Multiscale simulation of nanometric cutting of single crystal copper—effect of different cutting speeds

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A multiscale simulation has been performed to determine the effect of the cutting speed on the deformation mechanism and cutting forces in nanometric cutting of single crystal copper. The multiscale simulation model, which links the finite element method and the molecular dynamics method, captures the atomistic mechanisms during nanometric cutting from the free surface without the computational cost of full atomistic simulations. Simulation results show the material deformation mechanism of single crystal copper greatly changes when the cutting speed exceeds the material static propagation speed of plastic wave. At such a high cutting speed, the average magnitudes of tangential and normal forces increase rapidly. In addition, the variation of strain energy of work material atoms in different cutting speeds is investigated.

KEY WORDS Multiscale simulation; Nanometric cutting; Single crystal copper; Propagation speed of plastic wave

1 Introduction

Nanometric cutting is a mechanical machining method to fabricate micro- and nano-components. To understand the properties and mechanisms of nanoscale processing, much work has been performed using different simulation methods. Ikawa *et al.*^[1] and Shimada *et al.*^[2] investigated the effect of minimum cutting depth and the ratio of minimum cutting depth to the edge radius in the nanometric cutting processes of copper and aluminum. Liang *et al.*^[3] studied the mechanical properties of machined nanostructures using MD method. Fang and Weng^[4] studied the effect of the tool angle and the cutting depth on nanometric cutting process of single crystal copper using 3-D molecular dynamics (MD) method and found a linear relationship between the total force on the tool and the tool angle. Shimizu *et al.*^[5] analyzed the super high-speed grinding of ductile material using MD method, concluded that material deformation mechanism change greatly when the grinding speed exceeds propagation speed of plastic and verified their results by experiments. Pei *et al.*^[6] studied nanometric machining of copper with the model size of more than four million atoms and found that as the cutting depth decreases, the specific cutting force

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increases rapidly and a higher cutting speed results in more lattice defects at the cutting region and higher cutting forces. Lin and Huang^[7] proposed a method that combines MD with finite element deformation model (MDFM) to evaluate the chip formation and strain and stress distribution in nanoscale cutting of single crystal copper. Recently, Shiari *et al.*^[8] used a multiscale method (Coupled atomistic/discrete dislocation method) to research the features of dislocation distribution in nanoscale material removal process of single crystal aluminum.

As known from the above Refs.^[4–8], the influence of cutting speed on cutting force is minor in a lower speed (20–200 m/s) and the deformation mechanism and forces change obviously in a higher speed (200–1000 m/s). However, there are no consistent results about this problem due to the differences of simulation methods and machining parameters. In order to investigate the effect of the cutting speed on the deformation mechanism and the variation of cutting forces and strain energy in nanometric cutting, a multiscale method based on quasicontinuum method (QC) is used to simulate the nanometric cutting process of single crystal copper at five different cutting speeds (20–800 m/s).

2 Multiscale Simulation Methodology

2.1 QC method

QC method was developed by Tadmor *et al.*^[9] in 1996. In the local region where the deformation gradient changes gradually on the atomic scale, it is not necessary to explicitly track the displacement of each atom. Instead, only the displacements of a small fraction of the atoms (called representative atoms or “repatoms”) need to be explicitly tracked, and the displacements of the remaining atoms approximately are calculated through FE interpolation. In this region, macro deformation gradient F is considered to be fit for fine scale deformation. Deformation gradient F maps an undeformed configuration X onto deformed configuration $x=X+u(X)$,

$$F(X) = \frac{\partial x}{\partial X} = I + \frac{\partial u}{\partial X} \quad (1)$$

where I is unit tensor and $u(X)$ is the displacement tensor. The first Piola-Kirchhoff stress tensor P and Lagrangian stiffness tensor C are defined respectively in Eq.(2)

$$P = \frac{\partial W}{\partial F^T}, \quad C = \frac{\partial^2 W}{\partial F^T \partial F^T} \quad (2)$$

where W is strain energy density function that is calculated directly from the interatomic potentials by using the Cauchy-Born rule. Thus nonlinear finite element technique can be used to solve this kind of problems.

