MD Simulation of Effect of Crystal Orientation and Cutting Direction on Nanometric Cutting Using AFM Pin Tool

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Three-dimensional molecular dynamics simulations of nanometric cutting monocrystalline copper using atomic force microscopy pin tool are conducted to investigate the effect of crystal orientation and corresponding cutting direction on the deformation characteristics. EAM potential and Morse potential are utilized respectively to compute the interactions between workpiece atoms, interactions between workpiece atoms and tool atoms. The results reveal that the nanometric cutting processes are significantly affected by crystal orientation and cutting direction. Along the [110] cutting direction, better quality of chip pattern and smaller workpiece material deformation region can be obtained than along the [100] cutting direction. Cutting the workpiece material (110) crystal orientation, smaller chip volume and smaller subsurface deformed region can be obtained than cutting the workpiece material (100) crystal orientation. The variations of workpiece atoms potential energy in different cutting processes are investigated.

Key words: Nanometric cutting, Atomic force microscopy, Molecular dynamics, Crystal orientation, Cutting direction

I. INTRODUCTION

Recently, the atomic force microscopy (AFM)-based nanometric cutting technique has been proposed to directly machine material surfaces and fabricate micro- and nano-components in micro-electro-mechanical systems (MEMS) and nano-electro-mechanical systems (NEMS) [1-6]. The main challenge of this novel technique is to develop a fundamental understanding of the nanometric cutting mechanism and mechanics, such as the chip formation, elastic deformation and plastic deformation, and friction. Hence, theoretical analysis and investigation of the cutting mechanism at the atomic-scale greatly facilitate the development of high precision machining micro- and nano-components. However, as the nanometric cutting involves only a few atomic layers at the surface, it is inherently atomistic rather than continuous, so it is extremely difficult to observe the cutting process and to measure the process parameters through experiments, and the conventional continuum mechanics theory can not be applied to the analysis of the nanometric cutting process due to the size limitation. An alternative approach is molecular dynamics (MD) simulation, which has been confirmed to be best suited for the analysis of the nanometric cutting process [7-10].

Single crystal materials are anisotropic in their physical and mechanical properties, so workpiece materials elastic modulus are influenced during nanometric cutting process with different crystal orientations and corresponding cutting directions, consequently the elastic recovery degrees of machined surface vary, which significantly affects the finish, accuracy, and surface integrity. In order to achieve high precision machining in nanometric cutting, molecular dynamics studies of the effect of crystal orientation and cutting direction on deformation characteristics, such as chip formation and subsurface deformed behaviors are necessary.

Some typical works that investigated the effect of crystal orientation and cutting direction on the cutting process using MD simulation include that Komanduri et al. conducted MD simulation of nanometric cutting on single crystal aluminum in specific combinations of crystal orientation and cutting direction using diamond tool [11,12]. They investigated the nature of deformation and the extent of anisotropy of workpiece material. Kim et al. performed three-dimensional MD simulation of the nano-lithography process of monocrystalline copper using an AFM tip to evaluate the effect of crystallographic factors on the nano-deformation characteristics [13], and reported the crystal orientation and the ploughing direction had a significant influence on varying the force and surface quality of the machined material. Pei et al. performed a series of large scale MD simulation with the model size of more than four-million atoms to study the nanometric machining of copper, and the effect of crystal orientation and cutting direction were investigated [14]. They reported that the crystal orientation and cutting direction have a strong effect on material deformation, dislocation movement and cutting force.

However, previous studies mainly focused on the cutting force and nature of deformation, and haven’t inves-
tigate the effect of crystal orientation and corresponding cutting direction on the chip formation and workpiece material deformation region, which play a key role for fabricating fine surface quality nano-components.

Therefore, in this work three-dimensional MD simulations of nanometric cutting of monocrystalline copper using an AFM pin tool are performed to investigate the effect of specific combinations of crystal orientation and cutting direction ((010)[100], (010)[101], (101)[010], (101)[110]) on deformation characteristics, such as chip formation, subsurface deformed region, and variations of workpiece atoms potential energy in each cutting process.

