Molecular Dynamics Simulation of Local Structure Evolution in Cu Amorphous during Uniaxial Tension and Compression

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The local structural arrangement of the Cu amorphous was investigated during uniaxial tensile strain and compressive strain using molecular dynamics simulation, respectively. The amorphous of pure Cu system was get through high cooling rate in simulated situation. The amorphous phase of the system did not change in the tension process, whereas in the compression process the amorphous phase transform to bcc crystal structure. The tensile deformation promoted the expansion of the shear transition zones, whereas there is no similar result was observed in the compressive deformation process. [doi:10.2320/matertrans.MC201701]

Keywords: molecular dynamics simulation, uniaxial tension, uniaxial compression, amorphous structure, shear transition zone

1. Introduction

Amorphous alloys have been the subject of intense research in the past several decades, the scientific interest in this class of materials has been rapidly increasing. One of the attractions of amorphous are their unique mechanical properties³,⁴. Amorphous alloys exhibit elastic moduli on the same order as conventional engineering materials and strengths significantly in excess of polycrystals with same composition. Their strong tendency towards shear localization, which results in macroscopically brittle failure at room temperature, has imposed a barrier to broad commercial application⁵. Using the interesting properties of amorphous alloys for applications requires the understanding of the atomic scale mechanisms. However, amorphous alloys always have multi-element which results in complexity structure in amorphous alloys. And the present experimental techniques have difficulty to analyze atomic scale structure. The simulation method is a better choose to study amorphous material in atomic scale. One of the interesting research area using molecular dynamics is the deformation of metals⁶. R. Komanduri et al. used molecular dynamics to investigate uniaxial tension of some single-crystal cubic metals at nanolevel⁷. V. Yamakov et al. studied the deformation twinning in nanocrystalline Al by molecular dynamics⁸. Shin-Pon Ju et al. investigated the local structural rearrangement of Mg-Zn-Ca ternary amorphous⁹. However, the reports about pure element forming amorphous structure and local structure arrangement during uniaxial and compression are seldom reported.

The aim of this study is to show local structure arrangement of pure Cu amorphous using molecular dynamics (MD) simulations. The pure Cu amorphous was chosen as it is the least complex as compared to a multi-element amorphous with typically more than two constituting elements. Moreover, higher cooling rate might be easier get in simulation environment than laboratory condition. In this study, we compare the local structural atomic arrangement in uniaxial tension and compression of the Cu amorphous. The local structural properties are analyzed by radial distribution functions (RDF)⁴,⁹ and the Honeycutt-Andersen (HA)¹⁰,¹¹ and local atomic shear strain¹²–¹⁵.

2. Simulation Method

The MD simulation was used on the system containing 16000 atoms in a cube box with period boundary condition. The body-centered cubic (bcc) lattice was constructed with lattice constants set to 2.9 Å. All the atoms were assigned on the lattice sites. The Finnis-Sinclair embedded atom method (FSEAM) was selected for the interatomic interaction potential¹⁶. Newton’s equation of motion was integrated using the Verlet algorithm with a time step of 0.001 ps. To obtain the room temperature configuration of the amorphous, the system was melted at 2500 K under constant pressure and temperature (NPT ensemble), relaxed for 20 ps, and then quenched to 300 K with the cooling rate of 2.2 × 10¹³K/s. Uniaxial tension was applied in the microcanonical ensemble (NVE) under a constant strain rate of 1 × 10¹⁵m/s along the X-direction until the strain to 30%. Uniaxial compression was applied with the same condition but along the negative X-direction. Stress-strain responses were computed and local ordering analyzed using RDFs and the HA method for different magnitudes of strain. Local atomic shear strain was computed to visualize the patterns of atomic rearrangements.

3. Results and Discussion

The RDF, g(r), describes the probability of finding an atom in the spherical shell than has a radius, r, and a center positioned on another atom. Differences in RDF patterns of amorphous and crystalline can be used to identify the short and long ranged order of the atomic structure of metal. The position and intensity of the peaks provide insights about the local structure. Figure 1 (a) shows the RDF of the simulated Cu system after the cooling. The split in the second peak can be observed in the curve. The split in the second peak is the evidence of the amorphous phase¹⁷,¹⁸. This implies that
amorphous structure of Cu system was formed with the cooling rate of $2.2 \times 10^{12} \text{K/s}$.

To further investigate the local structural arrangement of atoms of the Cu system after cooling, we use the HA method. The HA structural pairs utilize a sequence of four integers to classify the local structure. According to the former literatures, amorphous and glassy structures is represented by the HA index 1551, 1541 and 1431. The bcc type has the type 1441 and 1661, the fcc structure has the type 1421, and hcp has the type 1421 and 1422. Figure 1 (b) shows the different HA types of the Cu system after cooling. HA types that occur less than 1.5 percent of the total number of atom pairs are ignored. Obviously the type 1551 is more than 50 percent of all bonded pairs in the system, indicating the amorphous phase of Cu system is formed after cooling.

Figure 2 shows stress-strain response of the amorphous Cu system under tensile strain (Fig. 2 (a)) and compressive strain (Fig. 2 (b)) from MD simulations. The stress is calculated using methods from Ref. 19. In Fig. 2 (a), stress increased linearly with strain at the beginning, indicating this stage is elastic deformation. Then the curve deviated from its initial linearity until to the critical strength. Finally, the Cu amorphous exhibited a sustained decrease in strength. In Fig. 2 (b), stress increased nonlinearly during the whole compression. By contrasting the curves of tension and compression, we have come to the tentative conclusion that different curve pattern maybe rise from different change of atomic structure of the Cu amorphous system by the different deformation.

