



# Influence of double-tip scratch and single-tip scratch on nano-scratching process via molecular dynamics simulation<sup>☆</sup>

Peng Zhang<sup>a</sup>, Hongwei Zhao<sup>a,\*</sup>, Chengli Shi<sup>a</sup>, Lin Zhang<sup>a</sup>, Hu Huang<sup>a</sup>, Luquan Ren<sup>b</sup>

<sup>a</sup> College of Mechanical Science and Engineering, Jilin University, Changchun 130025, China

<sup>b</sup> Key Laboratory of Bionic Engineering Ministry of Education, Jilin University, Changchun 130025, China



## ARTICLE INFO

### Article history:

Received 2 March 2013

Received in revised form 13 May 2013

Accepted 13 May 2013

Available online 18 May 2013

### Keywords:

Molecular dynamics

Nano-scratch

Double-tip

Single-tip

Mono-crystalline copper

## ABSTRACT

A three-dimensional molecular dynamics model was proposed to study the influences of scratch feed, depth and crystal orientation on the shape and surface quality of the scratched groove during nano-scratching process. In this paper, comparisons were made between the results of double tips simultaneously scratching the surface and those of single tip successively scratching the surface with the same scratch feed, depth and crystal orientation. EAM potential was used to model the interaction of copper atoms, and Morse potential was used to model the interaction between copper and carbon atoms. The residual profiles of scratched grooves and scratching forces were recorded during the simulations. Simulational results show that when single tip scratches the surface at an extremely small feed, the second time scratch significantly influences the previous groove. The second time scratch has a significant influence on the previous groove by increasing scratch depth. Compared with scratching along crystal orientation [1 0 0], scratching along crystal orientation [0 1 1] and [1 1 1] are easy to obtain two parallel grooves. However, when double tips simultaneously scratch the surface regardless of scratch feed, depth and crystal orientation, two parallel grooves are always obtained. Thus, in order to obtain scratched grooves of high quality, it is quite beneficial to design and machine multiple-tip tools.

© 2013 The Authors. Published by Elsevier B.V. All rights reserved.

## 1. Introduction

With the advancement of atomic force microscope (AFM) techniques, AFM can exert a very small vertical force on the contact area between AFM probe and material's surface, which can lead to material removal at macro/nano scale [1–4]. So it is available to obtain high surface finish quality and fabricate micro/nano components/devices in micro-electro-mechanical system (MEMS) and nano-electro-mechanical system (NEMS) [5,6]. At atomic scale, the traditional continuous mechanics theory cannot be applied to analyze nano-scratching process, and it is very difficult to experimentally reach a very small feed at nanoscale. Since the MD simulation method can reach such feed and trace the atomic structure behavior in the whole process, it provides a powerful and effective approach to investigate nano-scratching process [7,8].

Nowadays, many AFM-based nano-scratch studies have been carried out to investigate the deformation mechanism during

nano-scratching process [9–12]. Fang et al. carried out scratch experiments and MD analysis to study the feed on the machining characterization of the nano-lithography process [11,13]. They pointed out that scribing feed had a significant influence on surface roughness. Conclusion could be drawn that larger load produced deeper grooves and rougher surface, and the required surface could be obtained through changing scribing feed. Yan et al. investigated the effects of scratching velocity and tip shape on AFM nano-scratching processes of copper and silicon employing MD simulation [6,14]. It is found that lower scratching velocity resulted in less scratching resistance and dislocations glide along a more accurate beeline at an angle of 45° toward the scratching direction. Besides, the blunt indenter results in a bigger friction coefficient than the sharp indenter.

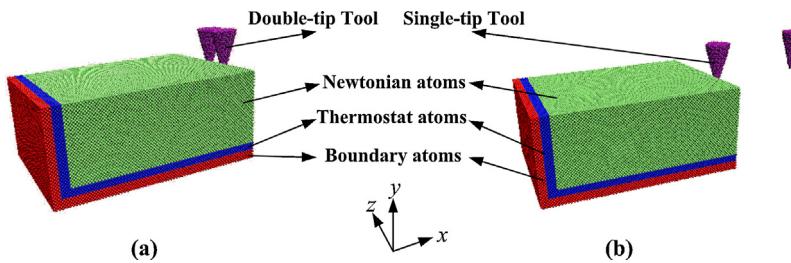
They also investigated the effects of the feed on the material removal mechanism of AFM-based nano-scratching process [15]. They found that the feed had significant effects on the cut depth, surface quality of the machined surface, and the smallest feed of obtaining parallel grooves was received.

