Molecular dynamics simulation of self-rotation effects on ultra-precision polishing of single-crystal copper

Yihan Yang, Hongwei Zhao, Lin Zhang, Mingkun Shao, Hongda Liu, and Hu Huang

Citation: AIP Advances 3, 102106 (2013); doi: 10.1063/1.4824625
View online: http://dx.doi.org/10.1063/1.4824625
View Table of Contents: http://scitation.aip.org/content/aip/journal/adva/3/10?ver=pdfcov
Published by the AIP Publishing
Molecular dynamics simulation of self-rotation effects on ultra-precision polishing of single-crystal copper

Yihan Yang, Hongwei Zhao, Lin Zhang, Mingkun Shao, Hongda Liu, and Hu Huang

College of Mechanical Science & Engineering, Jilin University, Renmin Street 5988, Changchun, Jilin 130025, China

(Received 12 July 2013; accepted 25 September 2013; published online 17 October 2013)

Understanding the behaviors of the material removal mechanism of ultra-precision polishing process has been a critical issue of generating well-formed surface. In order to make clear the abrasive self-rotation effects on material removal at the atomic level, a three-dimensional molecular dynamics (MD) model is conducted to study the mechanics of ultra-precision polishing on single-crystal copper with a diamond abrasive and the effects of abrasive self-rotation velocity and direction. Morse potential energy function and EAM potential energy function are applied to model the copper/diamond and copper/copper interactions, respectively. The simulation results show that the deformation mechanism of single-crystal copper is due to the formation and movement of dislocations in the specimen. In addition, with the increasing of abrasive self-rotation velocity, the deformation mechanism falls from cutting to plowing regimes. The abrasive self-rotation velocity and direction have effects on the morphology and quality of the specimen surface, distribution and evolution of defects under the surface of the specimen. Also, the interatomic force between abrasive and specimen is studied to account for the effects of different polishing conditions. © 2013 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License. [http://dx.doi.org/10.1063/1.4824625]

I. INTRODUCTION

In recent years, the demand for polishing material with higher planarity and nanometric surface finish has grown tremendously.1 Acquiring intricate features, low surface roughness, low-level residual surface stress, and smaller metamorphic region, the nano-scale ultra-precision machining technology is widely accepted in machining. Ultra-precision chemical mechanical polishing (CMP) is a powerful technique for fulfilling these requirements.2 However, one of the hindrances to the development of ultra-precision mechanical polishing process is the lack of a better understanding of the various micro and nano mechanisms of material removal and surface generation process.

The ultra-precision mechanical polishing process often involves complex micro-contact and micro-friction phenomenon. Moreover, since mechanical machining may cause substantial changes in the structural or other physical properties of machined substrates, a lot of studies are carried out to investigate kinds of machining process of single-crystal copper based on various experimental and theory methods, and have provided much help in understanding the machining parameters effects,3 machining mechanism4 and chip formation,5 etc. However, in spite of the rapidly developing fabrication techniques, our fundamental understanding of the structural changes taking place beneath the surface during polishing process is still far from complete. On one hand, the experiments which cannot trace the evolution of the physical essence inside the materials in this extremely small dimension in-site throughout the process lead to the experimental results lacking in convincing evidence. On the other hand, the previous method based on continuum mechanics to analyze the
macroscopic material removal process is not appropriate to analyze such a process limited in nano scale. Therefore, a useful approach like molecular dynamics (MD) which can describe the microcosmic world at atomic scale is imperatively needed to make a clear understanding of the physical essence of the machining process.

In contrast to computer simulations of nanoindentation or nanoscratching, only a few molecular dynamics studies have been performed for ultra-precision mechanical polishing. With the two-dimensional MD model, Han et al. studied chemical mechanical polishing of silicon specimen employing the hybrid potentials to investigate the phase transformation. They also investigated the edge radius of abrasive particle on the nano-scale polishing of monocrystalline silicon. However, the simplification of the abrasive particle to a cutting tool is inappropriate and inaccurate. Rentch et al. used MD to simulate the abrasive processes and found the pile-up phenomenon in the abrasive machining. Si et al. built a simulation of nanoscratching process to study the removal mechanism of single crystalline silicon in chemical mechanical polishing process and paid attention to the effect of scratching depth. Although many improvements have been done in their models, the abrasive particles are regarded as a rigid body without self-rotation and the self-rotation is not considered as an essential factor in the polishing process in those studies.

