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Effect of Machining Parameters on the Cutting Force and Microstructure in Nanometric Cutting of Cu$_{50}$Zr$_{50}$ Metallic Glass

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Abstract: Unlike the traditional crystalline metals, metallic glasses are lack of long-range order and have short-range order. Metallic glasses as amorphous alloys have excellent physical, chemical and mechanical properties, and have a broad application prospects in military, aerospace and sports equipment due to their unique microstructure. Cutting is an important shaping process for high efficient manufacturing of metallic glass components. Nanometric cutting simulation of Cu$_{50}$Zr$_{50}$ was carried out to investigate the effect of cutting speed and cutting depth on the cutting force by molecular dynamics simulation. The radial distribution functions and common neighbor analysis were calculated to analyze the microstructure of the chips and subsurface of the metallic glass workpiece. The results showed that there is no obvious change of microstructure during cutting process of Cu$_{50}$Zr$_{50}$ metallic glasses. The above simulation results were compared with those of nanometric cutting of single crystal copper with the same cutting parameters. It is found that, when nanometric cutting of Cu$_{50}$Zr$_{50}$ metallic glass, the average value and the fluctuation of cutting forces are larger than that of single crystal coppers. In addition, the normal cutting force was found to be substantially equal to the main cutting force during the cutting process of Cu$_{50}$Zr$_{50}$ metallic glasses. However, the normal force is smaller than the main cutting force during nanometric cutting process of the single crystal copper.

Keywords: Amorphous alloys; Nanometric cutting; Molecular dynamics simulation; Radial distribution function
1. Introduction

Metallic glasses (MGs) have aroused people’s attention because of its excellent mechanical properties such as high strength and hardness, etc\[1\]. The extensive application of new materials always needs to explore feasible processing methods. Consequently, various attempts have been made to examine processing technologies, such as welding\[2\], femtosecond laser micromachining\[3\], superplastic forming\[4\] and machining\[5\] to fabricate precision MGs components. Currently, machining has been considered as a promising method to obtain MGs components with low surface roughness and high dimensional accuracy\[1\]. In addition, cutting forces have direct impact on the stability of process parameters in the machining process. Therefore, understanding of the changing regularity of cutting force has great significance in processing of metallic glasses.

Due to the intrinsic property of short-range order in atomic clusters of MGs, it is essential to study the mechanical properties of MGs during the cutting process. However, it is difficult to observe various physical phenomena at micro scale during the cutting process of MGs through experiments due to the limitations of the detection resolution on the temporal and spatial scale. Therefore, the paper uses a numerical method, molecular dynamics (MD) simulation, which stems from statistical physics, as an effective method to observe the micro-phenomenon\[6\] in cutting process of MGs.

At present, the research on nanometric cutting of MGs is still on its nascent stage. Fang\[7\] et al. investigated nanometric cutting mechanism of amorphous alloys by varying cutting speed, cutting depth and tool edge radius. Zhao\[8\] et al. studied the potential/volume evolution of amorphous alloys in nanometric cutting process. It found that the normal cutting force is substantially equal to the tangential forces in nanometric cutting process of MGs by MD simulation, which is different with the phenomenon that main cutting force is smaller than normal force in the cutting process of crystal alloy. For this
phenomenon, traditional shear slip theory cannot provide a reasonable explanation because there are no dislocations and other microstructure defects in MGs. Therefore, the objectives of this paper are to investigate the effect of machining parameters on cutting forces in nanometric cutting process and analyze the microstructure evolution of the chips and subsurface of the metallic glass workpiece. Eventually, the above simulation results were compared with cutting process of single crystal coppers with the same cutting parameters. Details of modelling and simulation process are described in the rest of the paper.