Compared with the achievements in MD studies of nano-scratch simulation of mono-crystalline material, few papers have studied how to obtain parallel grooves with smaller feed. It is of great significance for precision machining. Therefore, a new processing method of multiple-tip scratch which is expected to obtain parallel grooves with smaller feed in micro/nano-machining is proposed. In this paper, MD simulations of double-tip and single-tip scratch at

<sup>☆</sup> This is an open-access article distributed under the terms of the Creative Commons Attribution-NonCommercial-No Derivative Works License, which permits non-commercial use, distribution, and reproduction in any medium, provided the original author and source are credited.

\* Corresponding author. Tel.: +86 431 85094594; fax: +86 431 85094594.

E-mail address: [hwzhao@jlu.edu.cn](mailto:hwzhao@jlu.edu.cn) (H. Zhao).



**Fig. 1.** (a) MD simulation model with double-tip simultaneously scratching the specimen's surface; (b) MD simulation model with single-tip successively scratching the specimen's surface.

different scratch feeds, depths and crystal orientations were performed, and the results of two models were compared to assess which were beneficial to obtain scratched surface of high quality.

## 2. Simulation methodology

### 2.1. Simulation model

The MD simulation model consists of two parts, a monocrystalline copper specimen and a diamond tip, as shown in Fig. 1. The AFM diamond tip used in current simulation has a configuration of cone shape with a tip angle of 30°, which is constructed with perfect diamond atomic lattice, consisting of 4944 carbon atoms. The apex of the cone is truncated by one atom. Due to the evidently higher hardness of diamond than copper, the diamond tip is treated as a rigid body during the process of scratching the specimen's surface.

The size of the specimen is  $70a \times 30a \times 50a$  along the X, Y and Z directions, consisting of 420,000 copper atoms, where  $a$  represents the lattice constant of copper (0.3615 nm). The copper atoms in the specimen are categorized into three kinds of atoms, namely: Newtonian atoms, Thermostat atoms and Boundary atoms, respectively. Boundary atoms are fixed in space to reduce the edge effects and maintain the proper symmetry of the lattice. Thermostat atoms are used to ensure reasonable outward heat conduction away from the machined zone. The motion of Thermostat atoms and Newtonian atoms is governed by Newton's second law. In order to reduce the effect of simulation scale, periodic boundary condition is set along Z direction in MD simulation model [16]. Moreover, the cutting speed is set at 100 m/s to reduce the computational time and memory requirements.

The MD simulations are conducted with the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) developed by Plimpton [17,18].

Fig. 2 shows the simulation procedure of two scratching tests. For convenience, the simulation model shown in Fig. 2(a) and (b) is named 'Simulation A' and 'Simulation B', respectively. In Simulation A, the double-tip tool simultaneously scratches the specimen's surface along X-axis. In Simulation B, firstly, the first tool scratches the specimen's surface along X-axis and the second tool moves forward on the X-Z plane. Then the first tool leaves the specimen upwards along Y-axis. Thirdly, the second tool feeds in the Z-axis and then scratches the second groove along X-axis.

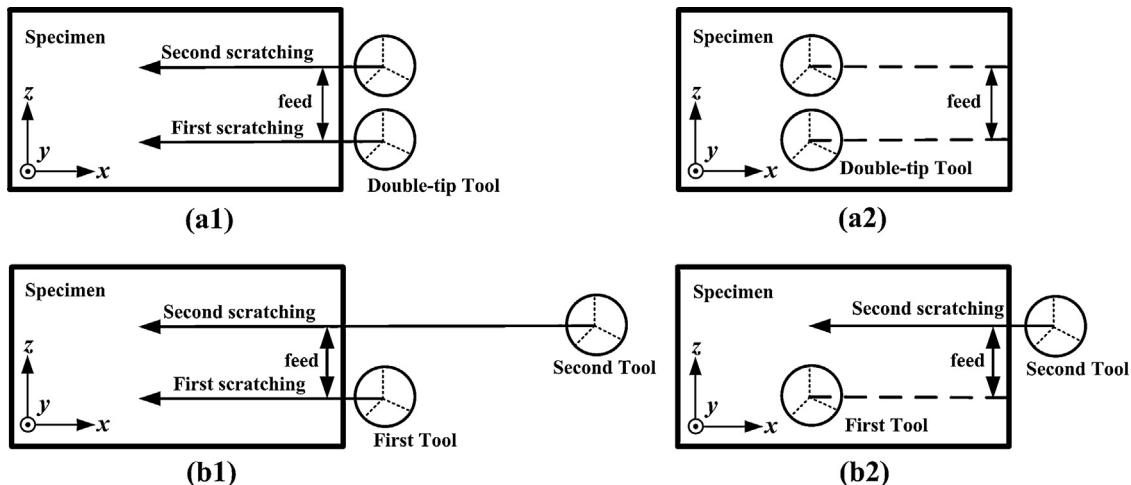
### 2.2. Selection of potential energy function

