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EFFECTS OF TEMPERATURE ON MECHANICAL RESPONSES OF $Cu_{50}Zr_{50}$ METALLIC GLASSES IN INDENTATION AND SCRATCHING PROCESS

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Abstract:

Through molecular dynamics simulations, the mechanical responses of $Cu_{50}Zr_{50}$ metallic glasses were investigated during the indentation and scratching process. The effects of different temperatures were analyzed through the surface morphology, pile-up height, hardness, machining forces, resistance coefficient, and radial distribution function (RDF) diagram. The results indicated that the pile-up height and the hardness reduce as the temperature increases. The chip height is the lowest and the scratching groove is the smallest at the highest temperature of 900 K. The forces and the resistance coefficient curves are very close in the temperature range from 300 to 700 K, while they are lower at 900 K. The peak point of RDF decreases as the increasing temperature.

Keywords: *$Cu_{50}Zr_{50}$ MGs, hardness, resistance coefficient, RDF.*

1. Introduction

As we know, it is necessary to survey and evaluate mechanical responses of materials because the mechanical properties are basic and very significant factors, which directly affect workability of the materials. During working process, heat is generated, which changes the characteristics of the material, especially the change of the mechanical responses. Therefore, the effects of heat on the mechanical responses of materials need to be carefully evaluated to help us prevent the material failures caused by heat. Many previous experimental studies [1,2] have been carried out to investigate the effect of heat on the material's mechanical responses. However, the experimental results are not really profound due to the very large size of the test samples, while the mechanical deformation of the material occurs at the atomic scale or nanoscale. This is an inherent disadvantage of experimental methods, which needs to be improved and replaced by more available methods. With rapid progress of software science and technology, the molecular dynamic simulation (MD) method was born and becomes a suitable choice in simulating and evaluating the properties of nanomaterials. With the advantages such as simple experiment setup, accurate simulation results, and diverse test processes, the MD simulation method is now widely applied in the materials science industry all over the world.

Nowadays, the CuZr metallic glasses (MGs) [3] are widely used for applications in electrical engineering, magnetic-sensing, chemical, and structural materials. The CuZr MGs dissolve better than the corresponding pure metal or metals. The addition of Zr to Cu, results in a medium strength, heat treatable alloy with an increased softening temperature compared to pure copper whilst maintaining excellent electrical and thermal conductivity. The indentation and scratching processes are usually performed to study the mechanical properties and deformation mechanisms of materials, however, the combination of these two processes is scarce, especially with the CuZr MGs.

From the analysis above, the mechanical responses and deformation mechanisms of the $Cu_{50}Zr_{50}$ MGs systems are analyzed and evaluated through the combination of indentation and scratching processes using MD simulation in this work. The machining processes are simulated at various temperatures. The results will supply a more penetrating understanding of the mechanistic abilities of $Cu_{50}Zr_{50}$ MGs.

2. Methodology

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is applied to create all MD simulations. The Open Visualization Tool (OVITO) is used to present the processing data from MD simulations. The embedded atom model (EAM) potential [4] is employed to depict the interaction between Cu and Zr atoms. The atoms interaction between the indenter and $Cu_{50}Zr_{50}$ MGs is employed by the Lennard-Jones (LJ) potential [5]. The indenter is set as a rigid body, therefore the interaction between C atoms of the indenter is ignored.

The $Cu_{50}Zr_{50}$ MGs model is created from the melting/quenching process [6]. First, the model is heated up to 2128 K (melting point of Zr component) at a heating rate of 2 K/ps. Then, the thermal equilibration process is kept at 2128 K for 500 ps. Finally, the model is cooled down to 300 K at a high cooling rate of 5 K/ps and then equilibrated at 300 K for 500 ps.

The simulation model system for the indentation and scratching process including a sphere diamond indenter and a $Cu_{50}Zr_{50}$ MGs sample is presented in Figure 1. To simplify the machining problem and focus on the deformation of the $Cu_{50}Zr_{50}$ MGs sample, the indentation, scratching, and retraction are performed with the ideal rigid indenter. The first experiment was performed at room temperature (300 K) to explore the properties and deformation mechanism of the $Cu_{50}Zr_{50}$ under normal working conditions. Then, to deeply appreciate the influence of temperature and the obvious change of the properties and deformation mechanism of the $Cu_{50}Zr_{50}$, three more different temperature levels were selected as 500 K, 700 K, and 900 K. The indenter radius is 2.0 nm. The dimensions of the $Cu_{50}Zr_{50}$ MGs specimen are 15 nm (length) × 6 nm (height) × 10 nm (width) corresponding to *x*-, *y*-, and *z*-axis, respectively. The periodic boundary conditions are determined in the *x*-, and *z*-axis, while the free boundary is applied along the *y*-axis. The NVT (canonical ensemble) is used in the simulation. Initially, the indenter is 1 nm from the surface of the sample. First, along the *y*-axis, the indentation stage is carried out with a depth of 2 nm and the indentation velocity of 50 m/s. After that, the indenter moves along the the *x*-axis by a distance of 5 nm with the velocity of 50 m/s to perform the scratching stage before retracts to the original position with the velocity of 100 m/s. The parameters related to the experimental process were selected based on previous studies [7].

