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# Subsurface defects structural evolution in nano-cutting of single crystal copper

Quanlong Wang [a,b], Qingshun Bai [a], Jiaxuan Chen [b,*], Yazhou Sun [a], Yongbo Guo [b], Yingchun Liang [a]

[a] School of Mechatronics Engineering, Harbin Institute of Technology, Harbin 150001, People's Republic of China
[b] Center for Precision Engineering, Harbin Institute of Technology, Harbin 150001, People's Republic of China

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ABSTRACT

In this work, molecular dynamics simulation is performed to study the subsurface defects structural distribution and its evolution during nano-cutting process of single crystal copper. The formation mechanism of chip and machined surface is interviewed by analyzing the dislocation evolution and atomic migration. The centro-symmetry parameter and spherical harmonics method are adopted to characterize the distribution and evolution of the subsurface defect structures and local atomic structures. The results show that stacking faults, dislocation loops, "V-shaped" dislocation loops, and plenty of point defects are formed during the machined surface being formed in shear-slip zone. In subsurface damage layers, stair-rod dislocation, stacking fault tetrahedra, atomic cluster defect, and vacancy defect are formed. And the formation mechanism of stair-rod dislocation is investigated by atomic-scale structure evolution. The local atomic structures of subsurface defects are icosahedrons, hexagonal close packed, body-centered cubic, and defect face center cubic, and the variations of local atomic structures are investigated.



## 1. Background

In nano-cutting, the mechanical property and lifetime of machined components are governed not only solely by their sizes and shapes, but also critically by the characteristics of surface and subsurface in the machined workpiece. The subsurface characteristics have great influence on machining precision and surface roughness, even affecting the mechanical performance and lifetime of machined components [1–3]. Residual stress release, as well as subsurface defect evolution, caused by the acute shearing interaction between workpiece and cutting tool during machining process, can generate the permanent deformation of the material, forming subsurface damage (SSD) layer underneath the machined surface. Further, the formation of the SSD layer has more significant effect on the machining performance and surface finish quality of nanoscale components. For instance, subsurface residual stress release and damage restoration will affect the machining accuracy and surface quality of micro and nano artifacts [4]. As for the ultra-precision optical crystal components, the SSD layer affects the light transmittance that can make the components absorbing laser energy, which result in the thermal damage of the optical components, even fail in the function [5,6]. The SSD layer basically is caused by the following three factors: foreign body embedment caused by chemical or physical adsorption [7], stress injury caused by residual stress [8], and the variation of material local crystal structure [9]. The observation for the subsurface damage layer in nano-cutting is extremely difficult to be verified by using experimental method. However, the atomistic computer simulation provides an effective and promising method to examine the subsurface defect and study its evolution mechanism.

The pioneering studies, in nano-cutting process, focused on cutting heat distribution, dislocation emission, and defect evolution. Zimmerman [10] analyzed the dislocation emission in nano indentation process by using the slip vector. Zhu [11] studied the formation mechanism of stacking-fault tetrahedra occurring in the deformation of single crystal gold nanowires. Inamura [12] researched the micro mechanisms of chip formation and slip deformation for crystalline material, and pointed out that the chip formation is mainly induced by the macroscopic shear-slip deformation which is caused by the external force in nano-cutting process. Pei [13,14] performed a series of large-scale 3-D MD simulations to study the effect of cutting parameter on material deformation, dislocation motion, and cutting force in nano-cutting process. It was found that the boundary effect became quite small when the workpiece size was 40 nm. Luo [15] demonstrated the shape transferability by using nanoscale multi-tip diamond tools in

* Corresponding author. Tel.: +86 451 86413840; fax: +86 451 86415244.
*E-mail address:* wangquanlong0@hit.edu.cn (J. Chen).

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the diamond turning for scale-up manufacturing of nanostructures. Kim [16] studied the plastic material deformation in machining with a round cutting edge by using MD simulation and analyzed the effects of cutting parameters. Based on the change of atomic potential energy, Zhang [17,18] realized the quantitative characterization of subsurface damage layer's depth in nano-cutting process of single crystal copper. Due to the limitation of analytical method, the plastic deformation, dislocation motion, and cutting force are concerned in the previous researches with macro perspective. However, little literature can be found for investigating the formation and transformation mechanisms of subsurface microdefect structure and local atomic structure, which are essential to the machining precision and surface finish.