There are three different atomic interactions between each other: (1) the interaction between copper atoms (copper–copper); (2) the interaction between carbon atoms (carbon–carbon); (3) the interaction between copper atoms and carbon atoms (copper–carbon).

Since 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. Hence, the EAM potential can well describe the properties of copper–copper [19]. The EAM potential can be expressed as follows:

$$E_{tot} = \frac{1}{2} \sum_{ij} \phi_{ij}(r_{ij}) + \sum_i F_i(\rho_i) \quad (1)$$

where  $E_{tot}$  is the total energy of all the atomic bonds;  $i, j$  label the atoms of the system;  $\phi_{ij}$  is the pair potential between atoms  $i$  and



**Fig. 2.** (a1–a2) Schematic of Simulation A; (b1–b2) schematic of Simulation B.

$j$ ;  $r_{ij}$  is the length of the  $ij$  bond, 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 systems, as follows:

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

where  $\rho_j(r_{ij})$  contributes to the electronic density at the site of atom  $i$ .

The interactions between the copper atoms in specimen and the carbon atoms in diamond tool are modeled by the Morse potential. The potential can be expressed as follows:

$$V(r_{ij}) = D(e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}) \quad (3)$$

where  $V(r_{ij})$  is a pair-potential function and  $D$ ,  $\alpha$  and  $r_0$  correspond to the cohesion energy, the elastic modulus and the atomic distance at equilibrium, respectively. The value of potential parameters adopted from Ref. [20] are  $D=0.087$  eV,  $\alpha=51.4$  nm $^{-1}$ ,  $r_0=0.205$  nm.

### 3. Simulation results and discussion

#### 3.1. Analysis of the scratch feed on nano-scratching process

The local top and cross-section views of the scratched surface of the specimen in Simulation A and Simulation B with different feeds are shown in Fig. 3. In our simulations, the scratch depth is 2 nm and the scratch feeds are 1.4 nm, 2.2 nm and 3.1 nm, respectively. Blue lines in Fig. 3 represent the residual cross-section profiles of the scratched grooves. It can be seen clearly that the cross-section profiles roughly resemble the shape of the tip with significant pile-ups around the edges under different feed cases. In Simulation B, the obtained cross-section profiles are a concave structure with smaller feeds of 1.2 nm and 2.2 nm and two parallel grooves with a feed of 3.1 nm, respectively. In the cross-section profiles of the concave structure, the previous groove distorts and the scratch depth of previous groove shallows. When scratches the second time, due to the lack of material support from the left side, the second time scratching chips move toward the previous groove, which leads the previous groove to shallow and the middle bulged material to tilt toward the left side. However, in Simulation A, two parallel grooves are always obtained on the specimen's surface with different feeds. From Fig. 3(a1–b3), the scratch depth of the distorted groove becomes shallower as scratch feed decreases. Fig. 4 is the section views of residual Von Mises stress distribution. From the section views of Fig. 4(a1–b3), the internal Von Mises stress has no significant change between double-tip scratch and single-tip scratch with different scratch feeds. It can be known that, scratch with different scratch feeds mainly influences residual cross-section profiles of the specimen's surface. It also reveals that

