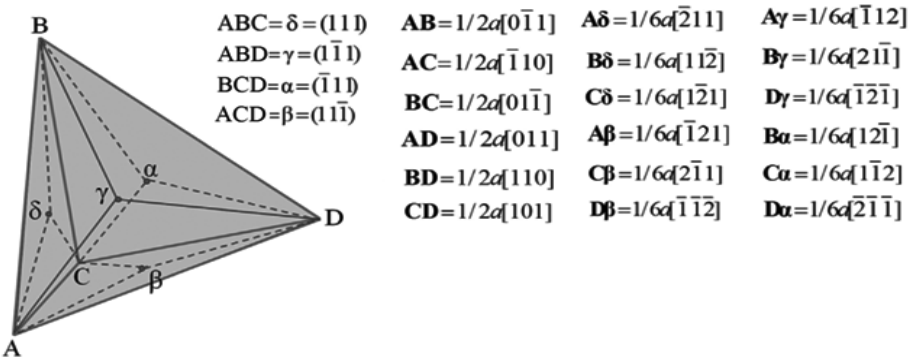

Fig. 5. *The Thompson tetrahedron used for indexing Burgers vectors and slip planes of FCC structure*

The dislocations and fracture structures of Cu/Ta nanofilms under the tension process over the peak stress at room temperature and a strain rate of 10^8 s^{-1} is shown in Fig. 6. The dislocations intensely appeared in the Cu elements. The generality dislocations are <112> and <110> in the Cu elements, and <111> in the Ta elements. This result is consistent with Lu et al. [4] and Zhang et al. [5] in previous studies.

The α and γ plane control all thplane control all the dislocation slip systems in Cu crystal. The Shockley partial dislocations [11] play a role as the leading partials. The glide of a leading partial in the swept areas under the tension process formed the intrinsic stacking faults. The intersection of the two leading partials on different [111] planes causes their movements being blocked and the stair-rod dislocation is generated, which is described as:

$\gamma\alpha = \gamma D + D\alpha$ or $1/6a\langle\bar{1}10\rangle = 1/6a\langle121\rangle + 1/6a\langle\bar{2}\,\bar{1}\,\bar{1}\rangle$ (in vector form) (2)

As a kind of sessile dislocation which is incapable of moving, the stair-rod dislocation is able to be dissociated into two trailing partials so that plastic deformation can proceed. The perfect dislocation is also formed according to the Shockley partial as follows:

$BD = D\alpha + B\alpha$ or $1/2a\langle110\rangle = 1/6a\langle211\rangle + 1/6a\langle12\bar{1}\rangle$ (in vector form) (3)

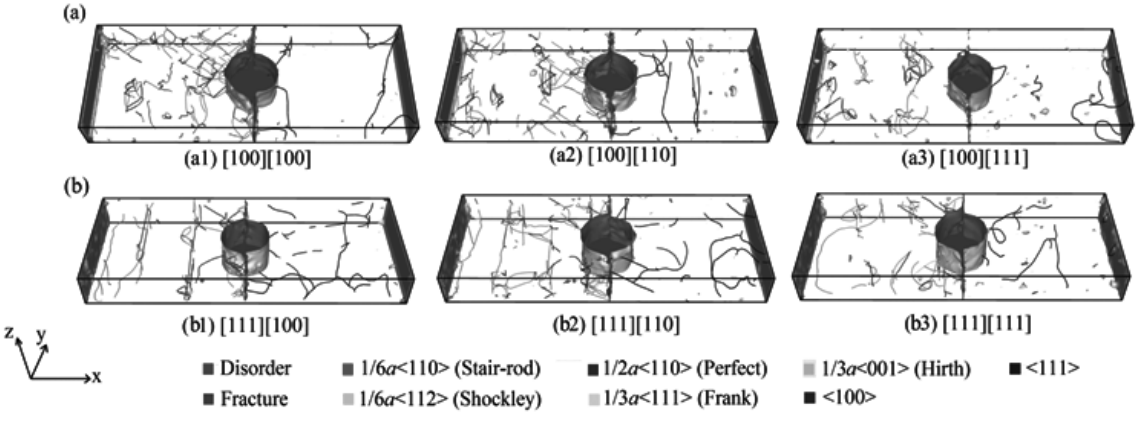

Fig. 6. *The dislocations and fracture structures of Cu/Ta nanofilms over the peak stress at room temperature and strain rate of 10^8 s^{-1}. (a) The growing orientation of Cu is [100] and (b) The growing orientation of Cu is [111]*

In addition to dissociating the stair-rod dislocations, the trailing partials are able to eliminate the stacking faults which result from the leading ones as well. Not only the stair-rod dislocation, but also another kind of sessile dislocation is formed, which is called Hirth dislocation [12]. This dislocation is the reaction product of a leading partial and a trailing partial and can be expressed as:

$\gamma\alpha/BD = \gamma B + \alpha D$ or $1/3a\langle001\rangle = 1/6a\langle\bar{2}\,\bar{1}\,1\rangle + 1/6a\langle211\rangle$ (in vector form) (4)

4. Conclusion

The mechanical properties and deformation mechanisms of Cu/Ta nanofilms with different growing orientations under tension process are studied using MD simulation. The conclusions are listed as follows:

(1) The Cu/Ta[100]/[111] nanofilms exhibits the most excellent mechanical properties.