The Brinell hardness (H) [8] is determined as

$$H = \frac{F_{max}}{A_c} \quad (1)$$

where F_{max} is the maximum normal force, A_c is the contact area between the indenter and specimen in the indentation stage. A_c is calculated as

$$A_c = \pi D h_c \quad (2)$$

where h_c is the indentation depth. The resistance coefficient (μ) [9] is determined as follows:

$$\mu = \frac{F_t}{F_n} \quad (3)$$

where F_t and F_n are the tangential and normal forces in the scratching stage, respectively.

3. Results and discussion

Temperature is an important working condition, which clearly affects the mechanical behaviors of the materials. In this part, the selected temperatures are 300, 500, 700, and 900 K, respectively.

Figure 2 shows the lateral cross-sectional-

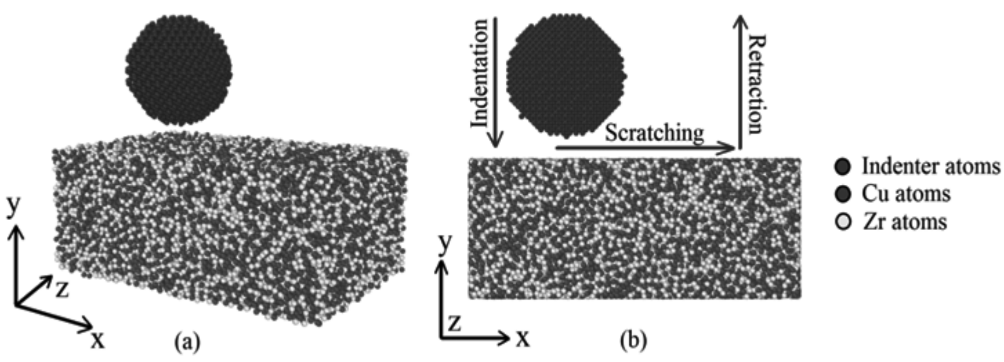

Figure 1. The $Cu_{50}Zr_{50}$ MGs model for the indentation, scratching, and retraction system

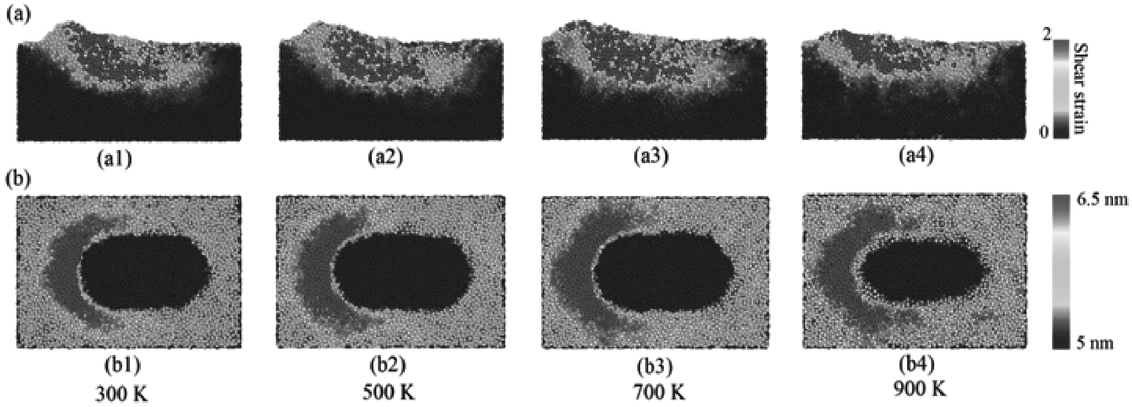

Figure 2. (a) The lateral cross-sectional-view of the pile-up and groove formed after the retraction of the indenter and (b) the surface morphology of the $Cu_{50}Zr_{50}$ MGs for the cases of different temperatures

