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

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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.

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 prospect [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 election 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 $Al_{90}Fe_5Gd_5$ 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 has been carried out. Molecular dynamics simulation of the deformation behavior of amorphous nickel under stress was 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 commonly used for material shaping. Cutting involves elastic and plastic deformation

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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/among copper atoms. The total atomic potential energy of a system is expressed as

$$E_{tot} = \frac{1}{2}\sum_{ij}\Phi_{ij}(r_{ij}) + \sum_{i}F_i(\overline{\rho_i}) \tag{1}$$

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

$$\overline{\rho_i} = \sum_{j\neq i}\rho_j(r_{ij}). \tag{2}$$

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

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

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].

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 $43.8 \times 18.1 \times 1.46$ nm^3.

Table 1
Morse potential parameters for Cu–C atom pairs [15].

Atom pairs	D (eV)	α (Å^{-1})	r_0 (Å)
Cu–C	0.087	5.14	2.05

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 that the potential functions and parameter settings in the simulation were effective.

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.

The geometry parameters of single crystal diamond tool are as follows: a cutting edge radius of 5 Å is used, the tool rake angle $\alpha = 15°$ and the tool clearance angle $\beta = 8°$. 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