Investigate the effect of temperature on the plastic deformation behavior of 3C-SiC and diamond tool wear during nano-scratching using MD

Zhipeng Li[1, a], Feihu Zhang[2,b*]

[1,2] School of Mechatronics Engineering, Harbin Institute of Technology, Harbin, China

[a]zplihit@163.com, [b] zhangfh@hit.edu.cn

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Abstract. Molecular dynamics (MD) simulation using the analytical bond order potential (ABOP) interatomic potential was employed to study the plastic deformation and subsurface defects formation mechanisms in nano-scratching of single crystal 3C-SiC within the temperature from 300 K to 1500 K. The scratching direction is on (110) <001>. To obtain better insights about structural changes, the radial distribution functions of SiC and diamond tool were plotted and analyzed. It is found that the intensity of plastic deformation of 3C-SiC increased with the increasing of temperature. Especially, when the temperature increased to 1500 K, high density of dislocations, stacking faults and structure changes formed during material removal process. Meanwhile, the interaction between frank type sessile partials and perfect dislocations and Shockley partials can be witnessed. More dislocation locks and dislocation loops were formed in 1500 K, which lead the depth of subsurface damage is deeper than 300 K. Nonetheless, the material removal initial response of 3C-SiC was found to be solid-state amorphization for all the temperature used in this study. Finally, the results revealed that the basic wear mechanism of the diamond tool is graphitization which make the bond of C-C easier to break.

Introduction

Due to superior physical, chemical and mechanical properties silicon carbide (SiC) has been regarded as a promising material for electronic and structural device [1,2]. However, the hardness and brittleness of SiC make it difficult to machine and easy to occur brittle fracture during grinding process. Therefore, achieving plastic removal mode in machining SiC is a challenge task. To solve this problem, the corresponding ductile and fracture mechanism and the critical transition condition need to be understand in urgent. To date, there are some studies have addressed the deformation mechanism of SiC in nano-metric. Szlufarska [3] et al. investigate the amorphization in SiC crystal generated in nano-indentation using MD. They found that dislocation loop is responsible for the crystalline to amorphous transition. Besides, the relationship between the load drops observed in the load-displacement and crystalline structure, dislocation activities are explained. Similarly, Goel et al. [4] claimed that 3C-SiC undergoes sp^3-sp^2 disorder in nano-metric cutting. On the contrary, Zhao [5] et al. revealed that the shear slip is the predominant deformation mechanism in 3C-SiC during indentation, which observed by transmission electron microscopy. They also point out the cracks always initiate at the intersection of shear bands or grain boundary. Kikuchi [6] et al. studied the brittle fracture dynamics for three crack surfaces, i.e. ((001), (111) and (100)) in cubic silicon carbide (3C-SiC). They verified the fracture of SiC exhibition significant orientation dependence. Moreover, to illustrate the heat contribution to the plasticity of crystal 3C-SiC during nano-metric cutting, Chavoshi and Luo [7] employed MD to elucidate the dislocation/amorphization-based plasticity mechanism across a range of cutting temperatures,

300 K to 3000 K. But the wear of diamond tool was not considered in their investigation. Therefore, this paper adopts MD simulation to analyze the temperature effect on scratching deformation mechanism of 3C-SiC and the diamond tool wear mechanism.

2. Simulation methods

Previous studies indicate that the grinding abrasive can be simplified as a spherical tip, especially when the cuting depth within nano scale. Therefore, we conducted MD simulations of scratching with a spherical tip over single crytal SiC with a zinc blende structure. **Fig. 1** shows the models for MD simulation which obtained after the equilibration process. The radius of diamond tool is 3 nm and the worpiece has dimensions of 19.6 nm × 17.4 nm × 8.7 nm. The scratching oriention is (110) <001>, y and z oriention is corresponding to (110) <110>, (110) <1-10>, respectively. The scratching depth is 2 nm.

The simulated temperatures of substrate of workpiece were 300 K, 900 K and 1500 K which realized via regulating a berendsen thermostat. The ABOP potential adopted for modelling the atomic interaction in SiC workpiece. This potential could describe the fracture toughness, elastic, dislocation formation and phase tranformation of SiC more accurate. In this study, all MD simulations are performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS). The visualization of MD data and the generation of MD snapshots during the grinding process is realized by OVITO software. The dislocations and defects induced during the scraching process was analyzed using Dislocation Extraction Algorithm (DXA).