view of the pile-up and groove formed after the retraction of the indenter (a) and the surface morphology (b) of the $Cu_{50}Zr_{50}$ MGs for the cases of different temperatures. As we can see, the pile-up height reduces, and the change in the size scratching groove as the increasing temperature. The changes are most clearly observed at a temperature of 900 K in Figure 2(a4) and (b4). The height of the chip is the lowest and the size of the scratching groove is the smallest. The maximum pile-up height diagram of the $Cu_{50}Zr_{50}$ MGs at different temperatures is presented in Figure 3. The maximum pile-up heights are 14, 13, 12, and 10 Å corresponding to temperature values are 300, 500, 700, and 900 K, respectively. This is due to the characteristics transformation of the material with the temperature change. At low temperatures, the brittleness of the material is more dominant, leading to the chip easy to form locally. The softness of the material prevails at high temperatures, the atoms can be compressed more tightly. Besides, the removed materials have not locally concentrated in front of the indenter that spreads around the indenter due to the strong activity of atoms. Therefore, the pile-up height is lower as the higher temperature. The above causes are also reasons to explain the decrease in hardness of the $Cu_{50}Zr_{50}$ MGs when the temperature increases.

Figure 3 shows the hardness of the $Cu_{50}Zr_{50}$ MGs at different temperatures under the indentation process. The hardness values of the $Cu_{50}Zr_{50}$ MGs are 8.72, 7.96, 7.14, and 5.38 GPa corresponding to temperatures of 300, 500, 700, and 900 K, respectively. The bonding stability between atoms becomes weaker as increasing temperature. So, the hardness of the $Cu_{50}Zr_{50}$ MGs is lowest at the highest temperature of 900 K, which is consistent with the previous studies [6,7].

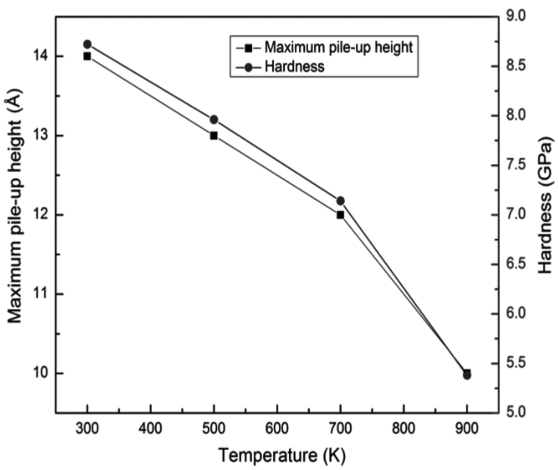

Figure 3. The maximum pile-up height and the hardness of the $Cu_{50}Zr_{50}$ MGs at different temperatures

Figure 4 presents the normal (a) and tangential (b) forces diagram of the $Cu_{50}Zr_{50}$ MGs during the indentation, scratching, and retraction process at different temperatures. Both F_n and F_t decrease as temperature increases. The material becomes weaker and softer with increasing temperature because the stability in the bonding between atoms reduces. Thus, the necessary force to realize the machining process is reduced. However, both F_n and F_t change slightly in the temperature range from 300 to 700 K, while the significant differences were observed at 900 K because the material is the weakest at the highest temperature of 900 K.

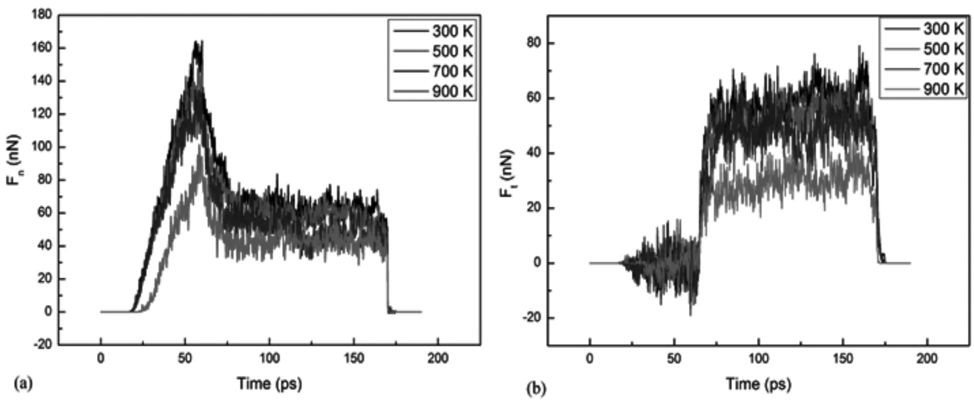

Figure 4. (a) Normal and (b) tangential force diagram of the $Cu_{50}Zr_{50}$ MGs during the indentation, scratching, and retraction process at different temperatures

Similar trends are also observed with the resistance coefficient diagram of $Cu_{50}Zr_{50}$ MGs at different temperatures under the scratching process in Figure 5. The resistance coefficient curves are very close in the temperature range from 300 to 700 K, while it is clearly lower at 900 K.

