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Crystallization of amorphous materials and deformation mechanism of nanocrystalline materials under cutting loads: a molecular dynamics simulation approach

Yan Zhao¹, Xunli Wei¹, Yan Zhang¹, Jiachun Wang¹, Dehong Huo^{2*}

¹*School of Mechanical Engineering, Yanshan University, 066004, China*

²*School of Mechanical and Systems Engineering, Newcastle University, Newcastle Upon Tyne, NE7 7QH, UK*

*Corresponding author: Dehong Huo, Tel: +0044 191 208 6230; email: dehong.huo@ncl.ac.uk

Abstract: The crystallization of amorphous and cutting process of nanocrystalline copper was investigated by the use of a molecular dynamics (MD) simulation. Stress-induced crystallization of amorphous in cutting process was observed. By the common neighbor analysis (CNA), it was found that nuclei were first formed in the larger stress region around the rake face and tip of the tool and then they grew quickly under stress. The growth and consolidation process of grains was analyzed, using relative atomic displacement vector method. When grains grew in contact with each other, a merger occurred. Grains were combined firstly in a local area, and rotated to discharge the excess free volume out of boundaries before the merging process completed. Through calculating the shear strain of atoms in the cutting process, the serrated chips and four shear bands were observed clearly. The radius distribution function (RDF) curve of the shear band shows that the cutting of crystalline was carried out in the amorphous state. The shear angle of less than 45° was observed in the simulation, which is consistent with the experiments reported and validates the simulation results in this paper.

Keywords: Amorphous alloys; Crystallization; Nanometric cutting; Molecular dynamics simulation

1 Introduction

Nanocrystalline materials generally refer to polycrystalline materials which have the grain size less than 100 nm. Due to their fine grain size, the volume fraction of its grain boundary becomes greater. This unique structural feature exhibits a series of excellent physical, chemical and mechanical properties, and has a high future prospects^[1].

There are mainly two methods for nanocrystals preparation. One method is to prepare nanocrystalline powders firstly, using inert gas condensation, RF sputtering, or mechanical milling, then, these powders are made to the block nanocrystals using sintering processes. The other method is the crystallization of amorphous alloys^[2]. Amorphous alloys are unstable thermodynamically and have the crystalline transition induced by heat or stress. By proper control of the crystallization condition, the bulk nanocrystalline materials can be obtained. Thermal annealing has been the typical method to obtain nanocrystals from an amorphous material^[3]. However, nanocrystals were also observed from amorphous alloys in some stress loading experiments. Chen *et al.* conducted bending experiments on Al-based amorphous alloys and found pure aluminium nanocrystals essentially by using transmission electron microscopy (TEM)^[4]. Kim *et al.* performed quasi-static nano-indentation experiments and proved the existence of nano-crystallites near the shear bands^[5]. Xu and Atzmon observed that nano-crystallites were formed by low-energy ball milling experiments^[6]. Guo *et al.* used Al₉₀Fe₅Gd₅ amorphous alloys to make uniaxial tensile tests and observed the Al-nanocrystals formation^[7]. In addition, Bakkel *et al.* observed nanocrystallization phenomenon in their cutting experiments^[8].

Atomic-level simulation^[9-10] on the process of crystallization of amorphous under stress

have been carried out. Molecular dynamics simulation of the deformation behavior of amorphous nickel under stress were researched by Lee^[9-10]. Under hydrostatic compressive pressure, it was found that the amorphous material crystallizes, and rotation and coalescence is the main mechanism of grain growth after completion of crystallization. Wang et al.^[11-12] carried out the study for the crystallization of amorphous copper under compressive deformation. From the perspective of microstructure, the nucleation and growth process of nanocrystals were analyzed. The result showed that the strain changed the amorphous metal structure from metastable state to a steady state, and some short-range order radicals first merged to smaller nuclei. The region of grain growth and consolidation occurred in the position of maximum shear strain, which is consistent with the Hertz contact theory. The physical images of grain growth process have been observed in these simulations. However, due to the simple simulation condition, many deformation mechanisms have not been revealed clearly. Cutting, as an efficient high-precision material processing method, is a commonly used for material shaping. Cutting involves elastic and plastic deformation together with fracture process at high temperature with very high strain and strain rate. Therefore, it has a different deformation mechanism from general material tests. If the machined surface achieves **nano-crystalline** formation in cutting process, it will be a new method of nanocrystals preparation. To our knowledge, there is very little research on crystallization and deformation mechanism of amorphous alloys under cutting loads and this will be the topic of this paper.

