An atomistic investigation of nanometric cutting process using a multi-tip single crystal diamond tool

Zhen Tong, Xichun Luo
School of Computing & Engineering, University of Huddersfield, Huddersfield HD3 3RR, UK

Abstract

In recent years great efforts are being made for the design and fabrication of periodic nanostructures used in emerging nano-products, such as plasmonic lens, nano-grating and high density hard disk etc. In our previous research work, a deterministic fabrication approach to cost-effectively manufacturing nano gratings over large area has been developed through single point diamond turning by using a multi-tip nano-scale single crystal diamond tool fabricated by FIB (Focus Ion Beam). However, the machining mechanism and technical limits of this approach i.e. the minimum dimension of nanostructures that can be obtained has not known yet. Due to the limitation of real-time detect equipment as well as the high research cost, it is difficult to obtain a quick answer through experimental work. On the other hand molecular dynamics (MD) simulation provides a cost-effective solution for this problem.
Based on the merit offered by the large-scale molecular dynamics simulation method and new progresses made in high performance computing (HPC) technique, this paper proposes a new MD model for nanometric cutting process using a multi-tip single crystal diamond (SCD) tools to machine single crystal copper workpieces. By using centrosymmetry parameter (CSP) method and combining it with the dislocation nucleation and propagation theory, the machining mechanism and generation of nanostructures are studied through MD simulation. In order to reveal the dependence of the depth of cut on the integrality of generated nanostructures, a number of MD simulations have been

carried out under depth of cut varying from 0.5, 1.0, 1.5, 2.0, and 3.0nm. The simulation results show that the depth of cut has significant influence on the integrality of the machined nanostructured surfaces and cutting force. A concept of maximum depth of cut to obtain high precision nanostructured surfaces in a single cutting pass is proposed based on analysis of the dimensional accuracy of the integrality machined nanostructures. In all simulations the cutting forces fluctuate around a constant value after chip formation.

1 Introduction

Nowadays, high precision micro/nano products have gained great demands in the fields of medical, biological and clean energies, etc.. Innovative machining methods are continually developed to meet the requirements on high precision and low cost for manufacturing these products. Using multi-tip single crystal diamond tools prepared by FIB in nanometric cutting is a newly developed method for cost-effective manufacturing of functional micro/nano structured surfaces on these micro- or nano-products [1-3]. It is noted that both the tools and the machined structures are in the range of sub-microns or even nano-meters. The main challenge in applying this novel technique is to develop a fundamental understanding of the mechanisms of material removal and formation of micro/nano structures during the machining process.

Due to the limitation of real-time detect equipment as well as the high research cost, it is difficult to obtain a quick answer through experimental work. In recent decades molecular dynamics simulation method has been extensively used by researchers to study the nanometric cutting process. Maekawa et al. carried out MD simulation to study the role of friction and tool wear in nano-scale machining [4]. Kim and his co-workers performed MD simulations to study the nano-indentation and scratching process. The study suggested that the nucleation of the dislocation plays more important roles in determining the abrupt drop during stick-slip than subsequent propagation of partial dislocations [5]. Yan et al. simulated the multiple scratching processes and investigated the effects of the feed rate on the deformation of the machined surface, scratching depth, and scratching forces [6]. The influence of tool geometry on scratching process has also been explored by Yan et al. which showed that four states exist between AFM pin tool and workpiece surface [7]. These studies confirm the feasibility of using MD simulation method to study nanometric cutting process. However, these studies are focused on nanometric cutting using single tip diamond tools.

Due to the fact that single cutting tool has ignored the specific geometry of multi-tip tool and cannot give details about the generation of structure in nano-scale, it is therefore required to develop a new MD model to study the nanometric cutting process using multi-tip SCD tools to machine Cu workpieces. The generation mechanism of nanostructures will be different from that using a single tip diamond tool. This paper will carry out MD simulation to study the mechanisms of chip formation and generation of nanostructures during mulit-tip SCD tool nanometric cutting process and quantify the

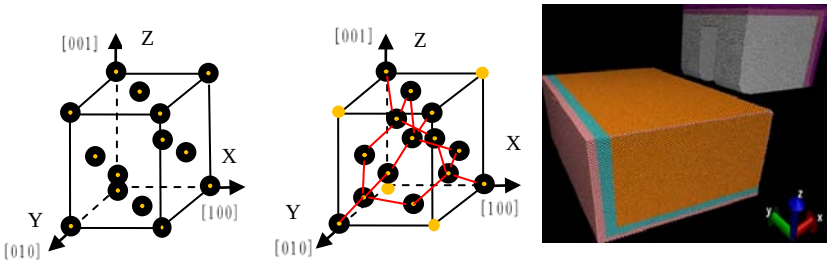
influence of depth of cut on the machined nanostructured surface.