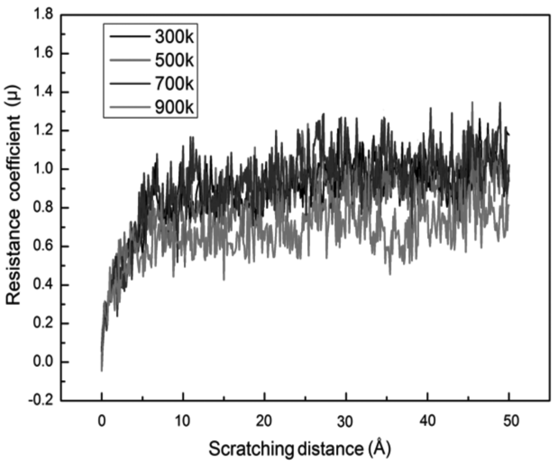

Figure 5. Resistance coefficient of the $Cu_{50}Zr_{50}$ MGs at different temperatures under the scratching process

The RDF of the $Cu_{50}Zr_{50}$ MGs at different temperatures under the machining process is shown in Figure 6. In order to examine the material's structure characteristics, the RDF of the $Cu_{50}Zr_{50}$ MGs are determined and calculated at temperatures of 300, 500, 700, and 900 K, respectively. The results indicate that the peak of RDF becomes lower as the temperature increases [8]. It means that at a lower temperature, the structure of the material is steadier. This result supplies good information about the disturbances of the material structure at various temperatures.

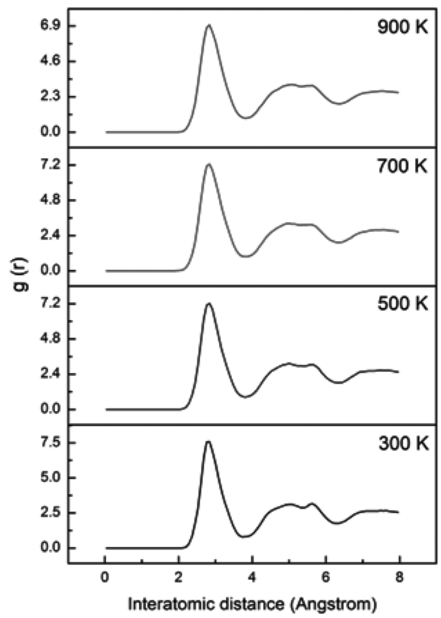

Figure 6. The radial distribution functions of the $Cu_{50}Zr_{50}$ MGs at different temperatures under the machining process

4. Conclusion

With the variation of testing temperature, the mechanical dynamic responses of the $Cu_{50}Zr_{50}$ MGs are significantly different. At a higher temperature, the pile-up height, the hardness, the force and the peak point of RDF decrease. At 900 K, the scratching groove is the narrowest. In the cases of 300 K, 500 K and 700 K, the resistance coefficient values are very close together and clearly higher than those at 900 K.

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ẢNH HƯỞNG CỦA NHIỆT ĐỘ ĐẾN CÁC PHẢN HỒI CƠ HỌC CỦA THỦY TINH KIM LOẠI $Cu_{50}Zr_{50}$ TRONG QUÁ TRÌNH TẠO LÕM VÀ CÀO XƯỚC

Tóm tắt:

Bằng phương pháp mô phỏng động lực học phân tử, các phản hồi cơ học của $Cu_{50}Zr_{50}$ thủy tinh kim loại được nghiên cứu thông qua quá trình tạo lõm và cào xước. Ảnh hưởng của các nhiệt độ khác nhau được phân tích thông qua hình thái bề mặt, chiều cao chất đống, độ cứng, lực gia công, hệ số cản và biểu đồ chức năng phân phối xuyên tâm (RDF). Các kết quả chỉ ra rằng chiều cao chất đống và độ cứng giảm khi nhiệt độ tăng lên. Chiều cao chất đống là thấp nhất và rãnh cào xước là nhỏ nhất ở nhiệt độ 900 K (nhiệt độ cao nhất). Các đường cong lực và hệ số cản rất gần nhau trong khoảng nhiệt độ từ 300 đến 700 K, trong khi chúng thấp hơn rõ rệt ở 900 K. Giá trị cao nhất của RDF giảm khi tăng nhiệt độ.

Từ khóa: *$Cu_{50}Zr_{50}$ thủy tinh kim loại, độ cứng, hệ số cản, RDF.*