In this paper, we perform a series of large-scale molecular dynamics (MD) simulations of ultra-precision mechanical polishing with hybrid potential functions to investigate the self-rotation effects of diamond abrasive. During the high-speed polishing on the Cu (010) surface by a single diamond abrasive with spherical shape, our special attention is laid on the correlation between defect evolutions and self-rotation conditions. In the following, the simulation methodology employed is firstly described in details. Then a detailed research on the effects of the diamond abrasive self-rotation velocity and direction on material removal is presented. It will show how self-rotation velocity and direction of the diamond abrasive influence the morphology and quality of the specimen surface, distribution and evolution of defects under the specimen surface.

II. MD SIMULATION

A. Initial physical model

In the current molecular dynamics simulations, a three-dimensional (3D) physical model is employed to describe an ultra-precision mechanical polishing process. For material removal from the substrate is largely influenced by such a process, the material removal mode is investigated as the mechanism of mechanical polishing process, as illustrated in Fig. 1. As shown in Fig. 1(a), in the typical chemical mechanical polishing process, a force is applied to the specimen fixed with the rotating clamp to press it into the rotating pad, which both clamp and pad have motion to create a relative velocity. Some abrasive particles are immersed in the slurry rolling across the specimen surface and some others are embedded in the polishing pad removing materials by plowing. To facilitate understanding, the model in Fig. 1(a) is simplified to a model of irregular shape of abrasives between the moving specimen and polishing pad, shown in Fig. 1(b). Then, it is necessary to investigate the deformation of a smooth copper surface subjected to a single abrasive. Moreover, the hard abrasive which is irregular in reality has been simplified to a spherical diamond ball of radius $R$, moving horizontally and rotating about its centre in the meantime, as shown in Fig. 1(c).
FIG. 2. Three-dimensional MD simulation model.

According to the simplification of mechanical polishing process, the schematic diagram of the physical model for the MD simulation is shown in Fig. 2. Because the abrasive is set to process in a defined depth, the polishing pad has no need in the simulation and is removed. The model consists of two parts, single-crystal copper specimen and diamond abrasive. Since the diamond abrasive is much harder than the copper specimen, it is appropriate to take the abrasive particle as a rigid body without any deformation in the polishing process. The abrasive is a diamond ball of radius $R = 4.346 \, \text{nm}$, moving horizontally along $X$-direction with a peripheral velocity rotating about its central axis, as shown in Fig. 2.

The specimen’s surface in the $X$-direction is to be machined, so the specimen surface of the $X-Z$ plane is built with free surface. The dimension of the control volume (primary cell) of the copper specimen has to be made sufficiently large to eliminate boundary effects. Taking this into consideration, an optimum control volume (primary cell) is chosen based on an iterative process of increasing the control volume (primary cell) size until further increases do not affect the displacement and velocities of the atoms due to the ultra-precision polishing process. Moreover, to reduce the computation, the periodic boundary condition is set along $Z$-direction in the model. The dimension of the specimen is $27.16 \, \text{nm} \times 9.235 \, \text{nm} \times 16.29 \, \text{nm}$, including 357,266 copper atoms. Copper atoms of the specimen are initially arranged in face-centered cubic (FCC) structure and vibrate around their perfect lattice structure positions. Atoms in specimen are divided into three kinds of atoms: Newtonian atoms, thermostatic atoms and boundary atoms. The boundary atoms are fixed in their initial lattice position to reduce the boundary effects and maintain the proper symmetry of the lattice. Thermostatic atoms are arranged to ensure reasonable outward heat conduction. The motions of Newtonian atoms and thermostatic atoms are determined by the force restricted by the classical Newton’s second law of motion.