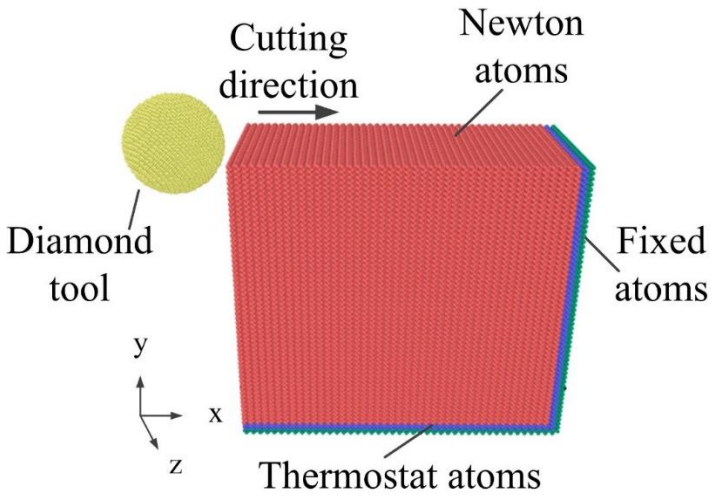

Fig. 1. Schematic model of the nanometric scratching simulation

3. Results and discussion

3.1 Analysis of crystal defects

Fig. 2 shows the crystal defects analysis results that obtained after scratch using the DXA in OVITO. It can be found that both of the removal chips and subsurface of substrate exhibited evident highly disordered atoms, which reveals that the amorphous transition is one of the removal mechanisms of 3C-SiC during scratching process. The results in agreement with the simulations of Goel et al. [8], which illustrated that the atoms in the chip and subsurface of the substrate lose their pristine diamond cubic lattice. Besides, high temperature could promote the intensity of amorphous atoms transition as seen in **Fig. 2a and c**, which the height of maximum amorphous chips at the final stage was increased from 2.82 nm to 3.18 nm.

Note that, some dislocations nucleated inside the subsurface of substrate when the temperature increased above 900 K. This phenomenon demonstrates that dislocations always formed beneath a layer of amorphous atoms, which means the amorphous transition was the first deformation mechanism in the substrate once the diamond tool contact with SiC. Most of the dislocations formed are Shockley partials with 1/6 <112> burgers vectors and perfect dislocations with 1/2 <110> burgers vectors.

Intersections of dislocations are also seen, especially when the temperature reached 1500K, which could cause formation of locks and dislocation loops. Furthermore, the total length of perfect dislocations was found to be about 5 times longer than that of 900K and higher density of dislocations were formed than that of 900 K. From the **Fig. 2c**, the formation and broken dislocation locks along with the process of scratching will not only hinder plastic deformation but also promote it. Moreover, it is interesting to see that comparing with the dislocations formed at 900 K, frank type sessile partials with 1/3<111> burgers vectors were observed to nucleate and joint with the perfect dislocation and Shockley partial dislocations at 1500 K. Also, stair-rod partials with 1/6 <110> Burgers vectors can be witnessed. Therefore, above mentioned evidences confirmed that temperature affects the deformation mode. As the temperature increased to a certain level, the deformation mechanism of 3C-SiC mainly controlled by the combination of nucleation, activity and movement of dislocations and amorphous transition.

In order to further illustrate the amorphous transition, the bond length variation was measured to gain further insights at atomistic level. **Fig. 3** shows the radial distribution function (RDF) of the SiC before and after the whole scratching for each setting temperatures. The RDF, namely, pair distribution functions which could describes the varies of bound length from a central particle:

$$g(r) = \frac{n(r)}{4\pi r^2 \rho \Delta r}$$

where n(r) is the number of the atoms located inside a shell within the region of $r=\pm\triangle r/2$. Here, $\triangle r$ denotes the thickness and $\rho=V/N$ is the bulk number density in which N represents the number of particles in the model volume V. It can be seen from **Fig. 3** various peaks occur in the RDF for each individual scratching temperature. The bond length at the peaks has a small discrepancy. The three peaks of RDF at the equilibrium bond lengths of 1.88 Å, 3.08 Å and 3.62 Å correspond to C-Si, C-C and C-Si bonds respectively. Obviously, the height of peaks is inversely proportional to the temperature of the substrate. This is because high temperature will cause high intensity vibrations of atoms, which will lead them deviated from their equilibrium positions. Meanwhile, the peaks width increases with the increase of temperature, which is an indication of enhanced structural changes. Furthermore, it is interesting to note that a small protrusion peak was emerged at the interatomic distance of 1.45 Å, which corresponding to the bond length of C-C, signifying the formation of C–C bond.

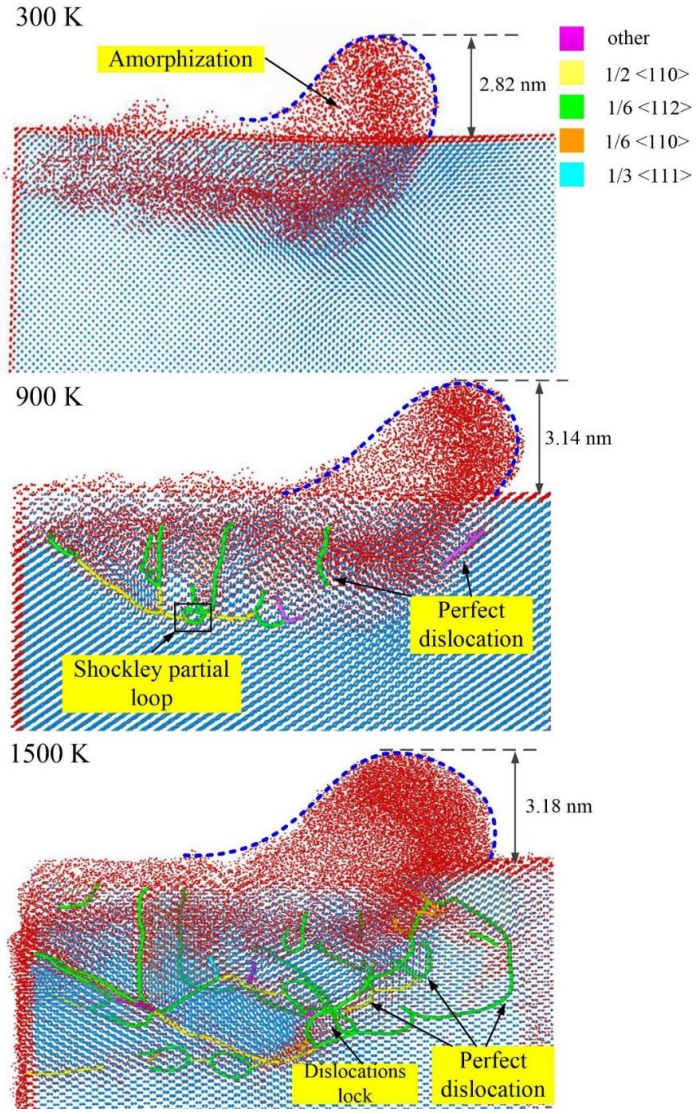

Fig. 2 Snapshots of surface and subsurface defects during scratching process.