In the nonlocal region such as dislocation cores, surfaces and interfaces, it is necessary to describe the energy accurately. In the energy-based formulation, the energy of model is calculated accurately by explicitly computing only the energy of repatoms ($N_{\text{rep}} \ll N$)

$$E^{\text{tot,h}} \approx E^{\text{tot,h}'} = \sum_{\alpha=1}^{N_{\text{rep}}} n_{\alpha} E_{\alpha}(u) \quad (3)$$

where n_{α} is the weight function for repatom α , which will be high for repatoms in regions of low repatom density and vice versa.

In the transition region where atomistic and continuum models are combined, the total energy is approximated through summing the energy of local and nonlocal repatoms as

$$E^{\text{tot,h}} \approx \sum_{\mu=1}^{N_{\text{loc}}} n_{\mu} E_{\mu}(u) + \sum_{\alpha=1}^{N_{\text{nl}}} n_{\alpha} E_{\alpha}(u) \quad (4)$$

where n_{μ} , n_{α} are the weight function for local and nonlocal regions respectively, E_{μ} is the energy of local elements and E_{α} is the energy of nonlocal repatoms.

2.2 Model system

Multiscale simulation was conducted on a copper single crystal workmaterial cutting along $[\bar{1}10]$ direction and (001) crystal orientation at 3 nm cutting depth and five different cutting speeds ($v=20, 200, 300, 400$ and 800 m/s).

Fig.1 shows the multiscale simulation model. The workpiece size is $100 \text{ nm} \times 100 \text{ nm}$ initially containing about 100 repatoms which increase as the cutting processes. The model is plane strain configuration with thickness in the out of plane direction equal to the minimal repeat distance in that direction and with periodic boundary conditions applied. The region close to the cutting surface is simulated with atomic resolution, while the remaining regions are simulated in a continuum sense. Fix boundary conditions are applied to the nodes in the left and bottom sides of the workpiece, and a circular tool is driven over the free surface of a block of copper atoms arranged in a 2-D triangular lattice. For the Cu-Cu interaction between the work material, the EAM^[10] potential is used.

Fig.1 Multiscale simulation model of nanometric cutting.

Each atom in the work material interacts with this idealized circular tool *via* the repulsive potential^[3,11]

$$V(r) = \begin{cases} A(r - R) & \text{for } r < R \\ 0 & \text{for } r \geq R \end{cases} \quad (5)$$

where $A=16021$ nN/nm is a force constant and is chosen according to Ref.[8], R is the indenter radius, and r is the distance from the atom to the center of the indenter sphere.

3 Results and Discussion

Multiscale simulation of nanometric cutting was conducted on a copper single crystal workmaterial using a workstation with Pentium (R) Dual-Core Processor @ 3.0 GHz to study the effect of cutting speed on deformation mechanism, cutting forces and strain energy.

3.1 Material deformation and chip formation process

Fig.2 shows the effect of cutting speed on the material deformation mechanism of single crystal copper under a cutting distance of 7 nm. It can be seen that more and more finite element nodes are meshed to atomistic size to simulate the nanoscale machining process as the cutting advances.

Fig.2 Chip formation process for five different cutting speeds: (a) 20 m/s; (b) 200 m/s; (c) 300 m/s; (d) 400 m/s; (e) 800 m/s.

In the case of Fig.2a, many atoms accumulate in front of the tool and form a chip. The dislocations which are generated at an angle of about 60° to the cutting direction are observed. This situation also can be seen from Fig.2b and 2c at 200 and 300 m/s, respectively. When the cutting speed is almost the same as the material static propagation speed of plastic wave, as shown in Fig.2c, plastic deformation in front of the cutting tool becomes smaller than the cases of Fig.2a–2c. Meanwhile, the number of the active slip planes decreases further than those of Fig.2a–2c. In the case of Fig.2d in which cutting

speed is higher than the material static propagation speed of plastic wave, the atoms in the chip are noncrystalline and in condition of melt rather than plastic deformation^[5]. This amorphous phase can be interpreted by radial distribution function (RDF) curves of local workpiece atoms. Fig.3 shows the variation of RDF in the deformation zone under the tool surface with an area containing 12 nm in the cutting direction and 6 nm in the perpendicular direction. It can be seen that the RDF shows the pattern of crystalline FCC when cutting speed range from 20–400 m/s. When cutting speed is 800 m/s, the peak values of RDF are reduced and some peaks become broad, which indicates an obvious decrease in the degree of lattice ordering. The disappearance of key peaks can be defined as a common feature of amorphous materials^[12,13].

