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Atomistic investigation of the wear of nanoscale diamond cutting tools shaped by focused ion beam

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Abstract
In recent years, micro/nanoscale diamond cutting tools shaped by focused ion beam (FIB) has been developed to the deterministic fabrication of micro/nano-structures owing to its unprecedented merits of high throughput, one-step, and highly flexible precision capabilities. However, the exposure of a diamond tool to FIB will result in the implantation of ion source material and the irradiation damage in cutting edges, and thus affect the tool life. In this work, molecular dynamics (MD) simulation has been carried out to study the effects of FIB induced damage on the wear resistance of nanoscale multi-tip diamond tool under different cutting conditions. A novel nanoscale multi-tip diamond tool model was built with the implanted Ga^+ and amorphous damaged layer around tool tips. A damage free tool model with the same tool geometry was built as a reference. The wear resistance of the cutting tool was characterized by the total number of defect atoms formed during nanometric cutting of single crystal copper. The results show that the FIB irradiation induced doping and defects significantly degrade the wear resistance of the diamond tool. For the damage free tool cutting, the sp^2 bonded carbon atoms were formed and accumulated on the surface layers. However, the sp^2 bonded carbon atoms were found both on the surface and the deep inside of tool when using the tool of predefined defects. The implanted gallium atoms were found to move to the tool surface and left vacuums inside diamond tool tip, which would further degrade the wear resistance of the tool. Moreover, the variation of the sp^2-bonded carbon atoms against the depth of cut and the cutting speed has been further analysed. The research findings from this study inform the in-depth understanding of tool wear of FIB shaped multi-tip diamond tool observed in previous nanometric cutting experiment.

Keywords: Tool wear, Nanometric cutting, Diamond cutting, Focused ion beam, Irradiation damage

1. Introduction

In recent decades, the single point diamond machining using micro tools have been widely used in the fabrication of periodic micro- and nanostructures in various materials [1-3]. With the advance of controlled FIB processing of micro diamond tools, varieties of tool geometries such as single tipped and dual-tipped tools having rectangular, triangular, and other complex shaped face designs have been produced to generate functional structured surface through ultra-precision lathe turning [2-3]. Most recently, nano-gratings with the pitch as small as hundreds of nanometres can also be generated by this technique using nanoscale multi-tip diamond tools [2-3].

Despite these breakthroughs, the exposure of a diamond tool to FIB will result in the implantation of ion source material and the irradiation damage of the milled area at the near surface. This modification would alternate the surface composition and cause surface instability. For the application of micro- and nanoscale diamond tools, the ion irradiation induced doping and defects will unavoidably degrade the cutting performance of the diamond tools fabricated by FIB. Therefore, the characterization of ion-induced damage layer and the in-depth understanding of the ion-solid interactions physics leading to tool wear in diamond machining process are significant to develop an effective way to improve the tool wear resistance and prolong the tool life of nanoscale multi-tip diamond tool.

In this paper, the nanometric cutting process using nanoscale multi-tip diamond tools has been stimulated by molecular dynamics (MD) simulation method. The effects of FIB induced damage on the wear resistance of nanoscale multi-tip diamond tool under different cutting conditions were analysed.

2. Mould and simulation method

In order to build multi-tip diamond tool model with FIB induced damage layer around tool tips, multi-particle collision of single crystal diamond has been carried out to bombardment the diamond cutting tool tips using the simulation method proposed in [4].The geometry of the multi-tip tool is shown in figure1. A damage free nanoscale multi-tip single crystal diamond tool was built with the same geometry. The cutting tool were set to cut along the X-axis (figure 1(d)). The cutting parameters were summarized in table 1. The MD simulations were implemented through an open source code, LAMMPS, complied on a high performance computing (HPC) platform using 32 cores.

Table 1 The processing parameters of **n**anoscale multi-tip tool cutting.

Component	Depth of cut (nm)	Cutting speed (m/s)
Ideal tool	3.0	50
Tool with damage	3.0	50, 100, 200
	1.0, 1.5, 2.0, 2.5, 3.0	50

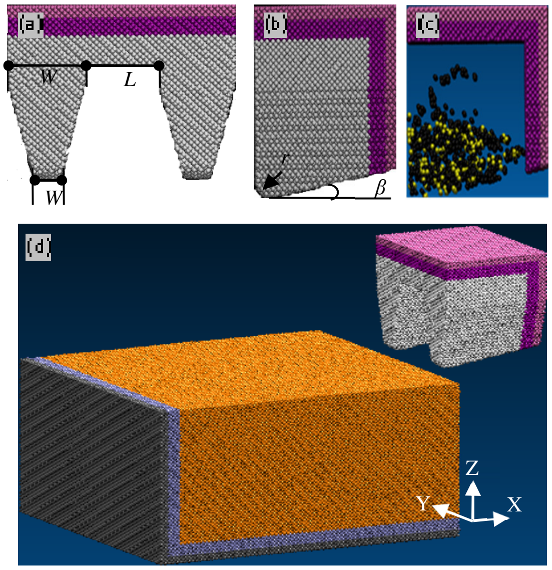


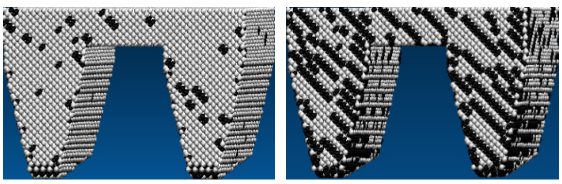
Figure 1. The MD model of nanometric cutting of copper using nanoscale multi-tip diamond tools. (a) Front view of the multi-tip tool model; (b) Right hand end elevation of the tool tip model; (c) Predefined damage inside diamond tools; and (d) the nanometric cutting model using multi-tip tool.