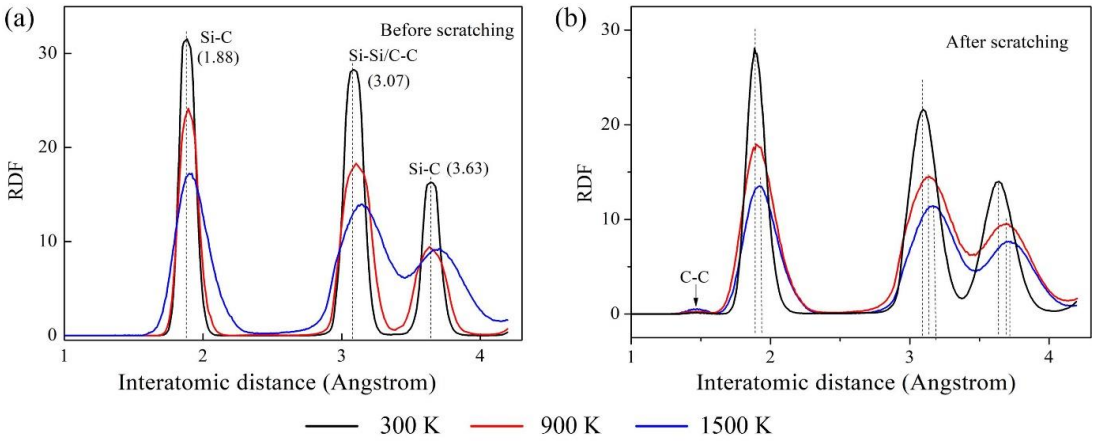

Fig.3 Radial pair distribution function at different temperature for SiC.

3.2 Structural changes

To clearly realize the development of local atomic structure, the atoms with hexagonal structure were characterized with different color as shown in **Fig. 4**. The phase transformations of SiC is of particular interest in the field of contact loading because of possibility of obtaining a ductile response from brittle materials. It can be seen from **Fig. 4a**, only a few of atoms transformed to hexagonal diamond structure at room temperature. However, when the substrate temperature raised to 1500 K (**Fig. 4c**), the number of hexagonal diamond structure atoms increased and accompanied by stacking faults. The basis of this transformation involves the motion of partial dislocations which change the stacking of planes from ABCABC…. to a hexagonal polytype.

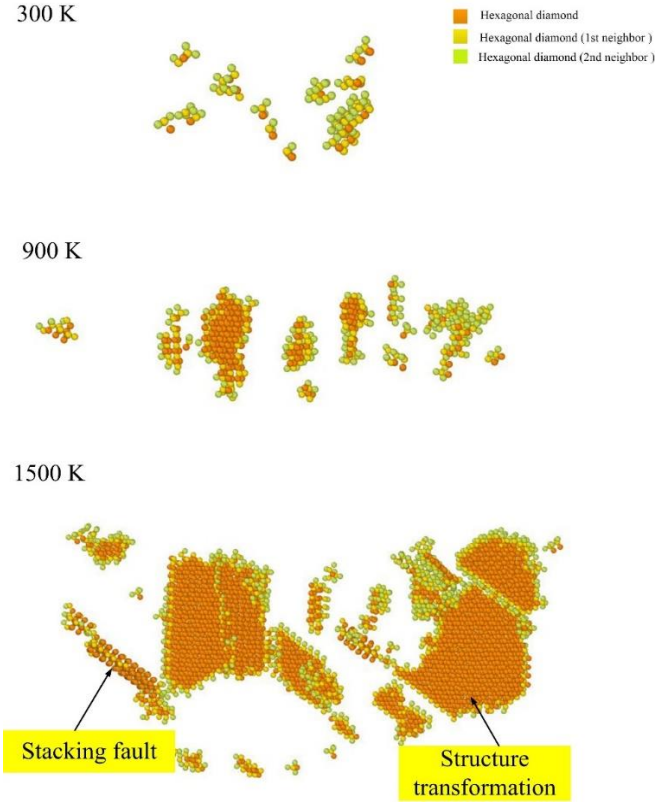

Fig. 4 Subsurface defects of structure transformation distribution in substrate of SiC.

3.3 The wear of diamond cutting tools

Fig. 5 described the wear state after scratching process at different elevated temperature. It is evident that the high rise of temperature (1500 K) could causes a severe wear around the tool cutting edge area. This wear phenomenon of the diamond tool suggests that the hardness of diamond tool was reduced with the temperature increase. The shorter length of Sp^3-Sp^3 bond in diamond lead it much harder than other allotropes of carbon. Hence, the bond length variation between C-C in diamond tools during scratching could further help to explain structure changes. For this purpose, radial distribution function for diamond tool was plotted before and after the scratching (1500K) which suggests graphitization of the diamond tool during the progress of scratching as shown in **Fig. 6.** It can be seen from the radial distribution function g(r), the first peak appears at 1.55 Å which is attribute to diamond bond length. After scratching, in the vicinity of 1.55 Å peak, a bow appeared at 1.42 Å which corresponding to another allotrope of carbon i.e. graphite. The graphite possessed layer structure make it much weaker than diamond and easier to break. That is to say, the cohesion bond of C-C is weaker. Thus, it can be

concluded that the graphite transformation was indeed occurred during scratching when the temperature achieved above 900K. Besides, the temperature has negative effect on the wear of diamond tool.