2. Simulation method and model

2.1 Interatomic potentials

In this paper, the workpiece is selected to be CuZr-based binary amorphous alloys which have a relatively outstanding glass forming ability and low packing density\cite{9}. Finnis-Sinclair (F-S) potential\cite{10} is employed to describe atomic interactions between Zr-Zr, Zr-Cu and Cu-Cu atoms in the workpiece. F-S is a many-body potential with tight-binding form based on the second-moment approximation and its general form is given in Eq(1)

\[
E = \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij} - \sum_i \rho_i^\dagger
\tag{1}
\]

The first term is a normal pair potential term representing the repulsive interaction, while \(\rho_i\) is the second moment of density of states representing the attractive term.

\[
\rho_i = \sum_{j \neq i} \Phi_{ij}
\tag{2}
\]

\(V\) and \(\Phi\) are both empirical functions of interatomic distance. Properties for Cu-Zr potential in F-S form, have been fit by Mendelev and his co-workers\cite{11}. 

\[\text{Finnis-Sinclair (F-S) potential}\]

\[\text{Properties for Cu-Zr potential in F-S form, have been fit by Mendelev and his co-workers}\]
A diamond tool which is considered as a rigid body was used for simulation. Morse pair potential\(^{[12]}\) is adopted to describe interaction between the diamond tool and the workpiece. The Morse potential function is written as

\[
E(r_{ij}) = D\left(e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}\right)
\]

(3)

where \(E(r_{ij})\) is a pair potential energy; \(D\) is the cohesion energy; \(\alpha\) is the bulk elastic modulus; \(r_{ij}\) and \(r_0\) are instantaneous and equilibrium distance between atoms \(i\) and \(j\), respectively. The value of parameters are listed in Table 1.

<table>
<thead>
<tr>
<th></th>
<th>(D_0)</th>
<th>(\alpha)</th>
<th>(r_0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu-C</td>
<td>0.087</td>
<td>5.14</td>
<td>2.05</td>
</tr>
<tr>
<td>Zr-C</td>
<td>1.56</td>
<td>3.3786</td>
<td>2.1187</td>
</tr>
<tr>
<td>C-C</td>
<td>3.10</td>
<td>4.9519</td>
<td>1.2419</td>
</tr>
</tbody>
</table>

### 2.2 Preparation for the workpiece

The \(\text{Cu}_{50}\text{Zr}_{50}\) MG was selected as workpiece material which was composed of 28,800 atoms. The workpiece was prepared by the melt-quench technology. Primarily, the workpiece of crystal was heated to 2,400K to ensure sufficient melting. Then, quenching the workpiece with cooling rate of \(1\times10^{12}\) K/s obtains the \(\text{Cu}_{50}\text{Zr}_{50}\) MGs. During this process, NPT (constant pressure and constant temperature) ensemble and periodic boundary condition (PBC) in all dimensions were applied in simulation. In order to ensure a successful preparation for MGs, i.e. full amorphous transformation, the radial distribution functions\(^{[14]}\) (RDF) of melting and quenching process was plot as shown in Fig. 1 and Fig. 2 respectively. Fig. 1 exhibits typical broad characteristics of liquid which demonstrates crystal workpiece has melted adequately. The second-peak splitting feature of RDF in Fig. 2 indicates that the correctness of preparation for \(\text{Cu}_{50}\text{Zr}_{50}\) MGs. Finally, the glass transition temperature \((T_g)\) was determined through the linear fitting\(^{[15]}\). Fig. 3 exhibits the curve of MGs volume variation with temperature during cooling process. The temperature on the turning point of the curve was determined to be approximately 770K.
which was regarded as $T_g$ of prepared MGs. Actually, the value of $T_g$ is slightly higher than the experimental value. Considering the influence of cooling rate, this result of simulation is considered to be reasonable. From what mentioned above, it is further proved that the setting of parameters is reasonable.