3. Results and discussion

3.1. Atomistic damage formed in multi-tip diamond tool

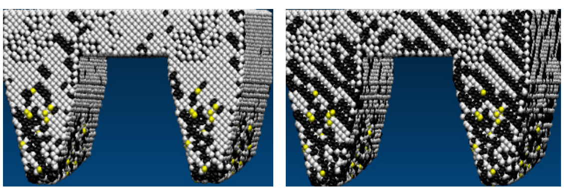
Figures 2 and 3 show the atomistic damage formed in diamond tools. The atoms were coloured according to the value of common neighbour analysis [4]. The wear resistance of the cutting tool was characterized by the total number of new defect atoms formed during nanometric cutting. For the damage free tool cutting, it is found that the sp^2 bonded carbon atoms were formed and accumulated on the surface layers of tool tips. However, the sp^2 bonded carbon atoms were found both on the surface and the deep inside of tool when cutting using the tool of predefined irradiation damage, which indicate that the FIB irradiation induced doping and defects can degrade the wear resistance of the nanoscale multi-tip diamond tool. Moreover, the implanted gallium atoms (yellow colour) were found to move to the tool surface and left vacuums inside diamond tool tip, which would further degrade the strength of the tool.

The temperature distribution in the tool tips are shown in figure 4. As compared with the damage free tool cutting, a higher cutting temperature was found when cutting with the tool of ion irradiation damage. The highest temperature region was found on the tool rake face.



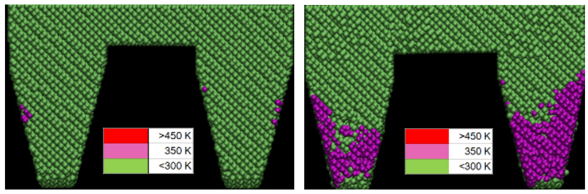
(a) Before cutting (b) After cutting

Figure 2. The atomistic damage formed in ideal cutting tool



(a) Before cutting (b) After cutting

Figure 3. The atomistic damage formed in tool with predefined defects



(a) Ideal cutting tool (b) Tool with predefined defects

Figure 4. The temperature distribution of tool tips in cutting process

3.2. The response of FIB-induced damage to cutting parameters

Moreover, the variation of the wear resistance of pre-damaged tool against the depth of cut and the cutting speed has been further analysed. As shown in figure 5, under the same cutting speed, the number of the sp^2-bonded C atoms increases with the depth of cut. Under the same depth of cut, the sp^2-bonded C atoms increases with the cutting speed (figure 6). The results indicated that the cutting parameters have significant effect on the formation of sp^2-bonded atoms in diamond. Low cutting speed can potentially prolong the nanoscale tool life.

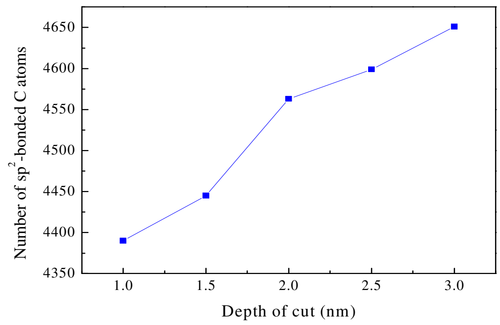


Figure 5. The variation of sp^2-bonded C atoms against depth of cut. (Cutting speed = 50 m/s)

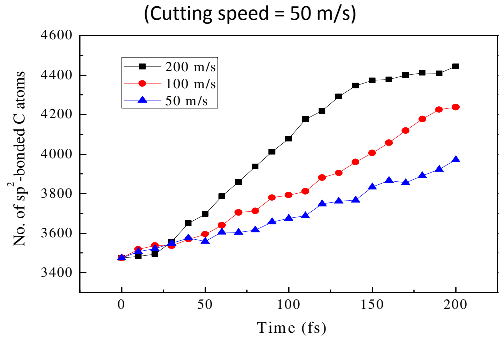


Figure 6. The variation of sp^2-bonded C atoms against the cutting speed. (Depth of cut = 3.0 nm)

4. Conclusions

In this paper, the effect of FIB induced damage on the wear resistance of nanoscale multi-tip diamond tool have been studied using the MD simulation method. The FIB irradiation induced doping and defects can cause the formation of sp^2-bonded C atoms inside the diamond and degrade the strength of diamond tool tip. The cutting parameters can affect the formation of sp^2-bonded C atoms. The research findings from this study inform the in-depth understanding of tool wear of FIB shaped multi-tip diamond tool observed in previous nanometric cutting experimental work.

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