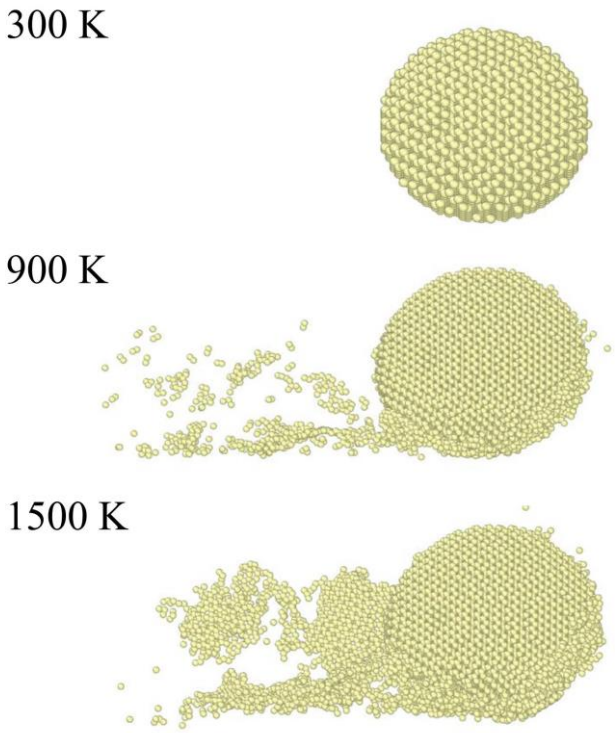

Fig. 5. The wear state of diamond tool after scratching at each temperature.

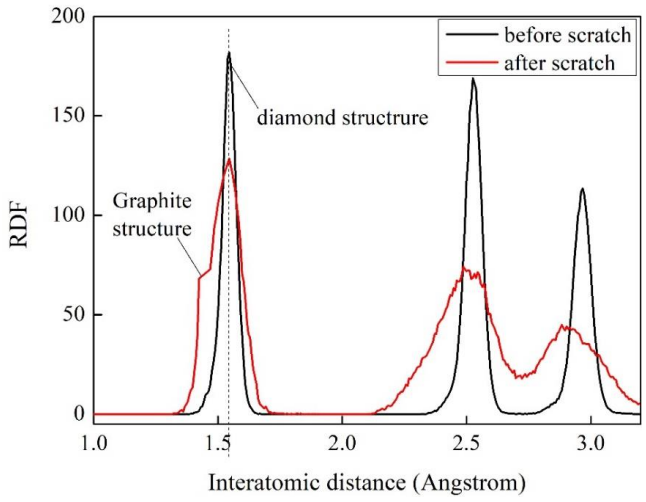

Fig. 6. The Radial pair distribution function at temperature of 1500 K for diamond.

Summary

In this paper, the plastic removal and deformation mechanism during nanoscale scratching of 3C-SiC within the temperature range from 300 K to 1500 K was investigated with the aid of MD. Besides, the wear mechanism of diamond tool and the temperature effect was also revealed. The conclusions can be drawn as following:

1. Amorphization is the dominate removal mechanism for 3C-SiC at all temperature. High temperature results in more intensity of amorphous transformation.
2. The subsurface defects including the dislocations, hexagonal structure transformation and accompanied stacking faults were induced when the temperature at 900 K and 1500 K, whereas at room temperature (300 K) only exhibit some disorder atoms. High temperature can accelerate the dislocations nucleation and propagation, the formation of dislocation locks and stacking faults.
3. The wear of the diamond tool depends on the temperature of substrate and the heat will decrease the hardness of the diamond. The RDF suggested that the graphitization indeed occurred during scratching of SiC and more serious in high temperature, which make the bond of C-C easier to break.

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