The main objectives of the present study include two aspects. One is the crystallization process of amorphous under the cutting stress loading conditions, such as the mechanism of

grain growth and consolidation. The other is the deformation mechanism of nanocrystalline materials under cutting loads after the full crystallization of amorphous, i.e. how the grains are to accomplish the deformation at high strain rate. In this paper, molecular dynamics simulation is used to simulate the cutting process of amorphous copper and details of the method and results are presented.

2 Method

2.1 Interatomic potentials

This study was carried out using an open-source parallel molecular dynamics simulation code, known as “large-scale atomic/molecular massively parallel simulator” (LAMMPS). Amorphous copper was chosen as the workpiece material and single crystal diamond tools were used in the computational experiments.

The EAM potential developed by Minish *et al.*^[13] was adopted to describe interactions between/amongst copper atoms. The total atomic potential energy of a system is expressed as

$$E_{tot} = \frac{1}{2} \sum_{ij} \Phi_{ij}(r_{ij}) + \sum_i F_i(\bar{\rho}_i) \quad (1)$$

Where Φ_{ij} is the energy of pair-interaction between atom i and j , and F_i represents the embedding energy of atom i . $\bar{\rho}_i$ is density of the host electron at site i which is induced by all other atoms in the system:

$$\bar{\rho}_i = \sum_{j \neq i} \rho_j(r_{ij}) \quad (2)$$

The Morse^[14] potential was adopted to describe the interaction of Cu-C atoms pairs. The Morse potential is written as

$$\phi(r_{ij}) = D \{ \exp[-2\alpha(r_{ij} - r_0)] - 2 \exp[-\alpha(r_{ij} - r_0)] \} \quad (3)$$

Where $\phi(r_{ij})$ is a pair potential energy function; D is the cohesion energy; α is the elastic modulus; r_0 and r_{ij} are the equilibrium and instantaneous distance between atoms i and j , respectively. And detailed Morse potential parameters were listed in Table 1^[15].

Table 1 Morse potential parameters for Cu-C atom pairs^[15]

Atom pairs	D (eV)	α ($\text{\AA}^{-1}$)	r_0 ($\text{\AA}$)
Cu-C	0.087	5.14	2.05

2.2 Preparation for the workpiece

Molecular dynamics (MD) simulations were carried out using the NPT ensemble that means constant temperature, constant number of atoms and constant pressure. The melt-quench procedure was applied to get glassy structures. At first, 96,000 copper atoms were set with initial zero velocity into a face-centered cubic (FCC) crystal lattice in a cell. The periodic boundary condition (PBC) was used in all three dimensions, and then all atoms were equilibrated at 2400 K for 1600 ps. It was then cooled down to 300 K after fully melting at rapid cooling rate of 2×10^{14} K/s. For achieving the thermodynamic equilibrium of the workpiece, the workpiece was kept relaxed with a thermostat of 300 K for 50 ps. Eventually glassy structures were obtained with the dimensions of $43.8 \times 18.1 \times 1.46 \text{ nm}^3$.

To verify the effectiveness of the simulation in generating glassy structures, the radial distribution function (RDF) was used to examine the molten copper and the amorphous copper respectively. The radial distribution function is a method to reveal the internal microstructure of materials, by calculating the probability of particles appearing around a particle in the space. Fig. 1(a) shows the RDF of the molten copper, which exhibits the typical broad characteristics of liquid. Fig. 1(b) shows the RDF of amorphous copper prepared in the simulation. The second-peak splitting feature as indicated in the diagram is

believed to be the main character of amorphous solids. The results of RDFs confirmed the potential functions and parameter settings in the simulation were effective.