2 Models and Simulation Methods

2.1 Multi-tip tool nano-cutting model

As shown in Fig.1 (a) and (b) the FCC (Face-Centred Cubic) crystalline lattice and diamond crystalline lattice are aligned for the single crystal copper workpiece and diamond tools respectively. The cutting tool is applied along the minus x direction at a constant speed of 200m/s. Free boundary conditions are enforced in the x, y and z directions.

To reduce the computational time a two -tip SCD tool (as shown in Fig. 1(c),) with a pitch of $10a$ (a = 3.567 Å) is employed in this paper to study the nanometric cutting process. The tool rake rake angle is set as 0°. The workpiece of dimension of $50a_0 \times 80a_0 \times 40a_0$ (a_0 = 3.615 Å) is utilized, and consists thicknesses of $2a_0$ and $3a_0$ for boundary layer and thermostat layer, respectively.



(a) FCC (b) Diamond crystal (c) Multi-tip tool cutting model

Figure 1: Model of MD cutting simulation

2.2 Simulation parameters

The interactions between Cu-Cu and C-C atoms are described by the embedded atom method (EAM) potential [8] and Tersoff potential [9], respectively. Morse potential function is selected to descript the interaction between Cu-C which has been widely used in MD simulations of nanometric cutting of Cu [6, 7, 10, 11]. The time step is set as 1 fs (10^{-15}s) and 90,000 steps are carried out in the relaxation process for fully free relaxation of the system. All simulations are run at a constant temperature of 293K and the system is controlled with NVE ensemble.

In order to obtain the cutting forces information, the virial formula for stress [12] is used to calculate the stress tensor for the atomistic system,

$$\sigma_{\alpha\beta} = -\frac{1}{V}\left(\sum_i \frac{p_\alpha^i p_\beta^j}{m^i} + \sum_i \sum_{j>1} r_\alpha^{ij} f_\beta^{ij}\right) \quad (1)$$

where the first term on the right hand is the kinetic contribution of atom *i* with mass m_i and momentum P^i_a, and the second term is the microscopic virial potential stress. The stress for the atomistic system is defined as the volume average of per-atom tensor.

2.3 CSP for post-processing

The visualization of the variation of atomistic configurations during the cutting process is realized by VMD (Visual Molecular Dynamics) software. The paper employs centro symmetry parameter P, which has been proven to be effective for FCC crystals [13] to view the evolution of defects in atomistic level,

$$p_i = \sum_{i=1}^{6} \left| \mathbf{R}_i + \mathbf{R}_{i+6} \right|^2 \quad (2)$$

where $\mathbf{R}_i$ and $\mathbf{R}_{i+6}$ are the vectors corresponding to the six pairs of opposite nearest atoms. The centro symmetry parameter P increases from 0 for perfect FCC lattice to positive values for defects and for atoms close to free surfaces. In the case of single crystal copper, the default value of P_i corresponding to those atomic defect structures and its represent color are indicated in Table 1.

Table 1: The default value of atomic defects structure in CSP

Lattice Structure	P_i	Represent Atoms Color
Ideal FCC structure	$P < 3$	Yellow
Partial dislocation	$3 < P < 5$	Cyan
Stacking fault	$5 < P < 8$	Blue
Surface atoms	$8 < P < 21.5$	Orange
Surface edge atoms	$P > 21.5$	Pink

3 Results and discussions

3.1 Machining mechanism

Fig. 2 shows the snapshots of nano-cutting process as well as the atomistic dislocation evolutions of workpiece with a depth of cut of 1.0 nm used. Each

workpiece atom is colored by CSP value according to Table 1. It should be pointed out that the isolated atoms with green color distributed inside the workpiece are not lattice defects. Those atoms having CSP above three result from the thermal vibration of atoms at finite temperature [10].
It can be seen from Fig. 2(a) that some dislocations initiate under the tool-workpiece contact region due to the compress stress induced by initial impact of tool tips. With the increase of the cutting distance, more and more dislocations nucleated and propagate along the (111) crystal slip planes systems. As shown in Fig. 2(b), the atoms accumulate and pile up in front of the tool rake face and form two independent initial chips. However, unlike single tip cutting, in multi-tip cutting process the dislocations generated under the tool tips tend to interact with each other and further form the surface of nano-structure between two adjacent tool tips, as shown by Fig. 2(c). A nanostructure with 1nm in height and 3.5nm in width is generated by this multi-tip SCD tool after a cutting distance of 6.4nm.