II. MD SIMULATION METHODOLOGY

As shown in Fig.1, a workpiece and a tool are assumed to consist respectively of monocrystalline copper and rigid diamond. The fixed integration step size is chosen as 0.5 fs.

![MD Simulation Model of Nanometric Cutting Using AFM Pin Tool](image)

FIG. 1 MD simulation model of nanometric cutting using AFM pin tool.

The size of workpiece utilized in the current MD simulations is $32a \times 12a \times 30a$, where $a$ is the lattice constant of copper (0.361 nm), and the number of workpiece atoms is corresponding to the workpiece crystal orientation. The workpiece includes three different kinds’ atoms, namely, boundary atoms, thermostat atoms, and Newtonian atoms, respectively. The motion of thermostat atoms and Newtonian atoms obey the Newton’s second law, and are determined by direct integration of the classical Hamiltonian equations of motion using Velocity-Verlet method. The two layers of boundary atoms in the left side of the workpiece and the bottom of the workpiece are kept fixed in space and server to reduce the edge effects. The initial temperature of the workpiece is 293 K, and in order to stabilize the average temperature of the thermostat layers at 293 K, heat dissipation is carried out through the thermostat atoms, whose velocities are adjusted by the presence of velocity reset functions at every 5 time steps of the computation [15]. The periodic boundary condition is used in z-direction to reduce the effects of simulation scale.

The AFM pin tool has the configuration of co-shape of sphere and cylinder, and the radius of the sphere is 1.07 nm. The pin tool employed is configured from 1762 atoms and is treated as a rigid body in the current simulations.

![Figure 2: Various Crystal Orientations and Cutting Directions](image)

For the Cu–Cu interaction between the workpiece atoms, the established EAM potential is used, which has been used successfully in nanometric cutting study [16–18]. For EAM potential, the total atomic potential energy of a system $E_{tot}$ is expressed as:

$$E_{tot} = \frac{1}{2} \sum_{ij} \phi_{ij}(r_{ij}) + \sum_i F_i(r_i)$$  \hspace{1cm} (1)

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

$$\rho_i = \sum_{j \neq i} \rho_j(r_{ij})$$ \hspace{1cm} (2)

for the Cu–C interaction between workpiece atoms and tool atoms, Morse potential is used, which is relatively simple and computationally inexpensive compared to the EAM potential [19–21]. The Morse potential is written as:

$$E_{tot} = \sum_{ij} D_0 \left[ e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right]$$ \hspace{1cm} (3)

where $E_{tot}$ is a pair potential energy function; $D_0$ is the cohesion energy; $\alpha$ is the elastic modulus; $r$ and $r_0$ are the instantaneous and equilibrium distance between atoms $i$ and $j$, respectively. The cutoff radius of the Morse potential is chosen as 902.5 pm, which ensures that the calculations will not consume large amounts of computational time.

In the current MD simulations, the cutting speed is selected as 200 m/s to keep the computational time to a reasonable value, though this high cutting speed is unrealistic. Previous studies have confirmed that there was little difference between the effects of a cutting speed of 20, 50, 100, 200, and 250 m/s on the surface quality [22,23].

Figure 2 shows the various crystal orientations and cutting directions for the monocrystalline copper in the current simulations (Table I).

III. RESULTS AND DISCUSSION

Nanometric cutting monocrystalline copper using an AFM pin tool with different combinations of crystal orientation and cutting direction, (010)[100], (010)[101], (101)[010], (101)[110], are conducted in the current simulations. All the simulations are performed using an AFM pin tool with radius of 1.07 nm, velocity of 200 m/s, uncut chip thickness of 0.54 nm.
FIG. 2 Crystal orientation and cutting direction utilized in the current simulations.