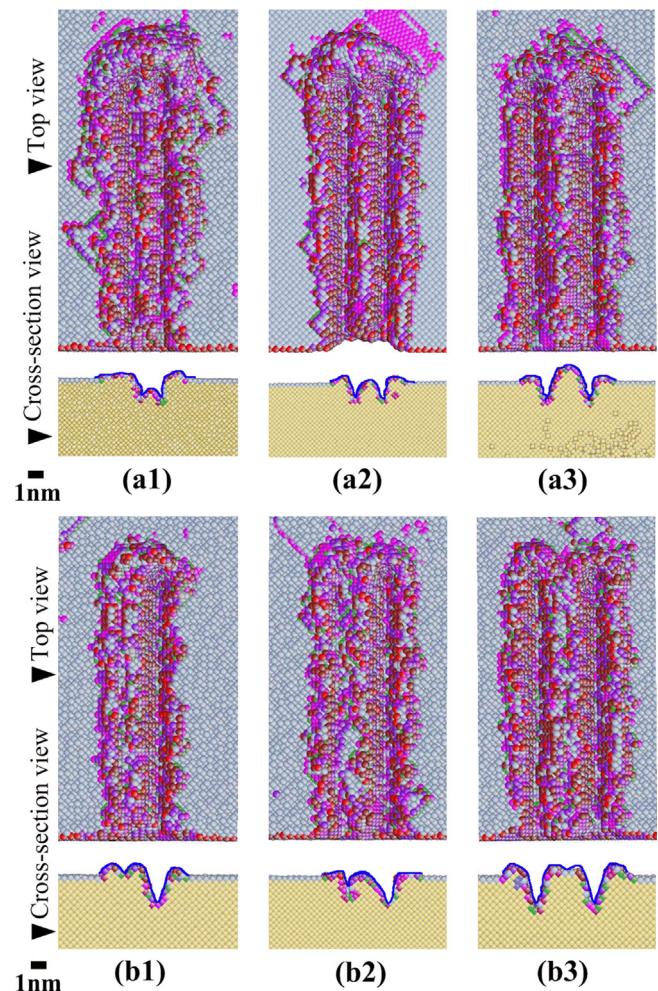


Fig. 3. Local top and cross-section views of scratched surface after scratching with scratch feeds equaling to 1.4 nm, 2.2 nm and 3.1 nm, respectively: (a1–a3) nanoscratch with double tip simultaneously scratched the specimen's surface; (b1–b3) nanoscratch with single tip successively scratched the specimen's surface.

when the feed decreases to some degree, the second time scratch has a significant influence on the first scratch.

The variations of scratching forces with different scratch feeds in Simulation B are showed in Fig. 5.  $F_x$  and  $F_z$  represent the average scratching force and the average lateral force, respectively.  $F_z$  is close to zero because of the perfect and symmetry lattice the specimen represents before the first scratch. Compared with the first scratch, in the subsequent scratch,  $F_z$  increases to 3.58 nN with the

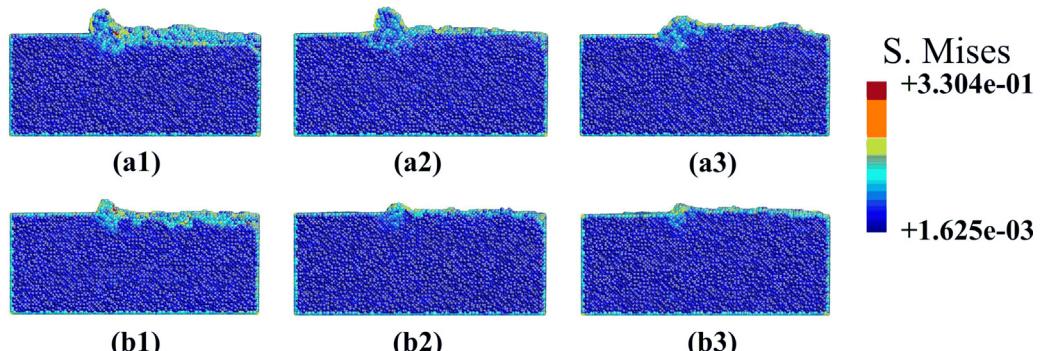
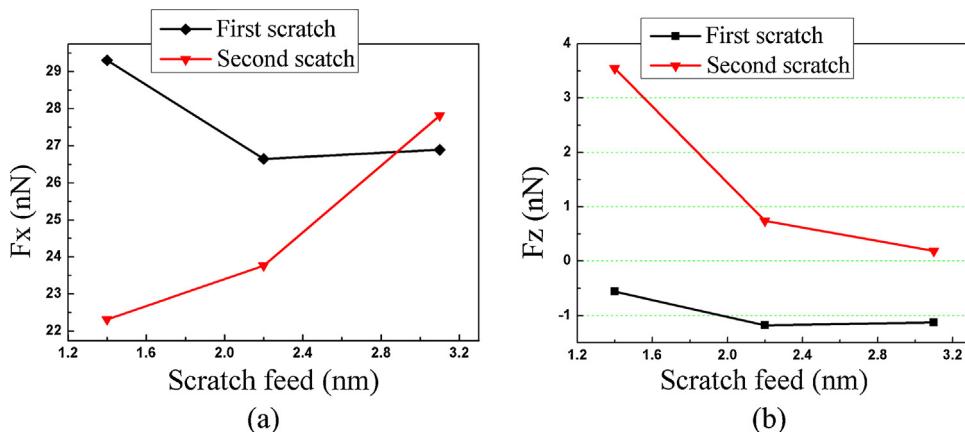