B. Selected potential energy function

For such a microcosmic atomic simulation, a reasonable and reliable potential function is a basic and critical prerequisite for accurate results. In this paper, there are two kinds of atoms in the nanometric model, which are C and Cu atoms. Therefore, there are three different atomic interactions between each other, which are the interaction between single-crystal copper atoms (Cu-Cu), the interaction between diamond carbon atoms (C-C) and the interaction between copper atoms and diamond atoms (Cu-C).

Between copper atoms in the specimen, the EAM potential is applied to describe the Cu-Cu interaction. The EAM potential, which is evolved from the density function theory, is based on the recognition that the cohesive energy of a metal is governed not only by the pair-wise potential of the nearest neighbor atoms, but also by embedding energy related to the “electron sea” in which the atoms are embedded. For EAM potential, the total potential energy of the system is expressed as
follows,

$$E_{tot} = \frac{1}{2} \sum_{ij} \phi_{ij}(r_{ij}) + \sum_{i} F_{i}(\rho_{i})$$

(1)

where $E_{tot}$ is the total potential energy of the system; $\phi_{ij}$ is the pair potential between atoms $i$ and $j$; $r_{ij}$ is the distance between the atoms $i$ and $j$, and $F_{i}(\rho_{i})$ is the embedded energy of atom $i$; $\rho_{i}$ is the host electron density at atom $i$ induced by all the other atoms in the system, as follows,

$$\rho_{i} = \sum_{j \neq i} \rho_{j}(r_{ij})$$

(2)

where $\rho_{i}(r_{ij})$ is the contribution to the electronic density at the site of the atom $i$, and $r_{ij}$ is the distance between the atoms $i$ and $j$.

Because diamond is much harder than copper, the tool is treated as a rigid body in the simulation and the wear and deformation of it are not considered in such a short distance polishing process. The force from the specimen to the abrasive is set to 0 in the simulation, while the force from the abrasive to the specimen is normally calculated. In addition, the atoms in the abrasive are fixed to each other relatively, and no potential is needed to describe the interaction between diamond atoms (C-C).

The Morse potential\(^{12}\) is used to describe the interaction between copper atoms and diamond atoms (Cu-C), which is relatively simple and computationally inexpensive compared with the EAM potential. What’s more, although EAM describe the metallic cohesion exactly, it is not appropriate to account for Cu-C interaction. For the Morse potential, the two-body potential energy is expressed as follows,

$$V(r_{ij}) = D \cdot (e^{-2\alpha(r_{ij}-r_{0})} - 2e^{-\alpha(r_{ij}-r_{0})})$$

(3)

where $V(r_{ij})$ is the cohesion energy; $D$ is the cohesion energy; $\alpha$ is the elastic modulus and $f_{ii}$ is the second derivative of the potential energy $V(r_{ij})$ with respect to the bond length $r_{ij}$; $r_{ij}$ and $r_{0}$ are the instantaneous and equilibrium distance between two atoms, relatively. The Morse potential parameters between C-Cu Morse potential are $D = 0.087$ eV, $\alpha = 5.14$ Å\(^{-1}\), and $r_{0} = 2.05$ Å.\(^{13}\)

The choice of the combination of EAM and Morse is supported by previous simulations and tests, which shows good agreement between simulation results and experimental data.\(^{14}\)

### C. Initial MD simulation

The simulation model is equilibrated to 296 K under the microcanonical ensemble (NVE) and the initial velocities of the atoms are assigned in accordance with a Maxwell-Boltzmann distribution. In order to keep the temperature close to the initial temperature, the direct velocity scaling method is applied to maintain the total kinetic energy at a constant value. More detailed parameters used in the simulation are listed in Table I.

