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The effect of stress on shear dilatation and cutting force during nanometric machining of amorphous alloys

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Abstract
Amorphous alloys have excellent physical and mechanical properties compared with traditional crystalline metals due to their unique microstructure. Previous research on nanometric cutting of amorphous alloys has observed several unusual phenomena, including high ratio of normal cutting forces to main cutting forces and distinct volume expansion of atomic clusters during shear deformation. With the aim to reveal the micro cutting mechanism of amorphous alloys, this paper investigates the effect of stress on shear dilatation and cutting force in nanometric cutting of $Cu_{50}Zr_{50}$ amorphous alloys by molecular dynamics simulation. In order to verify the calculated atomic true stress, stress-strain curves were obtained by the resolution of virial stress in the shear simulation of amorphous $Cu_{50}Zr_{50}$. The volume change before and after cutting process shows that due to the shear deformation the volume expansion phenomenon is much noticeable when nanometric cutting of $Cu_{50}Zr_{50}$ amorphous alloy. In addition, shear dilatation during shear deformation results in an increase of normal stress on the machined plane. The stress simulation results show that stresses on the rake face and flank face are approximately equal. The shear deformation simulation of micro units of the workpiece surface indicates that the normal stress on the shear plane increases significantly with the increase of shear stress, therefore normal force on the shear plane increase significantly. The paper concludes that the increase of normal stress causes the shear dilatation, and then results in the phenomenon that the normal cutting force is equal to the main cutting force in nanometric cutting of $Cu_{50}Zr_{50}$ amorphous alloys.

Keywords: amorphous alloy, molecular dynamics, shear dilatation, virial stress

1. Introduction

Amorphous alloys have excellent physical and mechanical properties [1] and have wide application prospects in aerospace, military and sports equipment due to unique atomic cluster structure. Previous experimental research on cutting of amorphous alloys has observed an unusual phenomenon that normal cutting forces are substantially equal to main cutting forces [2]. However, main cutting forces are usually much bigger than normal forcesin cutting of crystal materials. Zhao et al. investigated the effect of cutting parameters on cutting force by molecular dynamics simulation, which also found the main cutting force is approximately equal to the normal force [3]. The increase of normal cutting force will affect the machined surface quality and increase tool wear. This research aims to investigate the machining mechanism to explain this phenomenon and guide the processing of amorphous alloy effectively. In this paper, the volume expansion phenomenon was found in the clusters under the machined surface obviously. Shear simulation of micro units was conducted to testify that shear deformation induces the normal stress. The normal stress on machined surface and shear plane was investigated to explain the above mechanical properties.

2. Method

Molecular dynamics (MD) simulation was performed in nanometric cutting of $Cu_{50}Zr_{50}$ amorphous alloys. The structures of $Cu_{50}Zr_{50}$ were prepared by melt quench method. The parameters of Morse and F-S potential in Ref. [4] were adopted in this simulation. Firstly, we arranged Cu and Zr atoms proportionally in a super cell where periodic boundary condition was applied in all three dimensions. Then, it was heated up to 2400K to confirm melting sufficiently. After relaxing 0.1ns at 2400K, it was cooled down to 300K with cooling rate 10^{12}K/s. The amorphous state was verified by computing radial distribution functions and the glass transition temperature (T_g) was estimated as 800K.

During the simulation system, the virial stress of atoms is defined as Eq(1)[5]

$$\Pi^{\alpha\beta} = \frac{1}{\Omega}\left(-\sum_i m_i v_i^\alpha v_i^\beta + \frac{1}{2}\sum_i\sum_{j\neq i} F_{ij}^\alpha r_{ij}^\beta\right) \quad (1)$$

Where Ω is system volume; m_i and v_i are the mass and velocity of atom i respectively; F_{ij}^α is the interaction force between atom i and atom j; α and β are indexes of Cartesian coordinate components; r_{ij}^β is a component of vector $\vec{r}_{ij} = (\vec{r}_i - \vec{r}_j)$ along the β coordinate direction.

The true stress of atom i is obtained by resolution of virial stress, shown in Eq(2) and Eq(3).

$$\Pi^{\alpha\beta} = \frac{1}{\Omega}\sum_i \omega_i \sigma_i^{\alpha\beta} \quad (2)$$

$$\sigma_i^{\alpha\beta} = \frac{1}{\omega_i}\left(-m_i v_i^\alpha v_i^\beta + \frac{1}{2}\sum_{j\neq i} F_{ij}^\alpha r_{ij}^\beta\right) \quad (3)$$

$\sigma_i^{\alpha\beta}$ and ω_i are the true stress and effective volume of atom i; $\sum\omega_i = \Omega$.

3. Results and discussion

3.1. Stress calculation in cutting process

The shear simulation of $Cu_{50}Zr_{50}$ amorphous alloy was carried out to verify the calculated true stress with increment of strain rate of 0.05% at 0 K. The yield strength 1.4 GPa in our shear simulation is equal to that in ref. [6]

Fig. 1 shows the MD cutting model. In order to better explore the reason that normal cutting force is basically equal to main cutting force during nanometric cutting of $Cu_{50}Zr_{50}$. two regions were selected to calculate true stress during cutting process where one is in the chip layer(A) and the other is under machined surface area(B). During the cutting process, the normal stress of chip layer (A) along X direction (σ_{xx}) and surface area (B) along Y (σ_{yy}) direction was calculated.