Fig. 4. Section views of residual Von Mises stress distribution after scratching in MPa with scratch feeds equaling to 1.4 nm, 2.2 nm and 3.1 nm, respectively: (a1–a3) nanoscratch with double tip simultaneously scratched the specimen's surface; (b1–b3) nanoscratch with single tip successively scratched the specimen's surface.



**Fig. 5.** Comparison of forces during nano-scratching process with different scratch feeds: (a) comparison of forces  $F_x$  with different scratch feeds; (b) comparison of forces  $F_z$  with different scratch feeds.

scratch feed of 1.4 nm, as shown in Fig. 5(b). As there is no material support from the left side, the lateral force deviates from zero, which cannot be ignored. From Fig. 5(a),  $F_x$  deceases from 29.3 nN to 22.2 nN. It is because part material flows toward the previous groove, not moves forward, which results in less resistance along X direction during the second time scratch. As Fig. 5(a and b) shows, with the feed increasing to 2.2 nm, the differences of the average scratching force between the first time scratch and the second time scratch become less, and the average lateral force of the second time scratch is close to zero. When the feed increases to 3.1 nm, the average scratching forces of the first time scratch and the second time scratch become almost the same and the average lateral force of the second time scratch approaches to zero. It also verifies that the second time scratch has little influence on the first scratch when the scratch feed increases to 3.1 nm.

### 3.2. Analysis of the scratch depth on nano-scratching process

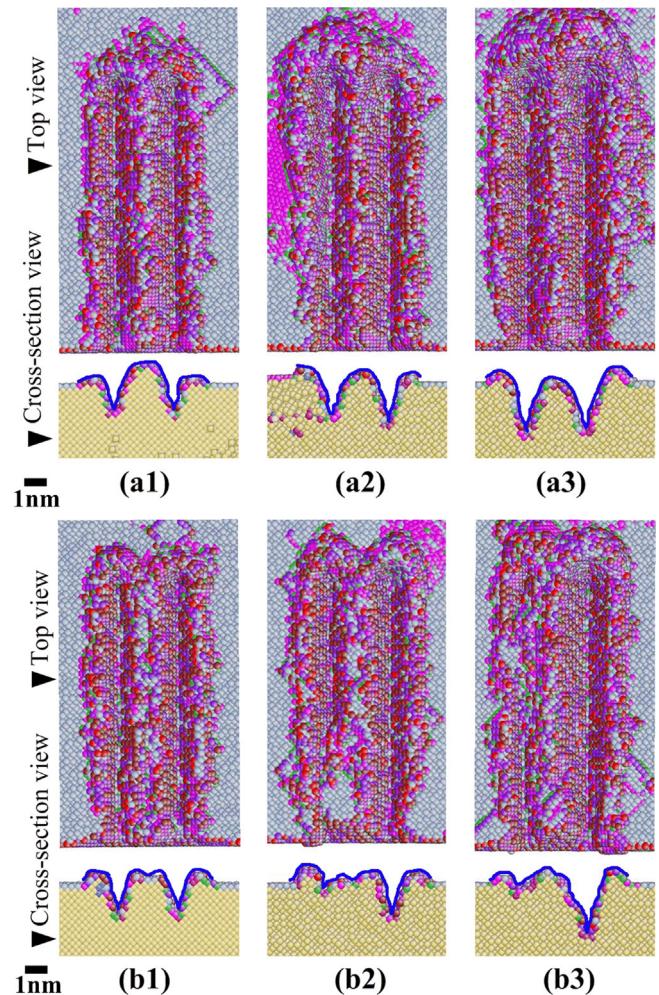
Fig. 6 shows the local top and cross-section views of the scratched surface of the specimen in Simulation A and in Simulation B when the scratch depth is 2 nm, 2.5 nm and 3 nm, respectively. In order to investigate the influence of scratch depth on nano-scratching process, uniform feed ( $f=3.1$  nm) is adopted. In Simulation B, two almost parallel grooves are obtained when the scratch depth is 2 nm, but when the scratch depths increase to 2.5 nm and 3 nm, the cross-section profiles present a concave structure. However, in Simulation A, two parallel grooves are always obtained regardless of the scratch depth. In Fig. 7, with scratch depth increasing, the chips become more. From the section views of Fig. 7(a1–b3), the internal Von Mises stress also has no significant change between double-tip scratch and single-tip scratch with different scratch depths. It can be drawn that two parallel grooves are easy to obtain at a shallower scratch depth.