The large scale three-dimensional MD simulations were performed by the Large-scale Atomic/Molecular Massively Parallel simulator (LAMMPS) developed by Plimpton.\(^{15}\) The parallel computing was realized under the help of message passing interface (MPI) library. Another software code—AtomEye—was used to visualize the simulation results.\(^{16}\)

### III. RESULTS AND DISCUSSION

After the initial relaxation at the environment temperature of 296 K, a stable structure of the specimen is obtained. The diamond abrasive begins to process along the X-direction with moving velocity of 50 m/s and self-rotation. Although such a velocity is extremely high compared with ultra-precision mechanical polishing experiments, the previous results confirm that there is little difference in deformation characteristics as well as the surface finish quality when the moving velocity ranges from 20 to 200 m/s.\(^{10}\)
TABLE I. Details of the model and simulation conditions in the mechanical polishing simulation.

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of copper specimen</td>
<td>$27.16 , \text{nm} \times 9.235 , \text{nm} \times 16.29 , \text{nm}$</td>
</tr>
<tr>
<td>Numbers of copper atoms in the specimen</td>
<td>357,266</td>
</tr>
<tr>
<td>Numbers of carbon atoms in the diamond abrasive</td>
<td>20,019</td>
</tr>
<tr>
<td>Diamond abrasive radius</td>
<td>4.346 nm</td>
</tr>
<tr>
<td>Polishing depth</td>
<td>2.173 nm</td>
</tr>
<tr>
<td>Specimen machining surface</td>
<td>(010)</td>
</tr>
<tr>
<td>Abrasive orientation and polishing direction</td>
<td>Cubic and [100]</td>
</tr>
<tr>
<td>Equilibration temperature</td>
<td>296 K</td>
</tr>
<tr>
<td>Polishing velocity</td>
<td>Moving velocity $v = 50 , \text{m/s}$</td>
</tr>
<tr>
<td></td>
<td>Self-rotation rate $w = 1.830 , \text{r/ns}$</td>
</tr>
<tr>
<td>Polishing distance</td>
<td>20.0 nm</td>
</tr>
<tr>
<td>Time step</td>
<td>1 fs</td>
</tr>
</tbody>
</table>

FIG. 3. The dislocations distributed in the specimen. (a) and (c) are at the instant of 5.75 nm polishing distance; (b) and (d) are at the instant of 17.0 nm polishing distance. (a) and (b) are the interior defects inside the specimen; (c) and (d) are the left views of the machining surface.

A. General description of interior defects and surface profiles in polishing

Rotation simulations are performed by a rigid diamond abrasive which is set in 2.173 nm polishing depth and processing on the single-crystal Cu substrate along with moving and rotation velocity. When there is no relative slip between the rotation abrasive and specimen, the rotation speed of the abrasive is approximately 50 m/s, which is equal to 1.830 r/ns.

Fig. 3 provides some different views of the machining-induced surface Cu (010) at the instant of 5.75 nm (Fig. 3(a) and 3(c)) and 17.0 nm polishing distance (Fig. 3(b) and 3(d)) with the moving velocity of 50 m/s and the rotation velocity of 1.830 r/ns, from different perspective angles. Colours in the figure represent the atomic coordination numbers of the copper atoms in the specimen. Note that atoms of which the coordination number is 12 are deliberately eliminated in these visualizations so that we can clearly observe any changes in the crystalline order. Therefore only boundary atoms and defect-related atoms as dislocations and vacancies are shown in Fig. 3.
According to Fig. 3(a) and 3(b), there are several types of defect generating during the process which are marked by the numbers in Fig. 3. The number 1 indicates a single vacancy, while the number 2 and 3 denote a vacancy cluster and a vacancy chain. There are lots of them underneath the surface so that they can be easily identified by the atomic coordination numbers. They are generated by the movements and interactions of dislocations. However, they are immobile throughout the polishing process, shown in the circle I and II, which are the typical cases of a single vacancy and vacancy cluster respectively. The number 4 and number 5 designate the dislocation loop. Unlike the vacancy-related defects, they are mobile in certain directions. In general, there are two sliding mode of dislocation loops. One is the bulk glide (marked 4) which emits from the around-the-abrasive region and glides toward the bottom surface. If a free boundary condition on the bottom surface is imposed, the dislocation loop will disappear, leaving a geometric projection step of itself on the specimen bottom. Yet another is the surface glide (marked 5) which moves along the top surface confinedly. It is generated mostly in front of the abrasive and slides hanging from the top surface, moving out of a side boundary and coming from the opposite side boundary due to the periodic boundary condition. In addition, most of the dislocations are partial dislocations as they have lower self-energies than perfect dislocations.17 The number 6 denotes a fixed dislocation loop generated by composition and decomposition of the dislocations. This type of dislocation is immobile and could be only bypassed through cross slip so that it blocks the motion of other dislocations except for its destruction in high temperature and high pressure.