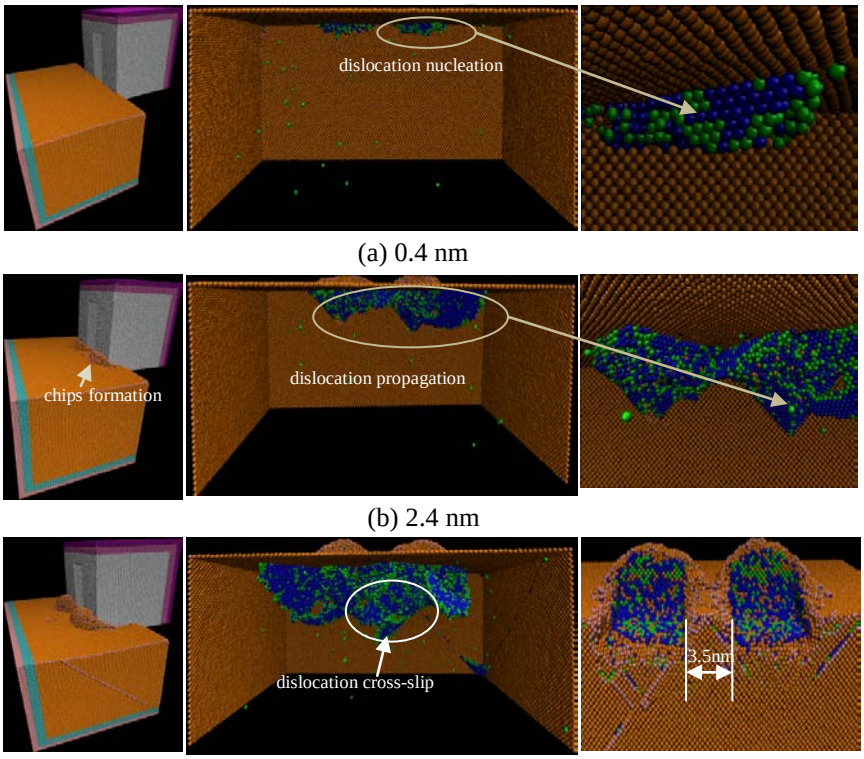


Figure 2: Snapshots of cutting process and dislocation evolution of workpiece at cutting distance of: (a) 0.4 nm, (b) 2.4 nm, and (c) 6.4 nm when a depth of cut is 1 nm.

The definition of cutting force and cutting force-displacement curves in the x, y and z directions during cutting process are shown in Fig. 3. The cutting forces

are obtained by summing the atomic forces of tool atoms. It can been clearly seen that both the tangential cutting force f_x and normal cutting force f_z fluctuate around a constant value after the cutting distance reaches 2.4nm. Correlating with the snapshot of MD simulation shown in Fig. 2(b), the simulations results indicate that the cutting forces tend to be in a steady state after the initial formation of chips. The main reason accounting for this phenomenon is that the plastic deformation of workpiece is dominated by the dislocation nucleation at initial cutting stage, the tool-workpiece contact area increases while the workpiece atoms pile up in front of the tool rake face to from chips. But the contact area is fixed at steady cutting stage. The plastic deformations are mostly dominated by the formation and movement of dislocations which lead to the release of the accumulated strain energy and further cause the temporary drop of the tangential cutting force and the normal cutting force [11]. However, the cutting force in the y direction has an average value near zero during the cutting process because of the balanced forces contributing from the two cutting tips.