### 3.3. Analysis of the crystal orientation on nano-scratching process

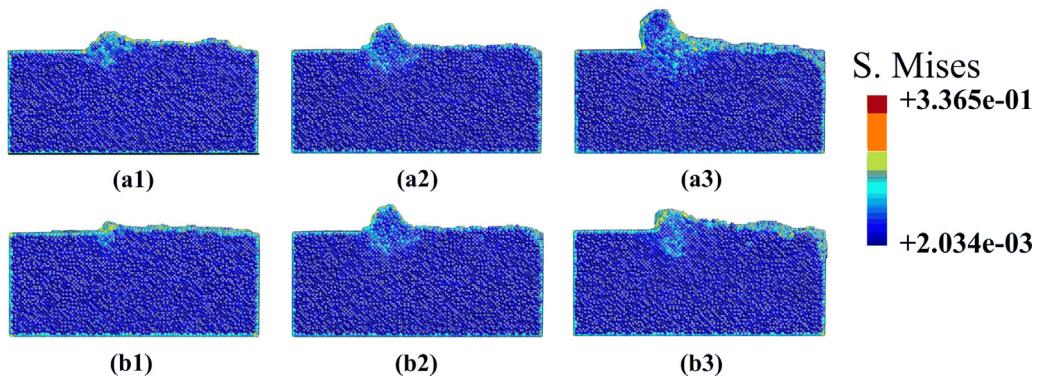
Fig. 8 shows the local top and cross-section views of the scratched surface of the specimen in Simulation A and in Simulation B scratching along crystal orientations [100], [011] and [111], respectively. In our simulation, the scratch feed and depth are 2.2 nm and 2 nm. From Fig. 8, in Simulation B, the cross-section profiles of scratching along crystal orientation [100] present a concave structure and the middle bulged material titles toward the left side. But the cross-section profiles have no significant change in Simulation A and Simulation B scratching along crystal orientation [011] and [111]. In Simulation A, two parallel grooves are

still obtained. From the section views of Fig. 9 (a1–b3), the internal Von Mises stress also has no significant change between double-tip scratch and single-tip scratch.

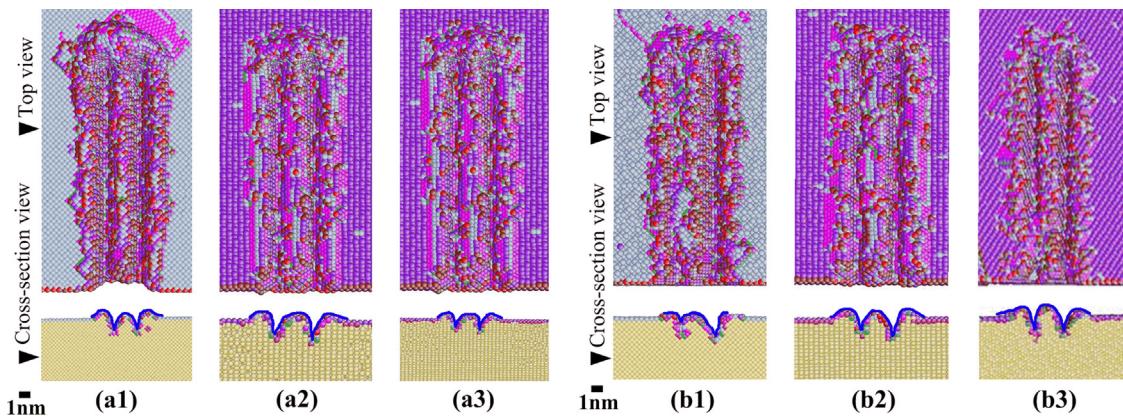
In order to obtain scratched groove of high quality, it is quite essential to get symmetrical and parallel grooves. When single tip



