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Atomistic investigation of FIB-induced damage in diamond cutting tools under various ion irradiation conditions

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Abstract

Focused Ion Beam (FIB) has been demonstrated as a promising tool to the fabrication of micro- and nanoscale diamond cutting tools. In-depth understanding of the ion-solid interaction in diamond leading to residual damage under different processing parameters are in high demand for the fabrication of nanoscale diamond tools. Molecular dynamics (MD) simulation method has long been regarded as a powerful and effective tool for analysing atomistic interactions with regard to its capacity of tracking each atom dynamically. Developing on the previous research work on single ion collision process in diamond, a novel Gauss random distribution multi-particle collision MD model was developed in this paper to study FIB-induced damage in diamond under various ion irradiation conditions. A multi-timestep algorithm was developed to control the whole collision process.

The results show that the proposed model can effectively track the impulse of each single ion leads to atomic displacements in diamond and finally to a U-shape residual damaged layer at the core irradiation area. The multi-timestep algorithm can increase the computing efficiency by 12 times while still holding high simulation accuracy in terms of the thickness of residual damaged layer and the range of incident gallium distribution. The simulation model was further used to study the ion-induced damage layer in diamond under various beam voltages (5 kV, 8 kV, and 16 kV) and incident angles (0˚, 15˚, 30˚, and 45˚). Less damage range were found under the beam energy of 5 kV with the ion incident angle of 45˚, which indicated that a post ion beam polishing process (low beam energy with large incident angle) would be an effective way in practice to remove/minimise the residual damage layer when shaping the diamond cutting tools.

Keywords: Focused ion beam, Irradiation damage, Molecular Dynamics, Diamond cutting tools

1. Introduction

In recent years, focused ion beam (FIB) milling technique has been widely applied in the fabrication of micro/nanoscale diamond cutting tools possessing complex geometry (e.g. single tipped and multi-tipped tools having rectangular, triangular, and other complex shaped face designs) owing to its suitability for top-down fabrication (down to submicron level or even few nanometres level). Several pioneering works have initially demonstrated the feasibility of using nanoscale diamond tools for scaling up fabrication of nanostructures through diamond turning operation[1]. However, the implantation of ion source materials and the formation of damaged layer at the machined surface was the two major defects on diamond tool tips. Most recently, it has been experimentally observed that the doping of gallium ions at tool rake face can cause a rapid diamond tool wear due to the increase of the adhesion of work materials to the tool surface[2]. The minimization of the FIB-induced damaged layer during the tool fabrication process will become more important when the dimensions of a diamond tool tip are approaching nanoscale.

As compared with other simulation methods, MD simulation method has long been regarded as a powerful and effective tool for analysing ion-solid interaction with regard to its capacity of tracking atoms dynamically. In our previous work, a random distribution multi-particle collision MD model has been developed to stimulate the FIB-induced damage in diamond [3]. This simulation work has shown the formation of atomic defects, the thermal spike and the recrystallization of atomic defects of each single ion collision process. However, the computing efficiency of this model is very low which limit the further application of this model to study the FIB processing process under different irradiation conditions.

In this paper, a novel Gauss random distribution multi-particle collision MD model was developed to study FIB-induced damage in diamond under various ion irradiation conditions. Inspired by the dynamic damage process of a single ion collision, a multi-timestep algorithm was developed to control and speed up the whole collision process.

2. MD model and simulation parameters

The Gauss random distribution multi-particle collision MD model was built as shown in figure 1. For the energetic ion collision process, it is important to make sure that the system size is able to track all the stopping processes of incident particles as well as the entire collision cascades happening subsequently. As shown in figure 1 (a) the diamond bulk has cylinder shape with a diameter of 25 nm. In order to save the computing load, the diamond bulk was cut with different surface angle θ (figures 1 (b)) to stimulate the ion irradiation process with different incident angles. Except the collision surface, all the rest surfaces were built with a thermal layer with thicknesses of $2a_1$ (a_1 = 3.567 Å is the lattice constant of diamond) to control the temperature at 297 K. For the purpose of concision, the other important simulation parameters used in this work were summarised in Table 1.

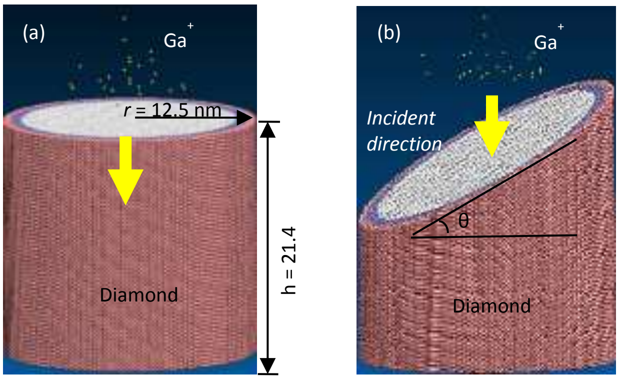

Figure 1. The MD model of FIB milling process. (a) Model I; (b) Model II.