Recently, some theoretical and experimental methods have been used to analyze the crystal structure defect in the crystallization processes of amorphous materials. Ackland [19] adopted the common-neighbor analysis (CNA) method to describe the local crystal structure of different crystalline materials. Zhao [20,21] described the kinetic details of the nucleation in supercooled liquid metals by means of the pair analysis (PA) method in MD simulation. It was shown that plenty of atoms nucleated in crystallization processes, which are icosahedra atomic in structure. Luo [22] characterized the icosahedral short-range order in amorphous solids using local environment probes, including normalized common neighbor pairs (CNP), and radial distribution functions (RDF). Hirata [23] studied geometric frustration of icosahedra in metallic glasses with the angstrom-beam electron diffraction (ABED) method. According to the reverse Monte Carlo (RMC) method, Sheng [24] carried on the extended X-ray absorption fine structure (EXAFS) experiments and obtained 3-D atomic configuration. Based on the model established by RMC, *ab initio* molecular dynamics simulations method was used to analyze the atomic packing and short-to-medium range order in metallic glasses. Rabkin [25] performed the uniaxial compression of cylindrical gold nanopillars and studied the structural change and plastic deformation mechanism by using spherical harmonic method(SHM). Cha [26] based on a series of MD simulations of single asperity contact and deformation, and then analyzed the dislocation evolution and the variation of local atomic structure by using the local bond order parameter and spherical harmonic method (SHM-Q6).

In this paper, a series of simulations on nano-cutting process of single crystal copper are implemented by using MD method. Firstly, the chip and machined surface formation mechanism are investigated by analyzing the dislocation-defect structure evolution and atomic migration. Secondly, the CSP and SHM are adopted to characterize the distribution and evolution of the subsurface defect structure and local atomic structure. Thirdly, the formation of stacking fault tetrahedra (SFT) and stair-rod dislocation are elucidated from atomic-scale evolution, which exist in the subsurface of workpiece after nano-cutting. Finally, the research was concluded in terms of the novel results obtained from the subsurface defects structural evolution in nano-cutting simulation. The research may give a distinct understanding for the machining mechanism and subsurface defective evolution of single crystal copper, and underpin the scientific development of nano-cutting.

## 2. Methods

### 2.1. Simulation model

The large-scale molecular dynamics simulation model adopted in this paper is shown as Fig. 1. The workpiece and tool are divided into Newton layer, temperature layer and boundary layer. In order to reduce the size effect, periodic boundary condition is adopted at [001] direction of the workpiece. The cutting tool is put 3 nm top right of the workpiece to avoid the interaction between cutting tool and workpiece at the initial state. At the beginning of the simulation, the conjugate gradient method is used to perform energy minimization to eliminate the initial unreasonable factors during modeling. And then the system is relaxed 100 picoseconds using the Nosé–Hoover thermostat which makes the system initial temperature up to 285 K. Thereafter, the cutting tool moves along [100] direction at the speed of 50 m/s to start the nano-cutting process. The maximum cutting distance is 38 nm. The others conditions and parameters related to the simulation are listed in Table 1.

### 2.2. Analysis methods

The centro-symmetry parameter (CSP) is adopted to analyze dislocation nucleation and defect evolution in the workpiece. The CSP of each atom is shown as Eq. 1 [27]:

$$CSP = \sum_{i=1,6} \left| R_i + R_{i+6} \right|^2 \quad (1)$$

where $R_i$ is the same length neighboring atoms and $R_{i+6}$ is the opposite direction neighbor atoms. The CSP values of FCC crystal, partial dislocation, stacking fault, and surface atoms are 0, 2.1, 8.3, and 24.9, respectively.

The CSP method can be used to identify the dislocation nucleation and defect evolution, but cannot be used to explain the local atomic crystal structure state of workpiece atoms. However, the spherical harmonics method (SHM) [28] can characterize the local atomic structure state by analyzing the relationship of relative position between an atom and its neighboring atoms. For the crystals materials with same atomic structure, the spherical harmonic $Q_6$ value is identical, but for the crystals materials with different atomic structure, the spherical harmonic $Q_6$ values are an imparity.

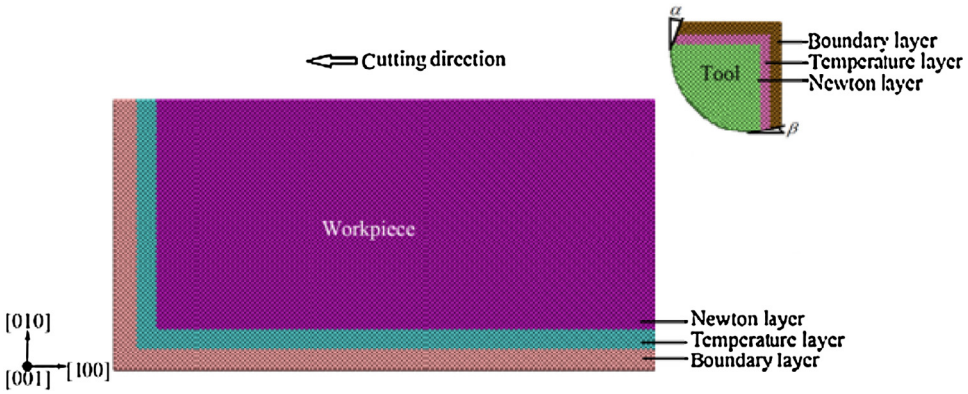


**Fig. 1.** The MD simulation model of nano-cutting process.