An atomistic investigation of FIB process damage on diamond

Zhen Tong, Xichun Luo, Liam Blunt, Xiangqian Jiang

School of Computing & Engineering, University of Huddersfield, Huddersfield HD3 3RR, UK

x.luo@hud.ac.uk

Abstract

Focused Ion Beam (FIB) is one of the important machining techniques to fabricate diamond sensors/detectors used for drug analysis, chemical analysis and bio-sensing applications. In-depth understanding of the high energy collision process and the residual damage induced along the trace of gallium ion could undoubtedly facilitate the development and improvement of performance of such devices through the optimization of machining processes. Based on the merit offered by large-scale molecular dynamics (MD) simulation method and the new progress made in high performance computing technique (HPC), a new atomistic modelling system was proposed in this paper to investigate the high energy collision process involved two gallium ions. The simulation results indicated that the energetic ion collision process comprises a bombardment event with a pulse temperature and a lateral relative long period annealing recrystallization process. The peak temperature for the second ion collision was 129.2 K higher than the first one, which indicates the alternation of the thermal conductivity of diamond due to the formation of amorphous (sp2 graphite-like) structure during the first ion collision and annealing process. Besides giving the damage configuration and distribution in diamond after fully recrystallization, the simulation also used coordination number (CN) and radius distribution function (RDF) to revel the change of diamond lattice structure after the collision process, which provided an insight of damage induced by FIB process.

1 Introduction

Due to its unique material properties, such as bio-compatibility, high PH/chemical surface sensitivity and high thermal conductivity etc., diamond has been proposed as

a good candidate material for sensors and detectors used for drug research and delivery applications [1], high-energy physics [2] and nuclear industry applications [3]. Focused Ion Beam (FIB) is one of the most important machining techniques to fabricate diamond sensors/detectors. However, with respect to the bright prospects in terms of applications of diamond sensors/detectors, the damage of diamond induced by ion bombardment during the fabrication process will undoubtedly affect the performances of these sensors/detectors, especially in high-resolution patterning where the incoming beam spot size is matching the characteristic lengths of collision cascades (< 10 nm). Although radiation damage in diamond caused by ions has been studied using a variety of techniques including Raman spectroscopy, AFM, x-ray diffraction, SEM and TEM, it is still difficult to track the incident gallium ions and get in-depth understanding of damage formation mechanism through experiment due to the limitations of real-time detect equipment as well as the high research cost. On account of these issues, it has been recognized that Molecular dynamic (MD) simulations constitute a powerful approach to address some of the fundamental issues of FIB machining process [4, 5]. Taking the advantage of this methodology, this paper therefore aims to gain in-depth understanding of residual damage induced by FIB processing through MD simulation of the high energy gallium ions collision process and verify the damage formation mechanism.

2 Modelling and simulation method

The diamond crystalline lattice and corresponding coordinate axes are shown in Fig. 1 (a). A collision system with two gallium ions has been built as shown in Fig. 1(b). The diamond models investigated for this study are rectangular boxes with the same computational region size of 60 a_0 × 60 a_0 × 45 a_0, composed of 1,314,166 diamond atoms in total, where the lattice constants a_0 is 3.567 Å for diamond materials. The direction of the ion incidence is along the negative direction of the z axis. The computing time step is set as 0.1fs and the initial temperatures in all simulations are 297 K after 60,000 time steps relaxation. After each bombardment event the system was equilibrated via a velocity scaling thermal layer until a point when the energy of the system has relaxed to a corresponding temperature of 297 K.

(a) (b)

Figure 1: FIB ion collision model. (a) The diamond crystalline lattice and corresponding coordinate axes; (b) Ion collision model.

3 Results and discussion

3.1 Ion collision process

The potential function used to describe the interactions between atoms has been reported in previous study [4]. As shown in Fig.2, for each ion collision, there is a sharp temperature rise during the instantaneous 16keV gallium ion collision process. This indicates that the whole single ion collision process comprises a bombardment portion up to a peak temperature and a lateral relative long period recrystallization process. The peak temperature can be defined as T_{max}, and they are 1255.86 K and 1385.06 K for the first and second ion collisions, respectively. The difference is mainly due to the alternation of the local thermal conductivity of diamond due to the ion-induced amorphous damage, which will be discussed in the subsequent sections.

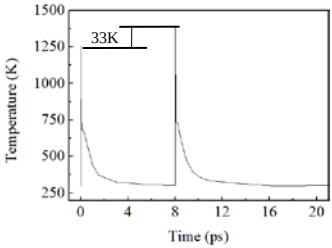


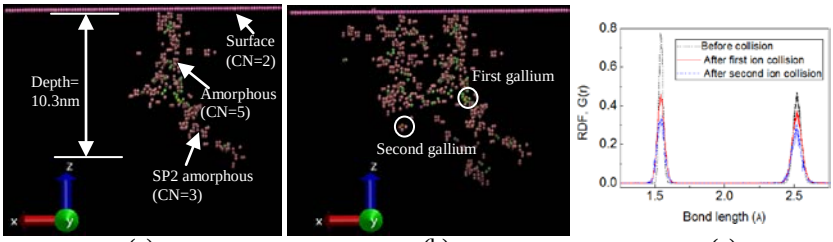
Figure 1: Variation of local temperature during 16keV ion collision process.

3.2 Damage induced by ions bombardment

As shown in Fig. 2(a) and (b), each impacting high energy gallium created a deeply buried highly damaged region inside the diamond sample. The nature of the damage is statistically around 15nm in thickness and the atoms are coloured according to their coordination numbers. However, the damage caused by the first gallium has changed the local properties of diamond as the second ion run deeply than the first one.

Moreover, as discussed before, its local thermal conductivity was also changed, which is mainly due to local amorphous structure induced by the first ion collision.

Detailed analysis using radial distribution function (RDF) further indicated that, during the collision process, the local bond disruption of the sp3 bonds and subsequent reconstruction on the equilibration process may result in the formation of sp2 rich region along the gallium-track (as shown in Fig.2 (c)). Indeed, the passage of MeV He+ or C+ through diamond-like (sp3 rich) layers has been shown by high resolution TEM scans to result in local graphitization [5]. Our simulation results confirm these results and further provide an insight of damage induced by single/double gallium ions, which further indicates that sp3 to sp2 transmission also happened around the ion-trace during each high energy single gallium collision process, and the damage induced by the former ion will change the local property of diamond and hence affect the process of next collision.



(a) (b) (c)

Figure 2: Residual damage analysis after ion collision. (a) Residual damage after first ion collision, (b) Residual damage after second ion collision, (c) RDF analysis

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