Comparing Fig. 3(b) to 3(a), many defects emerge not only under the groove surface gone through by the abrasive, but also under the unprocessed surface on both sides of the groove. The numbers of vacancy are more than 3(a) since the defects below the specimen surface increase significantly. And vacancies keep their position invariance, which turn into residual defects and largely alter the mechanical properties of the substrate after the polishing process. In addition, dislocation loops are generated continuously, with the bulk glide slipping downward to the bottom and the surface glide gliding along the specimen surface.

In Fig. 3(c) and 3(d), expect for the dislocation on machined surface, some dislocations can be seen on the unprocessed surface, marked with the number 6 and 7. The dislocations are parallel with the slip vectors [101] and [101] since the two directions are the easiest glide vectors in the single-crystal Cu (111) surface. The two directions make an angle of 45° with the polishing direction, reflecting as corresponding plastic deformation of the specimen. In addition, the groove surface in Fig. 3(d) implies the local breakdown of original perfect crystalline structure, revealing randomly distributed colours of atomic coordination numbers.

B. The effect of rotation velocity in polishing process

To study the effect of abrasive rotation velocity on ultra-precision polishing, simulations with rotation velocity of 0.915 r/ns (25 m/s) and 3.661 r/ns (100 m/s) have been also conducted. A special condition without rotation velocity is involved too. The force abrasive suffered is provided at the last of this part.

In a three-body contact sliding, specimen will experience different removal mechanism at different conditions. They are the no-wear, condensing, adhering, plowing and cutting mechanism. The no-wear means the specimen experiences pure elastic deformation. That the machined surface emerges remarkable condensing locally without material removal is referred to as the condensing. The adhering takes place when some surface atoms stick to the abrasive surface and move together with it. In general, no-wear, condensing and adhering just occur at very small polishing depth.18

In this simulation, 2.173 nm is chosen as the polishing depth. When the polishing depth is sufficiently large and self-rotation speed is small, cutting will happen.19 Fig. 4(a) and 4(b) present the state in which cutting state accents for the most part. It has features that the chips exist ahead of the diamond abrasive and its volume becomes large during the polishing process. At the same time, a groove is remained on the surface. According to the Fig. 4(a), when the specimen is machined by the abrasive without rotation velocity, it has good surface quality. What’s more, the end of the groove is flat (marked I). The specimen machined by the abrasive with the rotation velocity of 0.915 r/ns acquires the best surface quality in the four conditions. In addition, the volume of chips ahead
of the abrasive is smaller than the condition without rotation velocity, while some materials are pulled back to the end of the groove (marked II), as illustrated in Fig. 4(b). There is a state we called transition mechanism that both the states of plowing and cutting coexist. Shown in Fig. 4(c), which the rotation velocity is equal to the moving velocity of the abrasive, a certain amount of chips accumulates ahead of the diamond abrasive, with some materials distributing on the two flanks of the groove. With the increasing of rotation velocity, the amount of removal material reduces obviously and the materials squeezed out to the end of the groove grow in number (marked III). Fig. 4(d) shows the state in which plowing state plays the important role at the stage. Materials pile up on both sides of the grooves, which is the feature of the plowing state. As the abrasive rotation velocity is bigger than the moving velocity, the machined surface is rough. At this velocity, the volume of piled-up at the front of abrasive is the least but the amount of materials at the end of the groove is the biggest (marked IV). It is also observed that the order of atoms on the new generated surface and beneath the abrasive differs considerably from its original structure.