Fig. 1. The RDF of the molten alloy

Fig. 2. The RDF of the amorphous alloy
Fig. 3. The average atomic volume changes during cooling

2.3 Nanometric cutting model

Fig. 4 shows the nanometric cutting model used for MD simulation with the diamond tool. As shown in Fig. 4(a), the workpiece is divided into three parts: Newtonian layer atoms, thermostat layer atoms and boundary layer atoms. The boundary atoms with a thickness of 1 nm at the left and the bottom of the workpiece are kept fixed in space during the cutting process. The thermostat layer with a thickness of 1 nm adjacent to the boundary atoms is kept at a constant temperature of 300 K by velocity scaling method to imitate the heat dissipation in real cutting condition. The rest of atoms belong to Newtonian atoms whose motions obey the classical Newton's second law\(^{116}\). Periodic boundary conditions are imposed in the z direction, x and y directions are non-periodic boundary conditions.
Fig. 4. MD simulation model of nanometric cutting of Cu<sub>50</sub>Zr<sub>50</sub> MGs (Zr and Cu atoms are indicated in blue and pink respectively)

Table 2 shows the required parameters during all the cutting simulation process. The cutting process is simulated by moving a diamond tool at a constant velocity (cutting speed) along the negative x-direction with a fixed cutting depth. The velocity Verlet algorithm with a time step of 1 fs is used for the time integration of Newton’s equation of motion. The simulation processes are performed in microcanonical ensemble (NVE).

<table>
<thead>
<tr>
<th>Properties</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Workpiece material</td>
<td>Cu&lt;sub&gt;50&lt;/sub&gt;Zr&lt;sub&gt;50&lt;/sub&gt; MGs</td>
</tr>
<tr>
<td>Dimensions</td>
<td>19.6nm×9.8nm×2.6nm</td>
</tr>
<tr>
<td>Tool material</td>
<td>Diamond(C)</td>
</tr>
<tr>
<td>Tool dimension</td>
<td>3.0nm×3.5nm×2.6nm</td>
</tr>
<tr>
<td>Rake angle</td>
<td>0º</td>
</tr>
<tr>
<td>Clearance angle</td>
<td>0º</td>
</tr>
<tr>
<td>Tool edge radius</td>
<td>1nm</td>
</tr>
<tr>
<td>Ensemble</td>
<td>NVE</td>
</tr>
<tr>
<td>Timestep</td>
<td>1 fs</td>
</tr>
<tr>
<td>Initial temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>Cutting speed</td>
<td>100,200 and 400 m/s</td>
</tr>
<tr>
<td>Cutting depth</td>
<td>1, 2 and 3 nm</td>
</tr>
</tbody>
</table>
3. Simulation results and discussion

3.1 Investigation of cutting process with fixed parameters

3.1.1 Variations of cutting force

Firstly, the cutting forces ($F_r$) in MD simulation are obtained by summing the atomic forces of workpiece atoms on the tool atoms. In this study, the main cutting force ($F_x$) in feeding negative x-direction and the normal forces ($F_y$) to the machining surface in y-direction are respectively calculated. Fig. 5 shows the graph of $F_r$ during simulation process with the fixed parameters, where cutting speed and depth are 200 m/s and 2 nm, respectively. As it can be seen that at 200 m/s cutting speed the cutting force ($F_r$) exhibits large variation in the first 30 ps. In particular, cutting force ($F_r$) decreases suddenly when it reaches the maximum value. Due to the high strength, workpiece material will yield and then cutting force decreases after reaching the yield limit. Finally, the machining process steps into a stable cutting stage. It can be found that cutting force keeps in a range of stable value, which indicates that there is not obvious strain hardening in MGs nanometric cutting process because there is no grain dislocations and other defects in MGs. In addition, Fig. 6 provides the graph of main cutting force ($F_x$) and normal forces ($F_y$). As shown in Fig. 6, the normal cutting force is substantially equal to the main cutting force ($F_x$), which is clearly different from cutting process of single crystal metals. Further research will be carried out in this aspect.

3.1.2 Microstructure analysis in the process of cutting

In order to investigate the machining quality of the MGs, the microstructure of the chips and machined subsurface of the MGs were analyzed by using of RDF and common neighbor analysis\(^ {17}\) (CNA) which is used to analyze the lattice structure of atoms. Fig. 7 and Fig. 8 show the RDF of chip and subsurface of the MGs during cutting process. It is found that the phenomenon of the second-peak splitting still exists, which reveals that crystallization did not happen in cutting process of MGs. However, the phenomenon of
the second-peak splitting is not clearly obvious in Fig. 7. This can be attributed to temperature rise with increase of cutting speed and hence leading to melting of chips. In order to further investigate whether there are changes of microstructure, CNA was conducted and the results were given in Fig. 9.