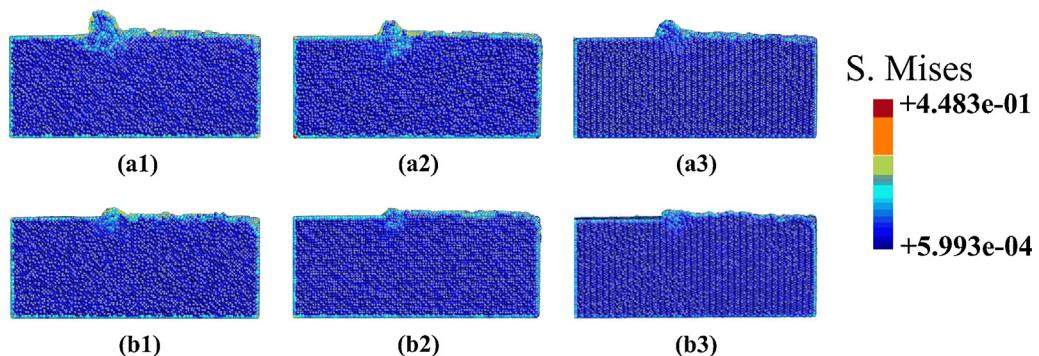
**Fig. 6.** Local top and cross-section views of scratched surface after scratching with scratch depths equaling to 2 nm, 2.5 nm and 3 nm, respectively: (a1–a3) nanoscratch with double tip simultaneously scratched the specimen's surface; (b1–b3) nanoscratch with single tip successively scratched the specimen's surface.



**Fig. 7.** Section views of residual Von Mises stress distribution after scratching in MPa with scratch depths equaling to 2 nm, 2.5 nm and 3 nm, respectively: (a1–a3) nanoscratch with double tip simultaneously scratched the specimen's surface; (b1–b3) nanoscratch with single tip successively scratched the specimen's surface.



**Fig. 8.** Local top and cross-section views of scratched surface after scratching with scratching along crystal orientation [1 0 0], [0 1 1] and [1 1 1], respectively: (a1–a3) nanoscratch with double tip simultaneously scratched the specimen's surface; (b1–b3) nanoscratch with single tip successively scratched the specimen's surface.



**Fig. 9.** Section views of residual Von Mises stress distribution after scratching in MPa with scratching along crystal orientation [1 0 0], [0 1 1] and [1 1 1], respectively: (a1–a3) nanoscratch with double tip simultaneously scratched the specimen's surface; (b1–b3) nanoscratch with single tip successively scratched the specimen's surface.

scratches the specimen's surface, two parallel grooves are easy to obtain under larger scratch feed and shallower scratch depth. Through changing crystal orientation, scratching along crystal orientation [0 1 1] and [1 1 1] are beneficial to obtain two parallel grooves compared with scratching along crystal orientation [1 0 0]. Therefore, scratch feed, depth and crystal orientation all influence the cross-section profiles when single tip scratches the specimen's surface. However, when double tips scratch the specimen's surface, two parallel grooves are always obtained with different scratch feeds, depths and crystal orientations. Although this kind of double-tip tool is difficult to machine, it is greatly beneficial to obtain scratched grooves of high quality.

#### 4. Conclusion

Using the MD simulation approach, the influences of scratch feed, depth and crystal orientation on the shape and surface quality of the scratched groove in two simulations were investigated. The following conclusions can be drawn:

- (1) During single-tip scratch, scratch feed, depth and crystal orientation all have a significant influence on the shape and surface quality of the scratched groove, especially when scratches with a small scratch feed and deep scratch depth. However,

- double-tip scratch can obtain two parallel grooves of high quality regardless of scratch feed, depth and crystal orientation.
- (2) With the scratch feed decreasing and the scratch depth increasing, the cross-section profiles present a concave structure and the second time scratch has an influence on the first scratch during single-tip scratch.
  - (3) Through changing crystal orientation, scratching along crystal orientation [0 1 1] and [1 1 1] are beneficial to obtain two parallel grooves compared with scratching along crystal orientation [1 0 0].
  - (4) Scratching forces results show that the lateral force cannot be ignored under small scratch feed. With the scratch feed increasing, the scratching force increases but the lateral force decreases during the second time scratch.