Table 1 MD simulation parameters of different irradiation conditions

Simulation Parameters	Model I	Model II
Beam size (d_{beam})	10 nm	10 nm
Incident angle θ	0˚	15˚, 30˚, 45˚
Incident voltage	5 kV, 8 kV, 16 kV	5 kV
Time step	0.1 fs	0.1 fs
Initial temperature	297 K	297 K

3. Results and discussion

3.1. The modelling of FIB milling process

In the simulation, an ion was only triggered having the correct mass of gallium and the velocity corresponding to the energy of beam when the former ion collision process has completely finished. Thus single ion collisions under different beam voltages were carried out firstly to determine the time slots between multi-particle collisions. In our previous research we found that although the whole collision process lasted about 18.5 ps (185,000 computing time step), the range and the distribution of defect remain unchanged when the local temperature at the core collision area cooled down to 600 K. This phenomenon inspired the design of a multi-timestep algorithm to further control and speed up the whole collision process by artificially re-set the system to 297 K when the system reached a certain point. For computational validation, 25 ions collision process (5 keV incident energy) have been performed using the optimised algorithm and the results were compared with the results calculated using non-optimised algorithm. It is found that the computing time reduced from 72 days to 6 days. The deviational rate of the simulation results on the damage features is less than 4.85%. A detailed comparison of the simulation results are summarised in Table 2.

Table 2 Comparison of optimized and non-optimized MD simulation results

	Non-optimised algorithm	optimised algorithm	Deviation rate (%)
***sp*^{2}-bonded C**	8139	8172	0.41
Thickness (nm)	10.4	10.1	2.88
Maximum depth of implanted Ga	10.3	9.8	4.85
Time (Day)	72	6	

3.2. The effect of processing parameters

Using the optimised algorithm, the FIB-induced damage in diamond under various ion irradiation conditions was further performed to study the dependence between the residual damage layer on FIB processing parameters (mainly the beam energy and the incident angle as shown in Table 1). Figures 2 and 3 show the damaged layers and the range of implant Ga^+ formed under different irradiation conditions. The simulation results indicate that the thickness of residual damage layer increased with beam energy but decreased with the incident angle. Less damage range were found under the beam energy of 5 kV with the ion incident angle of 45˚.

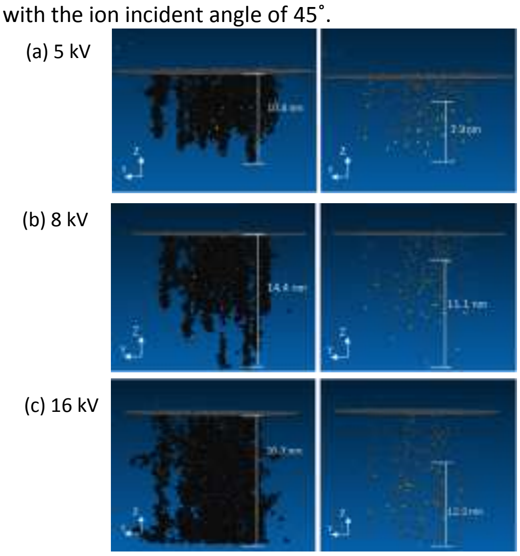

Figure 2. Residual damaged layer (left) and the range of implant Ga^+ (right) formed under different beam voltages.

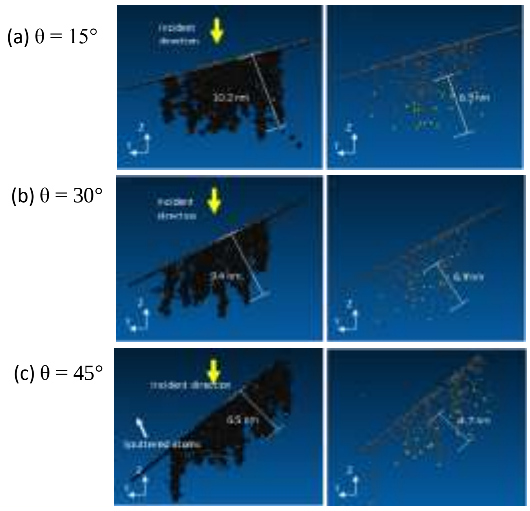

Figure 3. Residual damaged layer (left) and the range of implant Ga^+ (right) formed under different incident angles.

4. Conclusions

The proposed model can effectively stimulate the formation of residual damaged layer at the core irradiation area in diamond under different FIB processing parameters. The thickness of residual damage layer increase with beam energy but decrease with the incident angle, indicating that a post ion beam polishing process (with low beam energy and large incident angle) would be useful in practice to remove/minimise the residual damage layer when shaping the diamond cutting tools.

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