![Graph of Cutting Force](image1)

**Fig. 5** The graph of cutting force in nanometric cutting of MGs (Vc = 200 m/s)

![Graph of Fx and Fy](image2)

**Fig. 6** The graph of Fx and Fy in nanometric cutting of MGs (Vc = 200 m/s)

The analysis of microstructure mainly includes the structures of BCC (body-centered cubic), FCC (face-centered cubic), HCP (hexagonal close-packed), ICO (icosahedral), DIA (diamond) and amorphous. As shown in Fig. 9, before cutting, the proportion of the structures of BCC, FCC, HCP and ICO is only 0.2%, 9.5% of the atoms are in DIA structure and the rest are amorphous structure. After cutting, by comparing with the
atoms structure before cutting the workpiece, It can be clearly found that there are no obvious changes of lattice structure during cutting process of Cu_{50}Zr_{50} MGs.

Fig. 7 The RDF of the chip

Fig. 8 The RDF of subsurface of workpiece

Fig. 9 changes of microstructure by CNA before and after cutting process

3.2 The effect of different cutting parameters
In the conventional machining, cutting parameters have an great effect on cutting force, especially the cutting speed and depth. Therefore, we studied the variation of cutting force by increasing or decreasing cutting parameters.

3.2.1 Cutting speed effect

In order to investigate the effect of cutting speed on cutting force, three MD simulation trials have been made with different cutting speed. Due to the limitation of MD, cutting speed is set to 100, 200 and 400 m/s and cutting depth is 2 nm. The graph of the average cutting force was shown in Fig. 10. We can see that the main cutting force ($F_x$) increase gradually with increase of cutting speed, which is same as conventional machining. What’s more, the value of normal cutting force ($F_y$) is still close to the value of main cutting force ($F_x$) at different cutting speed and also increase with increase of cutting speed. In order to ensure the quality of machined surface, Table. 3 shows the expected value E and variance D of the normal cutting force ($F_y$) with different cutting speed in stable cutting process. E is the average of normal force when the cutting process steps into stable stage. D represents the status of fluctuations, which is the average of quadratic sum that instantaneous values minus E in stable cutting process. The fluctuation of normal cutting force ($F_y$) become intensive with increasing of cutting speed. It’s known that the fluctuation of the normal cutting forces is closely-related to the quality of the machined surface. In order to get an ideal machined surface, the cutting speed should be controlled as slowly as possible.
Table 3 E and D at different cutting speed

<table>
<thead>
<tr>
<th>V(m/s)</th>
<th>E(nN)</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>33.54</td>
<td>63.54</td>
</tr>
<tr>
<td>200</td>
<td>40.20</td>
<td>75.41</td>
</tr>
<tr>
<td>400</td>
<td>53.76</td>
<td>144.32</td>
</tr>
</tbody>
</table>

3.2.2 Cutting depth effect

The effect of cutting depth on cutting force was investigated with a fixed cutting speed 200 m/s. Fig. 12 shows the variation of tangential and normal cutting forces with different cutting depths of 1, 2 and 3 nm. The changes of the cutting force have shown that cutting force increase with the increasing of the cutting depth and the normal cutting force is roughly equal to the main cutting force. In order to study the fluctuations of normal force, the E and D of normal force versus different cutting depth are depicted in Table 4. As we can see, the value of variance is minimum when cutting depth is 3 nm. The edge radius of tool is 1 nm during MD simulation process. In the nanometric cutting, the phenomena of extrusion and ploughing from tool to workpiece are obvious when edge radius of tool and cutting depth are in the same order of magnitude, so the cutting force fluctuated wildly when cutting depth is equal to 1 nm. Therefore, we can draw a conclusion that cutting depth should be larger than edge radius of tool during nanometric cutting.
cutting process to ensure the machining quality. In addition, as shown in Table 3 and Table 4, due to the high hardness of MGs, the value of variance is still large regardless of the variation of cutting speed and depth, which also indicates that MGs is an intractable material.