Simulation results show that the cutting speed has a significant effect on the material deformation mechanism when the cutting speed exceeds the material static propagation speed of plastic wave. Fig.2 also reveals an uneven surface at the starting end of the machined workpiece and the material deformation tilts towards the left-hand side. The main reason for this phenomenon is that the cutting action is based on extrusion caused by a large negative tool rake.

3.2 Analysis of cutting force

The average tangential and normal forces are shown in Fig.4 as a function of cutting speed where both average forces are the mean values over the range of 5–7 nm cutting distance. The least square method is used to determine the best curves to fit the series of data points. Up to 200 m/s in cutting speed, the tangential and normal forces decrease. Then the two forces increase with the increase of the cutting speed. The low decrease of the cutting force from 20 to 200 m/s indicates that a lower cutting speed allows machined surface and cutting region experience elastic recovery because of the relaxation, which hinders the advancement of tool. The increase of cutting forces is because a higher cutting speed result in a shorter time for the dislocations to move away from the cutting region and thus the dislocations accumulate in the cutting region and strengthen the materials there, which cause a higher deformation force. Yet, the cutting forces do not change obviously when cutting speed range from 20–400 m/s. This can be interpreted from the fact that the cutting force represents the ability of overcoming the bond energy between

Fig.3 Radial distribution function of workpiece atoms with different cutting speeds.

Fig.4 Variation of average tangential and normal cutting forces versus cutting speeds.

the tool and the workpiece at atomic scale within every time step. Especially, the tangential and normal forces take a sudden increase at 800 m/s. The obvious differences can be related to the phase transition from crystal plasticity induced by lattice dislocation motion to an amorphous state in the workpiece atoms.

Simulation results show that speed variation in the range of 20–400 m/s has little effect on the cutting force at 3 nm cutting depth and the cutting forces increase obviously when the cutting speed exceeds the material static propagation speed of plastic wave.

3.3 Analysis of strain energy

Fig.5 shows the variation of strain energy of work material atoms obtained by multiscale simulation of nanometric cutting process with different cutting speeds. The strain energy increases as the cutting processes, and then the values of strain energy tend to be steady. It can be seen that the values of strain energy still fluctuate because of dislocation initiation events during the nanometric cutting process. The nucleation of dislocations causes the drop of strain energy of work material atoms.

The strain energy is lowest at 20 m/s cutting speed, and highest in 800 m/s cutting speed. The low strain energy indicates that the number of work material deformation atoms is less or work material experiences a larger elastic recovery due to the relaxation at 20 m/s cutting speed. The elastic recovery releases part of the energy. At 800 m/s cutting speed, atoms in the cutting region have lost their crystallinity. The instability of the crystal lattice leads to the collapse of workpiece atoms and the concomitant production of the amorphous solid in the deformation zone composed of a high concentration of defects and dislocations. As shown in Fig.5, the variation of strain energy is consistent at 200–400 cutting speeds, which shows that cutting speed has little effect on the strain energy for this speed range at 3 nm cutting depth.

Fig.5 Strain energy variation for various cutting speeds.

4 Conclusions

Multiscale simulation of nanometric cutting was performed to investigate the effect of cutting speed on the chip formation, the cutting forces and the strain energy of work material atoms. Following results were gained:

- (1) The material deformation mechanism of single crystal copper greatly changes when the cutting speed exceeds the material static propagation speed of plastic wave. Severe local surface plasticity and amorphization can be generated by increasing the cutting speed to higher than 400 m/s.
- (2) The lower cutting speeds have a little effect on the tangential and normal cutting forces. At cutting speeds over the propagation speed of plastic wave, the average magnitudes of tangential and normal forces increase rapidly.
- (3) Fluctuations of strain energy are related to dislocation generation events during the

nanometric cutting process of single crystal copper. The strain energy is independent on the velocity for the speed ranging from 200–300 m/s.

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