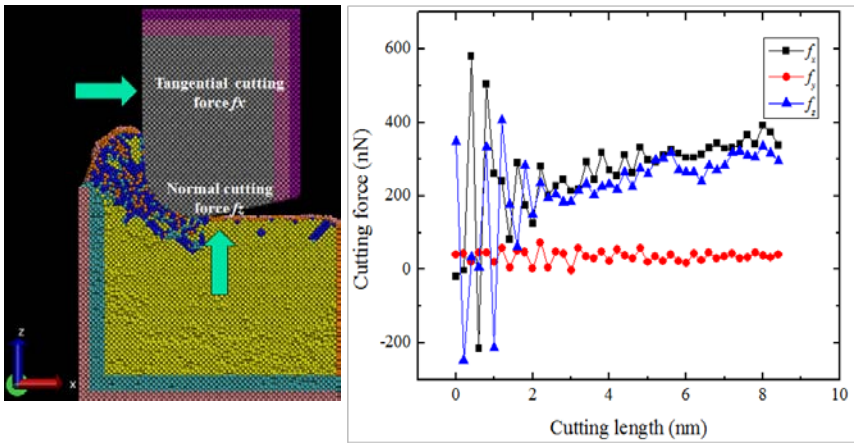


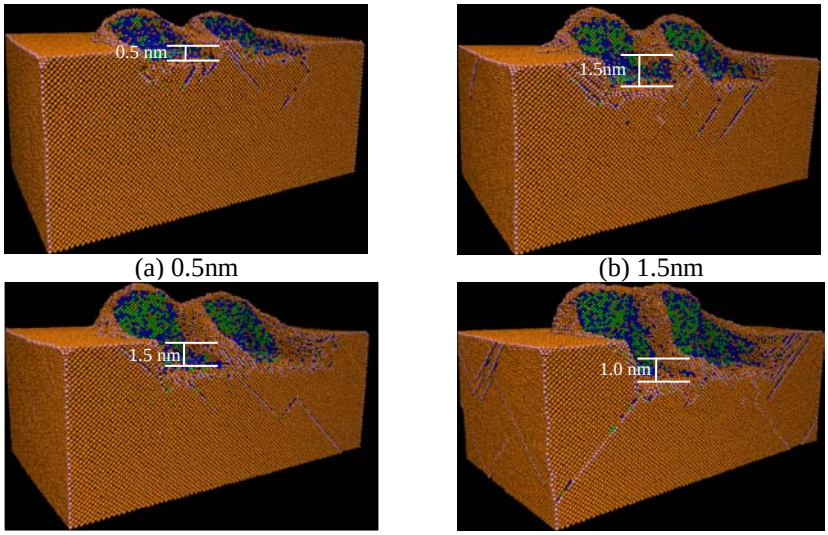
Figure 3: The definition of cutting force and force-displacement curves at the depth of cut of 1nm.

3.2 Effect of depth of cut

3.2.1 Machined nano-structure integrality

In order to study the effect of depth of cut on the generation of nanostructures, a series of simulation have been carried out with the depth of cut varying from 0.5, 1, 1.5, 2, and 3nm. Fig. 4 shows the formed nanostructured surface at the cutting distance of 8nm. It can be found that as the depth of cut increases, more workpiece atoms pile around the tool and the chips becomes larger. It should be

note that a fine nanostructure can be generated by using this two-tip SCD tools when the depth of cut is less than 1.5nm (as shown in Fig. 4(a)-(b) and Fig. 2(c)). When a depth of cut of 2nm is used the dimension of the machined nanostructure is not exactly the same as the design dimension. When a depth of cut of 3nm is used the height of the generated nanostructure is nearly 1nm, which is only 35% of the design dimension.
These simulation results indicate that there exists a cutting limitation when using multi-tip SCD tools to machine high precision nanostructures. For this two-tip model the limit of depth of cut in a single pass is around 1.5 nm.



(a) 0.5nm (b) 1.5nm

(c) 2.0nm (d) 3.0nm

Figure 4: Snapshots of machined nanostructures under different depth of cut.

3.2.2 Variation of cutting forces

The variations of cutting forces for different cutting depth are shown in Fig 5. It can be seen from Fig. 5 that the cutting forces in all the cutting models go to the steady states. The larger the depth of cut, the less the cutting distance needed for the cutting to reach the steady state. The average tangential cutting forces and normal cutting forces at the steady cutting state for the cutting distance of 6–8nm are also calculated. As shown in Fig. 6, both the tangential cutting forces and the normal cutting forces are increased with the increase of depth of cut. This is mainly due to the fact that the energy for breaking the Cu-Cu bonds is somehow proportional to the depth of cut. In addition, the chip volume which reflected the tool-workpiece contacts area is larger when using a large depth of cut.

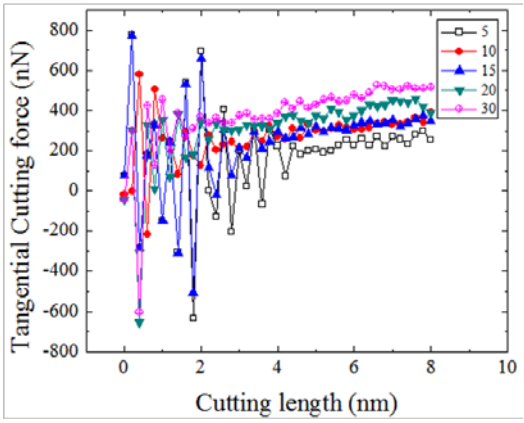


Figure 5: Force-displacement curves in the cutting process.