Fig. 1. The radial distribution functions, (a) the molten copper; (b) and the amorphous copper

2.3 Nanometer cutting model

Fig. 2 shows the atomistic model of nanometric machining, which was established on the basis of the conventional orthogonal machining. The model is made up of an amorphous copper workpiece and a rigid single crystal diamond tool.

The workpiece contains three different zones of atoms. The left and bottom of the workpiece were set to fixed boundary layer in order to prevent the workpiece from moving during machining. There is a thermostat layer between boundary layer and Newtonian layer whose behavior obeys the equations of motion due to their Hamiltonian. In order to keep thermostat layer at a temperature of 300 K, the velocities of the atoms are rescaled periodically. The thermostat layer imitates a heat sink which completes heat conduction across the workpiece. The Newtonian layer atoms satisfy a Gaussian distribution of atomic velocities at a temperature of 300 K. The top and right layers of the workpiece are assigned to

free boundary condition where the particles can move in the x and y direction freely. Finally, periodic boundary conditions are applied to the faces perpendicular to the z axis, which represents a plane stress orthogonal machining process.

Fig. 2. The atomistic model of orthogonal nanometric cutting of amorphous copper with a diamond tool

The geometry parameters of single crystal diamond tool are as follows: a cutting edge radius of $5 \text{ \AA}$ is used, the tool rake angle $\alpha = 15^\circ$ and the tool clearance angle $\beta = 8^\circ$. 1 fs was used as a time step of the velocity Verlet algorithm for the time integration of Newton's equations of motion. The nanometric cutting was simulated by advancing the tool atoms at every time step giving the tool a velocity of 200 m/s. In the simulation, the uncut chip thickness (cutting depth) and the cutting distance are 4 nm and 36 nm respectively.

3 Results and discussion

3.1 Crystallization of amorphous under cutting load

3.1.1 Atomic structure analysis

The Common Neighbor Analysis (CNA)^[16], a crystal structure analysis technology, was used to calculate the local lattice structure of atoms. The results are mapped according to the

following lattice structures:

- BCC (body-centered cubic)
- DIA (diamond)
- FCC (face - centered cubic)
- HCP (hexagonal close-packed)
- ICO (icosahedral)
- OTHER (the crystal structure is not identified)

The evolution of lattice structure of atoms during the cutting process is presented in Fig. 3, where the colored points represent the lattice structures as defined by the CNA. In addition to the long-range disorder atomic structure of amorphous as shown in Fig. 3(a), a small amount of crystal structures formed during cooling process are also observed. At the initial stage of cutting, the nucleation and growth of grains focusing on the region around the rake face of tool is clearly visible, and the original nucleus formed in the preparation stage grew rapidly induced by stress as shown in Fig.3 (b-e). With cutting progressing, the grains further grew until the full crystallization of amorphous occurred. In the end, the cutting of amorphous becomes the cutting of nanocrystalline copper as shown in Fig. 3 (f). This cutting is essentially a crystallization process **that is stress-driven**. According to the shear merger or shear deposition nucleation theory proposed by Lu^[17-18], when the shear strain accumulated to a certain extent, the atomic area near the short-range volume will give priority to the formation of ordered structure. This is similar to the pre-nuclei found by Sutton^[19] in the process of crystallization of alloy, which is a necessary condition for the occurrence of crystallization. Due to the large stress and shear deformation in the region around the tool

rake face and tool tip, grains nucleation occurs first in these areas. Since there is no need for long-range diffusion like multi-component alloys, these monopropellant nuclei are easy formed and grow rapidly under this condition. The entire crystallization process of amorphous completed within a short period of time, which is consistent to the result simulated by Lee^[10]. It can be seen from Fig. 4 that different lattice structures were produced during the nanometric cutting of amorphous copper. When the cutting process was in steady state, 40% of the copper atoms were in FCC structure, 13% of the atoms are in HCP structure and the rest are amorphous. BCC, ICO and DIA lattice structures are negligible in this state.