**Fig. 11 average cutting force at different cutting depth**

<table>
<thead>
<tr>
<th>Dp (nm)</th>
<th>E (nN)</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>33.26</td>
<td>153.16</td>
</tr>
<tr>
<td>2</td>
<td>42.75</td>
<td>87.21</td>
</tr>
<tr>
<td>3</td>
<td>55.36</td>
<td>82.23</td>
</tr>
</tbody>
</table>

3.3 Comparison with nanometric cutting of crystalline copper

In order to compare with single crystal metals, nanometric cutting of single crystal copper (Cu) with face-centered cubic (FCC) structure was simulated. The modeling process of single crystal Cu is same as the MGs. Fig. 12 shows the comparison of cutting force variations for cutting amorphous Cu_{50}Z_{50} and single crystal copper with fixed cutting speed (200 m/s) and depth (2 nm). By comparing the curve of cutting force, it has been found that the cutting force of single crystal Cu gradually increases during cutting process because of the influence of strain hardening, which indicates that the results of simulations are reasonable. Besides that, the cutting force of MGs is larger and the force fluctuations of cutting MGs are more obvious than cutting single crystal Cu. Considering the mechanical properties of MGs, it is believed that high strength and hardness can
explain these phenomena. High strength leads to materials yield under greater force, and high hardness would cause fluctuation of cutting force. In addition, under the action of external loading, ultra-thin localization shear band would form when the MGs are underwent plastic deformation. As stated in reference [18], the forming regularity of periodic shear band and the symmetry breaking of free volume flow are the primary cause[18]. Hence, the drastic fluctuation of cutting force can be thought of as the repeated formation of periodic shear band.

Fig. 12 Variations of cutting force for machining MGs and single crystal Cu

Fig. 13 shows the variations of main cutting force (F_x) and normal forces (F_y) during cutting of single crystal Cu process. Compared with Fig. 6, it can be seen that the main cutting force (F_x) is much larger than normal forces (F_y) of cutting crystal Cu, which is very different with amorphous cutting process. As shown in Fig. 14, due to the small elastic modulus of MGs, larger elastic deformation is generated under the same external loading. The atoms of machined surface contact closely with the flank face of the tool and the elastic recovery of machined surface are quite obvious as evidenced in Fig. 14. However, elastic recovery of machined surface in Fig. 15 during the cutting process of single crystal Cu is not evident. Due to small elastic modulus of MGs, the elastic deformation of machined surface results in increased normal forces (F_y) during cutting process of MGs.
Fig. 13 Variations of Fx and Fy for cutting single crystal Cu

Fig. 14 The nanometric cutting process of MGs

Fig. 15 The nanometric cutting process of single crystal Cu
4. Conclusions

In this study, the molecular dynamics simulation method has been applied to nanometric cutting of CuZr-based amorphous alloy. The RDF of the amorphous workpiece and effect of machining parameters on cutting force are investigated. In order to explore the differences with crystalline metals, comparative study with single crystal Cu was carried out. The following conclusions can be drawn:

1) The normal cutting force is substantially equal to the main cutting force during nanometric cutting of MGs because small elastic modulus causes larger elastic deformation.

2) The characteristics of amorphous state in MGs cause shear band forming in ultra-thin localization area. The repeated formation of periodic shear band causes the dramatic fluctuations of the cutting forces. Fluctuations of cutting forces of MGs are much greater than those in cutting of single crystal Cu. The normal cutting forces are strongly affected by the cutting parameters. To get an better machined surface of MG, the cutting speed should be controlled as slowly as possible and cutting depth should be greater than the cutting edge radius of the tool.

3) Nanometric cutting at room temperature does not change the microstructures of amorphous Cu50Zr50.

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