(2) The local stress concentration is intensely distributed at intersections between circle voids and interfaces of Cu/Ta specimens.

(3) The FCC structures are mainly transferred into HCP structures.

(4) The <112> and <110> dislocations mainly occur in Cu elements, <111> dislocations are found in Ta elements.

ACKNOWLEDGMENT

This study is conducted by the research team UTEHY.T016 and funded by the Center for Applied Science and Technology Research, Hung Yen University of Technology and Education.

References

[1]. Zhou, Q., Xie, J. Y., Wang, F., Huang, P., Xu, K. W., & Lu, T. J., The mechanical behavior of nanoscale metallic multilayers: a survey. *ActaMechanicaSinica*, 2015, **31(3)**, pp. 319-337.

[2]. Wang, T. H., Fang, T. H., & Kang, S. H., Nanomechanical response of indented multilayered nanofilms with size effect. *Current Nanoscience*, 2010, **6(2)**, pp. 173-177.

[3]. Stukowski, A., Structure identification methods for atomistic simulations of crystalline materials. *Modelling and Simulation in Materials Science and Engineering*, 2012, **20(4)**, 045021.

[4]. Lu, L., Huang, C., Pi, W., Xiang, H., Gao, F., Fu, T., & Peng, X., Molecular dynamics simulation of effects of interface imperfections and modulation periods on Cu/Ta multilayers. *Computational Materials Science*, 2018, **143**, pp. 63-70.

[5]. Zhang, Y., & Jiang, S., Investigation on dislocation-based mechanisms of void growth and coalescence in single crystal and nanotwinned nickels by molecular dynamics simulation. *Philosophical Magazine*, 2017, **97(30)**, pp. 2772-2794.

[6]. Abraham, F. F., Computational statistical mechanics methodology, applications and supercomputing. *Advances in Physics*, 1986, **35(1)**, pp. 1-111.

[7]. Qiu, R. Z., Li, C. C., & Fang, T. H., Mechanical properties and crack growth behavior of polycrystalline copper using molecular dynamics simulation. *Physica Scripta*, 2017, **92(8)**, 085702.

[8]. Hsu, K. C., Chen, J. Y., Fang, T. H., & Lin, M. H., Size-dependent strength and interface-dominated deformation mechanisms of Cu/Zr multilayer nanofilms. *Results in Physics*, 2018, **11**, pp. 684-689.

[9]. Daw, M. S., Foiles, S. M., &Baskes, M. I., The embedded-atom method: a review of theory and applications. *Materials Science Reports*, 1993, **9(7-8)**, pp. 251-310.

[10]. Stukowski, A., Bulatov, V. V., &Arsenlis, A., Automated identification and indexing of dislocations in crystal interfaces. *Modelling and Simulation in Materials Science and Engineering,* 2012, **20(8)**, 085007.

[11]. Hull, D., Bacon, D. J., & Hull, D., Chapter 5—Dislocations in face-centered cubic metals. *Introduction to Dislocations, 5th ed.; Butterworth-Heinemann: Oxford*, *UK*, 2011, pp. 85-107.

[12]. Hirth, J. P., A brief history of dislocation theory. *Metallurgical Transactions A*, 1985, **16(12)**, pp. 2085-2090.

ẢNH HƯỞNG CỦA SỰ ĐỊNH HƯỚNG NGUYÊN TỬ ĐẾN TÍNH CHẤT CƠ HỌC CỦA TẤM NANO Cu/Ta SỬ DỤNG MÔ PHỎNG ĐỘNG LỰC HỌC PHÂN TỬ

Tóm tắt:

Trong bài báo này, ảnh hưởng của sự định hướng nguyên tử khác nhau đến tính chất cơ học của tấm nano Cu/Ta với một lỗ trống hình tròn dưới tác động của quá trình kéo được nghiên cứu bằng cách sử dụng phương pháp mô phỏng động lực học phân tử. Mối quan hệ giữa sức căng-ứng suất, sự biến đổi cấu trúc nguyên tử, cơ chế xô lệch mạng tinh thể và ứng suất tập trung cục bộ được đánh giá. Kết quả cho thấy rằng tấm nano Cu[100]/Ta[111] thể hiện các tính chất cơ học tốt nhất. Các cấu trúc FCC chủ yếu bị chuyển biến thành cấu trúc HCP, và các hướng lệch mạng tinh thể <112>, <111> xuất hiện ở phần Cu. Ứng suất tập trung cục bộ được phân bố xung quanh các vùng giao nhau giữa lỗ trống của mẫu và giao diện của Cu/Ta.

Từ khóa: *Động lực học phân tử; tấm nano Cu/Ta; sự lệch mạng Hirth; tứ diện Thompson.*