Fig. 3. Evolution of lattice structure of atoms during the cutting process

Fig. 4. Percentage of different lattice structures during the cutting process

3.1.2 Grain growth and consolidation

From the simulation results of the nanometric cutting process, the nucleation, growth and combination process of grains can be clearly observed. In order to better observe the evolution of grains, the FCC structure of the nanocrystalline copper is selected and shown in the visualization software. Fig. 5 shows the distribution of FCC structure in the workpiece after the material preparation, and very few nuclei exist in the workpiece before cutting. It may be the reason for high nucleation rate of metallic glass with only one element.

Fig. 5. The distribution of FCC atomic structure in the workpiece

Fig. 6. The growth and mergence of grains

A rectangular region in Fig. 5 was chosen to study the nucleation evolution. There are two mini nuclei in this field. Fig. 6 (a) to (f) show the growth and consolidation process of the two nuclei. Amorphous metal is a metastable structure and has the tendency to crystalline transition under shear stress. In the cutting process, the growth and merger of grains are mainly caused by the shear stress. Driven by the shear stress, atom clusters moved to the two nuclei and then the atom transition occurred. Therefore, the two mini nuclei in Fig. 6 (a) gradually grow into large grains shown in Fig. 6 (b). The grown grains continued to move to

each other and stopped expanding when they touched. Since then, the rotation becomes the main mechanism of grain consolidation. Fig. 6 (c-f) show the process of grain rotation and consolidation. The atomic displacement vector method was used to trace the atomic movement under shear stress, which can label the atomic trajectories and orientation. The arrows shown in Fig. 7 display the rotation direction of the right grain. The simulation results of grain growth, rotation and coalescence are consistent with the conclusions of reference [20].

Fig. 7. The atomic displacement vector of grains

The enhancement of crystallization under high pressure is explained in terms of the volume difference between amorphous and crystallization phases contributing to lowering the thermodynamic nucleation energy barrier of crystalline nuclei^[21]. The combination of grains is a process of consuming excess free volume among the grain boundaries, i.e. the annihilation of free volume.

The process of grains growth and coalescence can also be illustrated by the RDF curves in Fig. 8. The curves shown in Fig. 8 correspond to different cutting time. Fig.8 (a) and (b)

represent the beginning of cutting. There is the second-peak splitting at the point where $r = 0.47\text{nm}$, which indicates the workpiece was in amorphous state at the initial stage of cutting. New peaks come out around the points where $r = 0.27\text{ nm}$ and $r = 0.55\text{nm}$ in Fig. 8 (c) and (d). And then, more and more peaks appear in the RDF curves shown in Fig. 8 (e) and (f) and the peak value are higher and higher. The RDF results show that under the shear stress the workpiece has gradually transformed from the amorphous to the crystalline state.

Fig. 8. The radial distribution functions of the workpiece with the tool advancing

3.1.3 Potential and volume changes of atoms

The average potential and volume of the system are the important parameters for the characterization of amorphous structure, so they were calculated in this study to characterize the crystallization process. The average potential energy was calculated according to the methods in Section 2.1 and the volume in this paper refers to the Voronoi volume which was proposed by Brostow^[22] in 1978. Two regions were chosen to represent chips and the materials below the machined surface respectively. As shown in Fig 9, Region 1 represents the region where the atoms will become chips after cutting, whilst the Region 2 represents the region where the atoms will remain in the machined workpiece after cutting. Both potentials and volume changes of the two chosen regions were studied.

As it can be seen from Fig. 10 and 11, the change of potential energy and volume during cutting is substantially similar. In Fig. 10, the potential energy value starts to increase slowly when these regions are subject to cutting stress. With the progressing of the cutting process, the potential energy increases constantly. When the potential energy accumulates to a certain level, the potential energy values start to decrease, indicating the crystallization of amorphous. In other words, the process of crystallization needs to consume some energy to take place. After the completion of crystallization, potential energy still increases under stress.

Fig. 9. The selected regions for calculated the potential and volume of atomics

Fig. 10. The potential curves of atoms in these two regions

Fig. 11. The volume curves of atoms in these two regions

A slight difference between the change of potential and volume is also noticed at the beginning of the effect of stress. As shown in Fig. 11, the volume begins to decrease under compressive stress, and then the value begins to become larger due to the effect of dilatancy.