TABLE I summarizes the numbers of workpiece atoms according with the four combinations

<table>
<thead>
<tr>
<th>Combination</th>
<th>Number of workpiece atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>(010)[100]</td>
<td>48750</td>
</tr>
<tr>
<td>(010)[110]</td>
<td>48394</td>
</tr>
<tr>
<td>(110)[010]</td>
<td>46971</td>
</tr>
<tr>
<td>(110)[110]</td>
<td>46410</td>
</tr>
</tbody>
</table>

A. On the nature of deformation behavior of nanometric cutting process

Figure 3 shows the representative nanometric cutting process with a tool travel of 2, 4, and 6 nm for a combination of workpiece crystal orientation (100) and cutting direction [100]. It maybe noted that the discussion of the results presented here is based not only on the MD simulations plots but also on the detailed study of the animations of the cutting process. Both of the plots and animations are created using VMD-VMD, an open source and free molecular visualization program [24].

There are two deformation states between the workpiece and tool, as ploughing state, cutting state. The workpiece material deformation region is localized around the tool. Some workpiece material atoms accumulated ahead of the tool edge, consequently formed chip. Simultaneity, some workpiece material atoms piled up on the left and right sides of the V-groove, consequently formed remarkable side-flow.

The deformation mechanism could be explained: In nanometric cutting process, with the ploughing of tool edge, workpiece material atoms surround the pin tool undergo complicated plastic deformation and elastic deformation, lattice of workpiece atom is deformed as buckled. When the strain energy stored in the deformed lattice exceeds a specific level, the atoms are re-arranged successively onto the lower lattice so as to relax the lattice strain, and a lot of dislocations are generated in the workpiece near the tool-work interface. Some of them move into the shear zone, and workpiece atoms accumulate ahead of the tool and formed chip, some workpiece atoms pile up on both side of the groove simultaneity. And some dislocations move downward and penetrate into the workpiece beneath the tool edge. After the passing of tool edge, machined surface experiences elastic recovery, almost all of penetrated dislocations begin to move back and finally disappear from the workpiece surface. However, considerable distorted atoms inevitably exist in the subsurface deformation region [25].

B. Effect of crystal combination on chip formation

Figure 4 shows the effect of crystal orientation and cutting direction on chip formation during deformation process. Each figure shows cross-section views of the $xy$ plane and with the same tool travel of 7 nm.

Figure 4(a) with a crystallographic combination of (010)[100] shows that there are clear workpiece material accumulation ahead of the AFM pin tool, and the chip volume is similar to the Fig.4(b) with a crystallographic combination of (010)[101]. However, there are small difference in chip pattern between the two crystallographic combinations. Under the crystallographic combination of (010)[100] the atoms at the chip surface are loosely connected to each other, while under the crystallographic combination of (010)[101] the atoms at the chip surface are more closely connected to each other. Figure 4 (c) and (d) shows that the atoms at the chip surface are more closely connected to each other under the crystallographic combination of (101)[110] than the crystallographic combination of (101)[001]. In both these crystal combinations as shown in Fig.4 (a) and (c), the cutting direction corresponds to the [100] family, and the cutting direction corresponds to the [110] family for Fig.4 (b) and (d). It indicates that along the [110] cutting direction family better quality of chip pattern can be obtained than along the [100] cutting direction family.

The chip volume is bigger under the crystallographic combination of (010)[100] than the crystallographic combination of (101)[001] as shown in Fig.4 (a) and (b), which with the same cutting direction but different workpiece material crystal orientation. It is the same case for Fig.4 (b) and (d), the chip volume is bigger under the crystallographic combination of (010)[101] than the crystallographic combination of (101)[110]. In Fig.4 (a) and (b), the crystal orientation corresponds to the (100) family, and the crystal orientation corresponds to the (110) family for Fig.4 (c) and (d). It indicates that

FIG. 3 Deformation behaviors of cutting process with different tool travel.
FIG. 4 Variations of chip formation for various combinations of crystal orientation and cutting direction.

cutting the workpiece material crystal orientation family (110) smaller chip volume can be obtained more than cutting the workpiece material crystal orientation family (100).

Therefore, it concludes that the crystal orientation and cutting direction have a significant effect on the chip formation, such as chip pattern and chip volume.