Fig. 5 shows views of dislocations and other lattice defects in the specimen with different rotation velocities at the instant of 11.75 nm polishing distance. Fig. 5(a) is the side view of specimen without rotation velocity. Fig. 5(b) to 5(d) show the side views of specimen with rotation velocity of 0.915 r/ns, 1.830 r/ns and 3.661 r/ns respectively. The fixed dislocation loop is marked I, the bulk dislocation loop is marked II and the surface dislocation loop is indicated III. It is clear that the specimen with rotation abrasive can generate more vacancy-related defects and dislocation loops. In addition, there are a lot of obvious differences between these simulations with different
rotation velocity, such as the number and distribution of defect. As the rotation velocity is smaller than moving velocity, the number and the volume of defect are getting larger with the increasing of the rotation velocity. Both the quantity and the volume of defect are the largest when the rotation velocity is equal to abrasive moving velocity. At this time, both the surface and bulk glide are generated actively. They are important because they mediate the plastic deformation. However, the two factors decrease with the rotation velocity keeping growth, demonstrated by the yellow dotting line in the Fig. 5.

In the MD simulation, the force is the interatomic forces between the specimen and the abrasive, and it is calculated as the summary of all the interaction forces that the copper specimen atoms act on the diamond abrasive atoms. The variation of the tangential force $F_t$ with different abrasive rotation velocity is shown in Fig. 6. The tangential force tends to be in a steady state after a big fluctuation at the initial stage. A larger tangential force is present for a lower abrasive rotation velocity.

FIG. 5. The dislocations distributed in the specimen at the instant of 11.75 nm polishing distance with rotation velocity of (a) 0 r/ns; (b) 0.915 r/ns; (c) 1.830 r/ns; (d) 3.661 r/ns.

FIG. 6. Polishing MD simulation force–displacement curves with various rotation velocity.
FIG. 7. A scheme of rotation angle in the simulation. The abrasive moves horizontally along X-direction and rotates about its rotation axis (parallel to X-Z plane). The rotation angle is between abrasive moving direction and rotation direction.

FIG. 8. Dislocation distribution in the specimen at the instant of 15.50 nm polishing distance with abrasive rotation angle of 45°. The moving velocity is 50 m/s, which is equal with the rotation velocity. (a) the right view on the groove; (b) the left view on the machining surface; (c) the front view of the interior defects inside the specimen; (d) the back view of the interior defects inside the specimen.

C. The effect of rotation direction in polishing process

In order to investigate the rotation direction effect on the surface profile and defect generations, we simulate four different rotation angles: 0°, 30°, 45°, and 90°, with 50 m/s moving velocity and 1.830 r/ns rotation velocity. The rotation angle is illustrated in Fig. 7, which is between the abrasive moving direction and rotation direction. The initial parameters are identical with the ones in Table I. At first, the simulation with the rotation angle of 45° at the instant of 15.50 nm polishing distance is discussed. This direction is particular since it coincides with one of the slip directions on the FCC (111) surface.

Fig. 8 are the snaps of internal atoms in the specimen, with the side view of (a), the top view of (b), the front view of (c) and the rear view of (d). It is obvious that the volume of the pile-up along the direction of [101] is more than rotation direction of [10]̅, and the profile of the groove differs the simulation in part B. In addition, the (010) is the surface of low Miller index which generally implies a lower surface energy to reconstruct. In the Fig. 8(b), pieces of pink region distribute on
FIG. 9. The morphology of the patterned surface at the instant of 15.50 nm polishing distance with different rotation direction. The rotation angle is (a) 0°; (b) 30°; (c) 45°; (d) 90°.