3.2 Deformation mechanism of cutting of nanocrystalline materials

The shear strain of atoms in the cutting process is calculated according to Shimizu^[23], and the maps based on its deformation value are shown in Fig 12. Fig. 12 (a) shows the initial

strain diagram without cutting. At the beginning of cutting, the workpiece materials deformed under the compression of the cutting tool and the strain occurs mainly around the tip of tool as shown in Fig. 12 (b). With the tool advancing, the deformation becomes larger, and gradually extended from the tool tip to the free surface of the chip (the outer surface of the chip). Periodic shear instability appears in the shear zone evidenced by the four shear bands and serrated chips as shown in Fig. 12 (c-f). Meanwhile, the tool-chip interface and the machined surface have undergone large deformation due to the intense friction between the tool and the workpiece materials. In the high-speed cutting of crystalline metals, the chip is usually jagged^[24]. In this simulation, although the scale of nanometric cutting is much smaller than that of the conventional cutting, it can reflect the formation process of serrated chip in some level. The distance between each of the four shear bands shown in Fig. 12 (f) are 4.07 nm, 3.64 nm, and 4.57 nm respectively. And the average distance of the shear bands in this simulation is 4.09 nm.

Fig. 12. The atomic shear strain diagram during the cutting process (the unit of spacing between the shear bands is nanometer)

In order to better understand the formation of periodic shear bands and reveal the cutting mechanism, instantaneous atomic structure images of these shear bands were constructed. Figure 13 (a-d) corresponds to figure 12 (c-f) respectively. The elongated ovals in Fig. 13 (a) and (b) represent the location of the shear zones at different cutting time. Judging from the images, the shear bands may be amorphous. To prove this speculation, 3 small areas around the point A, B, and C in the shear band (shown in Fig. 13 (c)) were selected and their radius distribution functions were calculated. The three RDF curves are similar to each other and one of them is shown in Fig. 14 (a). The general trend of the curve in Fig. 14 (a) is similar to Fig. 1 (b). Although there are some slight fluctuations along the curve, the atomic structure in **the shear band is still amorphous**. The reason for the shear-slip which was in the amorphous region is that the bulk metallic glasses are pressure-sensitive materials. The free volume in the shear band is increased under the shear stress. Therefore, the viscosity of the shear zone is declined and the plasticity increased. The cutting adiabatic rise contributes to this process at the same time.

In Fig. 13 (c), φ is the shear angle which represents the angle between the shear band and the cutting direction. It is clear that the shear angle φ is less than 45° , which is consistent

with many experimental results of the tension and compression tests of metallic glass. The metallic glass has the property of tension/compression asymmetry. The simulation result in Fig. 13 (c) proves that this conclusion holds true even in the case of nanometric cutting with such a high strain rate.

When the cutting is in the steady state, **three parallel fields in the end of the chip can be seen** in Fig. 13 (b), (c) and (d). Judging from the images, those fields have been totally crystallized. Fig. 14 (b) shows a representative RDF curve of No.1, No.2 and No.3 field as shown in Fig. 13 (d). From this curve, it is believed that those fields have been crystallized. During the nanometric cutting process, the shear energy of the chip gradually released, the materials with high temperature in the shear zone were crystallized at a relatively lower cooling rate which is much smaller than that of amorphous preparation.

Fig. 13. The instantaneous structural analysis diagram corresponding to the formation of the shear bands

Fig. 14. The radial distribution functions of the shear band and the chip end

4 Conclusions

Using molecular dynamic simulations, the crystallization behavior of amorphous and cutting deformation process of nanocrystalline copper was observed. The following conclusions can be drawn:

- The crystallization of amorphous copper was observed. The FCC is the main lattice structure produced in the cutting process.
- The growth and consolidation process of grains were analyzed based on the RDF curves and atomic displacement vector method. The crystallization was induced mainly by the shear stress. The grains consolidation completed through the annihilation of excess free volume at the grain boundaries.
- The shear deformation in cutting of nanocrystalline copper took place in amorphous state. The shear angle during the cutting process is less than 45° which is consistent with the compression experiments of metallic glass.

Future work will be directed to study the tool geometry and cutting parameters effect for the formation of shear bands.

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