C. Effect of crystal combination on workpiece material deformation region

Figure 5 shows the effect of crystal orientation and cutting direction on workpiece material deformation region during nanometric cutting process. Each figure shows the plane view of the xz plane as shown in Fig.5(e) with the same tool travel of 7 nm. In the current study the area of workpiece material deformation region is pointed out by the black line manually in order to denote it efficiently, as shown in Fig.5 (a)-(d).

As shown in Fig.5(a) with a crystal combination of (010)[100], it is clear that the range of workpiece material deformation is limited to the workpiece atoms surrounding the tool, and a remarkable side-flow on the two sides of the tool. It is the same case for Fig.5(b) with a crystal combination of (010)[101]. But there are slight difference for the two crystal combination, which is with the same workpiece material crystal orientation but different cutting direction. The workpiece material deformation region is smaller for Fig.5 (b) than (a). Furthermore, Figure 5 (c) and (d) show that the workpiece material deformation region is smaller for the crystal combination of (101)[110] than the crystal combination of (101)[001]. It indicates that along the [110] cutting direction family results smaller workpiece material deformation region than along the [100] cutting direction family.

Figure 5 (a) and (c) show the workpiece material deformation regions for crystal combination with the same cutting direction but different workpiece material crystal orientation. It is clear that both the workpiece material deformation region and side-flow volume are bigger with the crystal combination of (010)[100] than the crystal combination of (101)[001]. It is the same case for Fig.5 (b) and (d), both the workpiece material deformation region and side-flow volume are bigger with the crystal combination of (010)[101] than the crystal combination of (101)[110]. It indicates that cutting the workpiece material crystal orientation family (110) results smaller subsurface deformed region than cutting the crystal orientation family (100).

Figure 6 shows the variations of workpiece atoms potential energy obtained by MD simulation of nanometric cutting process with different combinations of crystal orientation and cutting direction. The workpiece atoms potential energy increase with the tool advancement. It can be seen that potential energy-time step diagrams of nanometric cutting process with different combinations of crystal orientation and cutting direction seem parallel to each other. However, the potential energy is larger for the workpiece material crystal orientation family (1101) than the workpiece material crystal orientation family (100). It indicates that the number of workpiece deformation atoms is smaller with the crystal orientation (101) than the crystal orientation (010), which basically agrees with the result that

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cutting the workpiece material crystal orientation (101) results smaller workpiece material deformation region than the workpiece material crystal orientation (010).

Komanduri [11-12] and Kim [13] both reported that for (100)[100] combination, dislocation generated at about 45° to the cutting direction. In (100)[110] combination, dislocation generated parallel to the cutting direction. In (110)[100], dislocation generated normal to the cutting direction. In (110)[110], dislocation generated parallel as well as perpendicular to the cutting direction. In the current study, this effect of crystal orientation and cutting direction on chip formation and workpiece material deformation region can be explained by the conclusions above, as in term of the different directions of the workpiece dislocation slip direction to the cutting direction. For example, there is less workpiece deformation for the (110) crystal orientation family than the (100) crystal orientation family, as the direction of slip direction to the cutting direction is smaller for the (110) crystal orientation family than the (100) crystal orientation family.

IV. CONCLUSION

Three-dimensional MD simulations of nanometric cutting using AFM pin tool are performed to investigate the effect of crystal orientation and cutting direction on deformation characteristics, such as chip formation, workpiece material deformation region, and variations of potential energy. Based on the study, conclusions are given as follows:

MD simulations of nanometric cutting monocrystalline copper using an AFM pin tool reveal that workpiece material crystal orientation and cutting direction have a significant effect on the chip formation and workpiece material deformation region during the deformation process. Along the [110] cutting direction family, better quality of chip pattern and smaller workpiece material deformation region can be obtained than along the [100] cutting direction family. Cutting the workpiece material crystal orientation family (110), smaller chip volume and smaller subsurface deformed region can be obtained than cutting the workpiece material crystal orientation family (100). The potential energy required for removal of workpiece atoms was larger for the workpiece material crystal orientation family (110) than the workpiece material crystal orientation family (100).

V. ACKNOWLEDGMENTS

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