## Acknowledgements

This research is funded by the National Natural Science Foundation of China (Grant No. 50905073, 51275198), 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), and Key Projects of Science and Technology Development Plan of Jilin Province (Grant No. 20110307), Program for New Century Excellent Talents in University of Ministry of Education of China (NCET-12-0238).

## References

- [1] B. Bhushan, *Handbook of Micro/Nano Tribology*, CRC Press, New York, 1995.
- [2] A. Chahboun, R. Coratger, F. Ajustron, J. Beauvillain, P. Aimar, V. Sanchez, Comparative study of micro-and ultrafiltration membranes using STM, AFM, and SEM techniques, *Ultramicroscopy* 41 (1992) 235–244.
- [3] A. Chatterjee, A.A. Polycarpou, J.R. Abelson, P. Bellon, Nanoscratch study of hard HfB<sub>2</sub> thin films using experimental and finite element techniques, *Wear* 268 (2010) 677–685.
- [4] B.D. Beake, V.M. Vishnyakov, A.J. Harris, Relationship between mechanical properties of thin nitride-based films and their behaviour in nano-scratch tests, *Tribology International* 44 (2011) 468–475.
- [5] L.L. Sohn, R.L. Willett, Fabrication of nanostructures using atomic-force-microscope-based lithography, *Applied Physics Letters* 67 (1995) 1552–1554.
- [6] J.J. Zhang, T. Sun, Y.D. Yan, Y.C. Liang, Molecular dynamics study of scratching velocity dependency in AFM-based nanometric scratching process, *Materials Science and Engineering A* 505 (2009) 65–69.
- [7] K. Mylvaganam, L.C. Zhang, Nanowinning in monocrystalline silicon upon nanoscratching, *Scripta Materialia* 65 (2011) 214–216.
- [8] T.H. Fang, C.I. Weng, Three-dimensional molecular dynamics analysis of processing using a pin tool on the atomic scale, *Nanotechnology* 11 (2000) 148–153.
- [9] T.H. Fang, W.J. Chang, Effects of AFM-based nanomachining process on aluminum surface, *Journal of Physics and Chemistry of Solids* 64 (2003) 913–918.
- [10] K. Cetinkaya, An effect of feeding system on the scratches of sheet metal strips, *Materials & Design* 28 (2007) 362–367.
- [11] T.H. Fang, C.I. Weng, J.G. Chang, Molecular dynamics simulation of nanolithography process using atomic force microscopy, *Surface Science* 501 (2002) 138–147.
- [12] Y.D. Yan, T. Sun, S. Dong, X.C. Luo, Y.C. Liang, Molecular dynamics simulation of processing using AFM pin tool, *Applied Surface Science* 252 (2006) 7523–7531.
- [13] T.H. Fang, C.I. Weng, J.G. Chang, Machining characterization of the nanolithography process using atomic force microscopy, *Nanotechnology* 11 (2000) 181–187.
- [14] P.Z. Zhu, Y.Z. Hu, H. Wang, T.B. Ma, Study of effect of indenter shape in nanometric scratching process using molecular dynamics, *Materials Science and Engineering A* 528 (2011) 4522–4527.
- [15] Y.D. Yan, T. Sun, S. Dong, Y.C. Liang, Study on effects of the feed on AFM-based nano-scratching process using MD simulation, *Computational Materials Science* 40 (2007) 1–5.
- [16] 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 Research Letters* 4 (2009) 444–451.
- [17] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, *Journal of Computational Physics* 117 (1995) 1–19.
- [18] H.W. Zhao, C.L. Shi, P. Zhang, L. Zhang, H. Huang, J.W. Yan, Research on the effects of machining-induced subsurface damages on mono-crystalline silicon via molecular dynamics simulation, *Applied Surface Science* 259 (2012) 66–71.
- [19] S.M. Foiles, M.I. Baskes, M.S. Daw, Embedded-atom method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys, *Physical Review B* 33 (1986) 7983–7991.
- [20] Z.C. Lin, J.C. Huang, A nano-orthogonal cutting model based on a modified molecular dynamics technique, *Nanotechnology* 15 (2004) 510–519.