FIG. 10. The dislocations distributed in the specimen at the instant of 15.50 nm polishing distance with the abrasive rotation angle of (a) 0°; (b) 30°; (c) 45°; (d) 90°.

the unprocessed surface, included in the right area of the dotted line which is parallel with [101] direction. It will be shown that it is very different from the ones with the rotation angle of 0°, 30° and 90°. This result provides evidence that the rotation direction can make an effect on the morphology of the patterned surface. In accordance with the pile-up, the volume of defects under the surface in the front view is bigger than the one in the rear view. During the process of polishing, the interaction of dislocation in [101] direction produces dislocation frequently, resulted in more volume of defects under the specimen surface. Besides, vacancies mostly appear below the groove rather than the place ahead of the abrasive.

The morphology of the patterned surface is diverse in different rotation angles conditions, shown in Fig. 9. It can be seen that when the abrasive rotates along the moving direction, no pink region appears. With the angle increasing to 45°, the distribution of the pink region enlarges and reaches the maximum. Then the pink region diminishes with the larger angles. Compared with these four
machined surface, the simulation with 45° angle acquires the best surface quality after polishing process. Moreover, the distribution of piled-up is quite different with each other, marked by the yellow dotted line.

The views of dislocations and other lattice defects in the specimen at four different angles of 0°, 30°, 45°, and 90° are given by Fig. 10. All of them are processing at 15.50 nm distance. The amount of the piled-up becomes bigger with the rotation angle increasing. However, the volume of dislocation reaches biggest at 45° angle yet diminishes with the angle rising sequentially (marked yellow dotted line). Comparing with the process of the four simulations, the simulation of 45° rotation angle that the abrasive rotation direction is one of the slip directions on FCC (111) surface generates dislocation loop most actively and generates most vacancy. It is because that the rotation direction belonged to (111) [¯10¯1] slip system can activate more dislocation than others as a result.

The variation of the tangential force $F_x$ with different abrasive rotation angle is shown in Fig. 11. The tangential force does not appear to be much different at various rotation angles. It reveals that the rotation angle of the abrasive has little effect on the tangential force.

IV. CONCLUSION

The present investigation has shown that how the polishing abrasive rotation velocity and direction affect the specimen surface morphology and internal dislocation at atomic level of single-crystal copper on the (010) surface by molecular dynamics simulation. The combination of Morse and EAM potential energy function are used to describe the interactions of copper/diamond and copper/copper, respectively. The polishing simulation is carried out with the abrasive moving velocity of 50 m/s. Some interesting conclusions are summarized as following,

(1) With increasing of rotation velocity, the deformation of single-crystal copper specimen falls from cutting to plowing regimes.

(2) The rotation velocity directly affects the surface quality and the distribution of interior defects. When the rotation velocity is smaller than the moving velocity such as $w = 0.915 \text{ r/} \text{s}$, the specimen has good surface quality. While the abrasive rotation velocity is equal with moving velocity, the specimen generates the most dislocation. As the abrasive rotation velocity is bigger than the moving velocity, the machined surface quality will deteriorate.

(3) The rotation direction has also been shown to play an important role in the surface profile as well as the formation of interior defects. The patterned surface is more favoured to be faced when the rotation angle is 45°. In this situation, the rotation direction is special because the
[101] coincides with one of the slip directions on the (111) surface of FCC. Moreover, the machined surface quality is the best and the dislocation generated is the most.

ACKNOWLEDGMENTS

This research is funded by the National Natural Science Foundation of China (grant no. 50905073, 51275198, 51105163), Special Projects for Development of National Major Scientific Instruments and Equipments (grant no. 2012YQ030075), National Hi-tech Research and Development Program of China (863 Program) (grant no. 2012AA041206), Key Projects of Science and Technology Development Plan of Jilin Province (grant no. 20110307) and Graduate Innovation Fund of Jilin University (grant no.20121084).

5 Y. Ye, R. Biswas, J. R. Morris, A. Bastawros, and A. Chandra, Simulation of Nanoscale Polishing of Copper with Molecular Dynamics. Materials Research Society, 2002