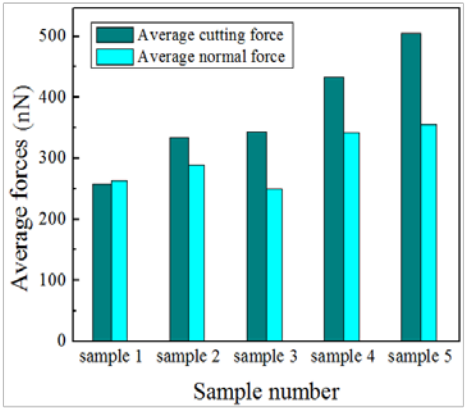


Figure 6: The average cutting forces under different depths of cut.

4 Conclusions

In this work, a new MD model is developed to study nanometric cutting of single crystal copper when using a two-tip diamond tool. Based on the simulation results, conclusions are drawn as follows:

(1) Unlike single tip cutting, in multi-tips cutting process the dislocations generated under the tool tips tend to interact with each other and further form the nanostructures between the tool tips.

(2) The cutting forces tend to be in a steady state after the initial formation of chips. At initial cutting stage the plastic deformation of workpiece was dominated by the dislocation nucleation and then by the propagation of dislocations at steady cutting stage. The cut force in the y direction has an

average value near zero during the cutting process because of the balanced forces contributing from the two cutting tips.

(3) The cutting depth has significant influence on the cutting force and integrality of the machined nanostructures. The larger the depth of cut, the larger the cutting forces and the less the cutting distance needed for the cutting to reach the steady state. Maximum depth of cut to be used to obtain high precision nanostructured surfaces in a single pass is around 1.5 nm when using for a two-tip diamond tool.

5 Acknowledgments

The authors would like to acknowledge the technical supports from the HPC team at the University of Huddersfield and the use of Huddersfield Queensgate Grid for performing MD simulations in this study.

6 References

[1] D. P. Adamsa, M. J. Vasile, A.S.M. Krishnan, “Microgrooving and microthreading tools for fabricating curvilinear features”. Precision Engineering, 2000, 24: 347–356.

[2] Xu, Z., et al., “Fabrication of micro DOE using micro tools shaped with focused ion beam”, Optics Express, 2010, 18 (8): 8025-8032.

[3] J Sun, X Luo, W Chang, M J Ritchie, J Chien and A Lee. “Fabrication of periodic nanostructures by single-point diamond turning with focused ion beam built tool tips”. J. Micromech. Microeng. 2012, 22: 115014.

[4] K Maekawa, A Itoh. “Friction and tool wear in nano-scale machining—a molecular dynamics approach”. Wear, 1995, 188 (1-2): 115–122.

[5] MH Cho, SJ Kim, DS Lim, H Jang. “Atomic scale stick-slip caused by dislocation nucleation and propagation during scratching of a Cu substrate with a nanoindenter: a molecular dynamics simulation”. Wear, 2005, 259(7-12): 1392–1399.

[6] Y Yan, T Sun, S Dong. “Study on effects of the feed on AFM-based nano-scratching process using MD simulation”. Computational materials science, 2007, 40 (1): 1–5.

[7] Y Yan, T. Sun, S Dong, XC Luo, and YC Liang, “Molecular dynamics simulation of processing using AFM pin tool”. Applied surface science, 2006, 252 (20): 7523–7531.

[8] S. M. Foiles, M. I. Baskes and M. S. Daw. “Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys”. Phys. Rev. B., 1986, 33(12): 7983-7991.

[9] Tersoff J, “New empirical approach for the structure and energy of covalent systems”. Phys Rev B, Condens Matter. 1988, 37(12): 6991-7000.

[10] Q. X. Pei, C. Lu, H. P. Lee, Y. W. Zhang, “Study of materials deformation in nanometric cutting by large-scale molecular dynamics simulations”, Nanoscale Res. Lett. 2009, 4: 444–451.

[11] P. Z. Zhu, Y. Z. Hu, T. B. Ma, and H. Wang. “Study of AFM-based nanometric cutting process using molecular dynamics”. Applied Surface Science, 2010, 256 (23): 7160–7165.
[12] M.P. Allen and D. J. Tildesley. “Comput. Simulation of Liquids”. Oxford University Press. 1987.
[13] Kelchner C. L., Plimpton S. J. and Hamilton J. C., “Dislocation nucleation and defect structure during surface indentation”. Phys Rev. B., 1998, 33(17): 11085-11088.