Figure 3 shows the RDFs of the simulated Cu amorphous subject to uniaxial tensile strain (Fig. 3 (a)) and compressive strain (Fig. 3 (b)). In Fig. 3 (a), the split in the second peak can be observed in all the curves. This implies that the structure remained amorphous during the entire tensile process. With increased strains, the intensities of the two peaks increased and their positions shifted towards smaller distances, indicating tensile deformation increases the packing density of the local structure. In Fig. 3 (b), the split in the second peak gradually disappear in the curves with increased strains. This implies that the structure did not maintain amorphous during the entire compressive process. With the increased strains, the intensities of the two peaks decreased and their positions shifted towards smaller distance, indicating compressive deformation decreases the packing density of the local structure.

Figure 4 shows tensile strain (Fig. 3 (a)) and compressive strain (Fig. 3 (b)) as a function of interatomic distance, $r$ of the Cu system from simulations after cooling. (b) Relative numbers of bonded atomic pairs of the different Honeycutt-Andersen structural types of the system after cooling.
strain (Fig. 3 (b)) dependent fractions, expressed in percentage, the different HA types of amorphous Cu extracted from simulation. HA types that occur less than 1.5 percent of the total number of atom pairs are ignored. In Fig. 4 (a), it is clear that the type 1551 change very small throughout the entire duration of the tensile process, indicating deformation does not change the amorphous phase of the system, which agrees with our inference from the RDF curves mentioned above. The relative numbers of atomic pairs of the 1441 and 1661 types that correspond to the bcc crystal structure decreases with tensile strain. The 1561 and 1671 types slightly increase as tensile strain increase. Tensile deformation can transform 1551 to 1561, and 1661 to 1671, which discussed in one of our papers. Combined 1551 change very small with 1561 slightly increase, we could be inferred that the tensile deformation help the formation of 1551 type in Cu amorphous system. Meanwhile it break the bcc crystal structure (the 1441 and 1661 types decrease more than the 1671 type increase). In Fig. 4 (b), the 1551 type decreases dramatically as compressive strain increase. Meanwhile the 1441 and 1661 types dramatically increase with the compressive strain. The 1671 and 1561 types have little change during the entire process. These results show that the 1551 type transform to the 1441 and 1661 types in the compressive process, indicating that the compression deformation transform amorphous phase to bcc crystal structure in the system.

Figure 5 shows the snapshots of the microscopic strain filed \( \eta_{Mises} \) in the tension process (Fig. 5 (a)) and compression process (Fig. 5 (b)) of the simulated Cu amorphous system. Local atomic shear strain, \( \eta_{Mises_i} \), was used to trace the evolution of shear transition zones (STZs) and the definition of \( \eta_{Mises} \) can be found in Ref. 7). A large value of \( \eta_{Mises} \) implies the atom \( i \) is under local plastic and shear deformation, whereas a small value of \( \eta_{Mises} \) indicates that the atom \( i \) is under local elastic deformation. In Fig. 5 (a), at the strain of 10 percent, STZs distribute randomly. At the strain of 20 percent, STZs expand with maximal value of \( \eta_{Mises} \), STZs further expand at the strain of 30 percent. In Fig. 5 (b), at the strain of 10 percent, STZ distribute randomly as same
as Fig. 5 (a). At the strain of 20 and 30 percent, however there are no STZs expansion observed. These results maybe show that the tension deformation has deeply promoted on STZs expansion in the Cu amorphous system. The compression deformation has no the effect on STZs expansion, whereas the compression deformation has greatly promoted amorphous phase transform to bcc crystal structure in the Cu amorphous system.

4. Conclusions

In this study, we have used molecular dynamics simulation to study the local structural arrangements in the amorphous phase of the Cu under uniaxial tensile strain and compressive strain, respectively. We have analyzed the structural changes by using the radial distribution function, the Honey-Andersen method, and computing the magnitudes of local atomic shear strain. The conclusions are summarized as follows:

(1) The pure Cu system can be get amorphous phase in the MD simulation through high cooling rate.

(2) In tensile process, the stress-strain curve shows three different stages. The RDFs show that the amorphous is retained and the atomic structure becomes more closely packed with the tensile strain increases. In compressive process, stress increases non-linearly during the entire process. The RDFs show that the amorphous gradually disappear and the atomic structure becomes more loosely packed with the compressive strain increases.

(3) The Cu amorphous under uniaxial tension has a greater of atomic pairs of the icosahedral structural type (1551) than of the bcc crystal types (1441, 1661), whereas under uniaxial compression the icosahedral structural type transform to the bcc crystal types.

(4) The tensile deformation has deeply promoted on shear transition zones (STZs) expansion in Cu amorphous system, whereas the compressive deformation has greatly promoted the amorphous structure transform to bcc crystal structure in the system.

Acknowledgments

This work was supported by the Shanxi Key Laboratory of Precision Machining, Shanxi Province Science Foundation for Youths (Grant No. 201601D202028), and Shanxi Provincial Department of materials science and Engineering (Grant No.201606), and Taiyuan institutes of Technology.

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