Figs. 2 shows the normal stress calculation results of region A and B. From the normal stress curves, the difference of maximum value between σ_{xx}(from A) and σ_{yy} (from B) is about 0.4GPa. For the sake of comparison, we simulated the normal stresses of region A and B in nanometric cutting of single crystal Cu. It was found that the difference of maximum value between σ_{xx} and σ_{yy} of Cu is about 1 GPa. Therefore, the above special cutting force phenomenon may be due to the similar stress value of region A and B in the orthogonal cutting model shown in Fig.1.

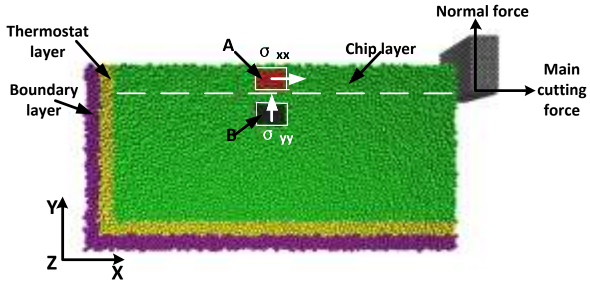

Figure 1 The MD simulation model in nanometric cutting of $Cu_{50}Zr_{50}$

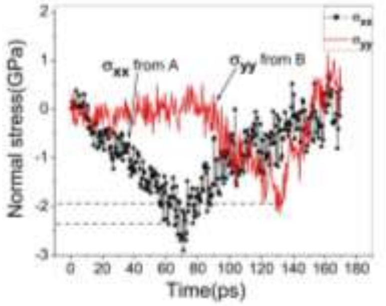

Figure 2. Normal stress calculation of region (A) and (B)

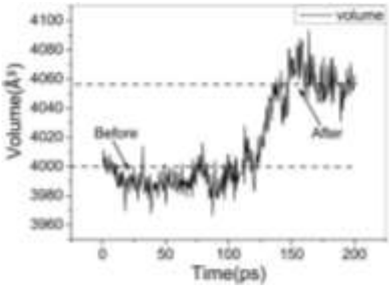

Figure 3. Volume change curves of machined surface region (B)

Moreover, Figure 3 shows the volume change curves of machined surface region (B) in cutting process. It is found that the volume expansion phenomenon is obvious and volume growth rate is 1.5% approximately before and after nanometeic cutting of $Cu_{50}Zr_{50}$ amorphous alloys.

3.2. Shear dilatation during shear deformation

Clusters close-packed structures possess distinct shear dilatation phenomenon (volume expansion during shear deformation) based on solid mechanics theory. In section3.1, we have verified $Cu_{50}Zr_{50}$ amorphous alloy has distinct volume expansion phenomenon during cutting process. Therefore, the shear deformation simulation of micro units (a small rectangular cell of 30 000 atoms) is applied to explore the reason of volume expansion.

Fig 4.shows the stress-strain curves of micro units under shear deformation. The shear modulus and strength are estimated to be 13 and 0.75 GPa respectively. Moreover, the shear deformation induces the normal stress σ_{yy}, which is perpendicular to the shearing place x-z, and normal stress σ_{xx} and σ_{zz}. With the proceeding of shear deformation, shear stress τ_{xy} and normal stress increase constantly. Up to ~12% shear strain, the normal stress is trend to stabilize. Therefore, the extrusion and overturn among clusters induce normal stress. And then, the normal stress leads to volume expansion of micro units during shear deformation and the increase of σ_{yy} perpendicularly the shearing place causes the increase of normal force during nanometric cutting process.

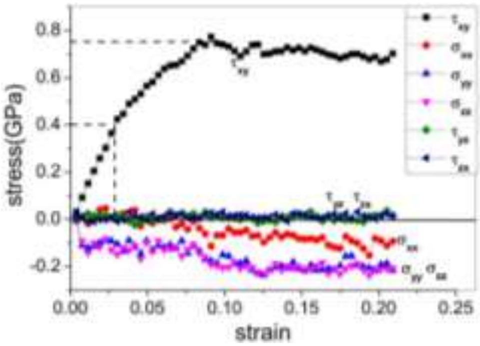

Figure 4. Stress-strain curves of micro units under shear deformation

4. Summary

The effect of stress on shear dilatation and cutting force in nanometric machining of $Cu_{50}Zr_{50}$ amorphous alloy was investigated by molecular dynamics simulation.

The extrusion and overturn among clusters induce normal stress during the shear deformation of amorphous alloy, which leads to shear dilatation. Meanwhile, the increase of normal stress on tool flank surface caused by shear deformation of machined surface micro units leads to the phenomenon that the normal force is nearly equal to the main cutting force during nanometric machining process. The effect of stress on free volume will be investigated in the future work.

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