Possible mechanism of strength change of diamond depending on thermal histories based on molecular dynamics analysis

H. Tanaka[1], S. Honda[2], S. Shimada[1]
[1]*Osaka Electro-Communication University, Japan*
[2]*Technology Research Institute of Osaka Prefecture, Japan*

hiroaki@isc.osakac.ac.jp

Abstract

Molecular dynamics (MD) simulations of indentations and heat treatments of diamond were carried out to understand the mechanism of strength change of diamond depending on thermal histories. In the simulations, a pre-existing micro crack on diamond surface disappeared by complete healing at 1070 K for 55 ps while no crack healing took place at 590 K for 2000 ps. The length of Hertzian crack decreased and dislocations moved to the crack and vanished at 1700 K. Graphitization was also observed around the crack and the area of graphitization gradually increased. The results of the simulations suggested that the strength increased by crack healing and decreased by graphitization depending on the heating temperature.

1 Introduction

The tool life in diamond turning is mainly governed by the occurrence of fatal cutting edge chipping which deteriorates the quality of turned surfaces. The cutting edge chipping takes place as a result of sudden extension of a pre-existing micro crack under a certain stress field produced by cutting force. It was reported by the authors [1, 2] that the strength decreases of the diamonds subjected to the temperature higher than 800 K for 30 min in air under atmospheric pressure. The specimen heated in copper powder also showed strength decrease even at 523 K. On the other hand, the specimens heated under the temperature between 500 K and 700 K showed strength increase. The temperature for the highest increase rate was shifted to higher temperature under low oxygen partial pressure. However, the mechanisms of the strength change of diamond have not been fully understood. In this paper, in order to

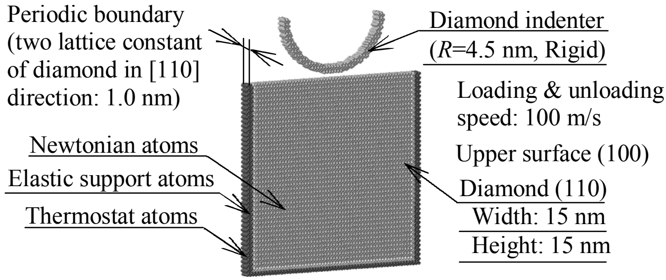


Figure 1: Initial model for crack healing

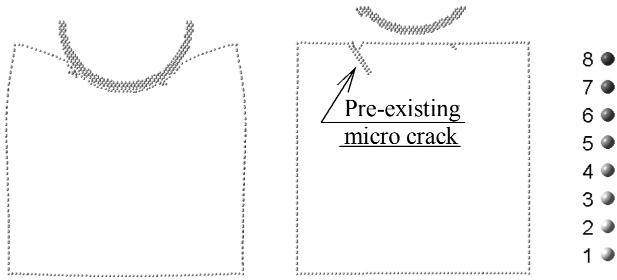
understand the mechanism of the strength change of diamond, MD simulations of indentations and heat treatments of diamond were carried out.

2 Molecular dynamics simulation

The model used for the analysis consisted of a defect-free mono-crystalline diamond specimen and a rigid diamond indenter as shown in Figure 1. The specimen consisted of Newtonian atoms, thermostat atoms and elastic supported atoms [3]. Tersoff type three-body potential [4] was used for diamond specimen while Morse type two-body potential was employed to reflect the interaction between specimen and indenter atoms. Periodic boundary condition was applied in the [110] direction because of generating continuous crack on (111) crystal orientation. MD simulations were processed as follows. The specimen was indented by the indenter so as to induce micro cracks at 293K with a speed of 100 m/s. After unloading, the specimen was heated gradually and kept under various thermal conditions. After cooling down, the second indentations were performed to test strength change. In the simulations, comparatively higher temperatures were applied to accelerate the thermal activities. These processes were equivalent to the experiment under high vacuum.

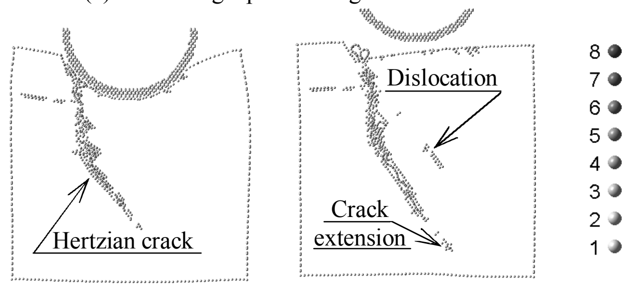
3 Results of molecular dynamics simulation

The first indentations was performed to induce two types of cracks supposing a pre-existing micro crack and a Hertzian crack, respectively as shown in Figure 2. The cracks extended spontaneously during unloading. Then heat treatments of diamond were carried out under several temperature conditions after unloading. Figure 3 shows that the pre-existing micro crack was completely healed at 1070 K for 55 ps



(i) Indentation (d=3.50 nm) (ii) Unloading

(a) Generating a pre-existing micro crack



(i) Indentation (d=3.65 nm) (ii) Unloading

(b) Generating a part of Hertzian crack

Figure 2: Crack initiation by indentation and crack extension during unloading. Gray scales of atoms represent the number of nearest neighbours (N_n).

while no crack healing took place at 590 K for 2000 ps. The length of Hertzian crack decreased and dislocations moved to the crack and vanished at 1700 K for 2375 ps. Graphitization was also observed around the crack and the area of graphitization gradually increased as the heating time increased. After cooling down, second indentations were performed to test the strength change. Figure 4 shows the effect of heating temperature on Hertzian strength. The results of MD simulations suggested that the strength increased by crack healing and decreased by graphitization depending on the heating temperature.

4 Conclusions

In the simulations, a pre-existing micro crack was completely healed at 1070 K while no crack healing took place at 590 K. The length of Hertzian crack decreased and dislocations moved to the crack and vanished at 1700 K. Graphitization was also

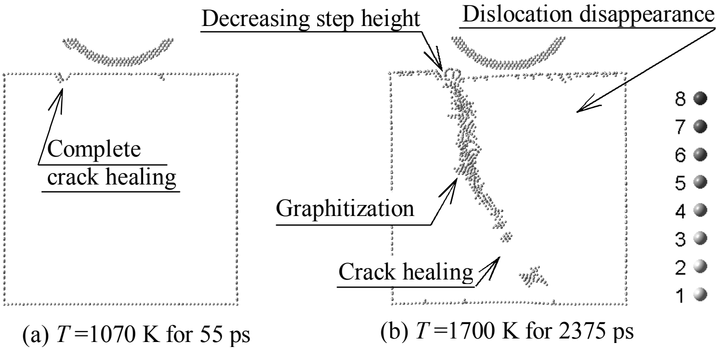


Figure 3: Effect of heat treatment on crack behaviours.

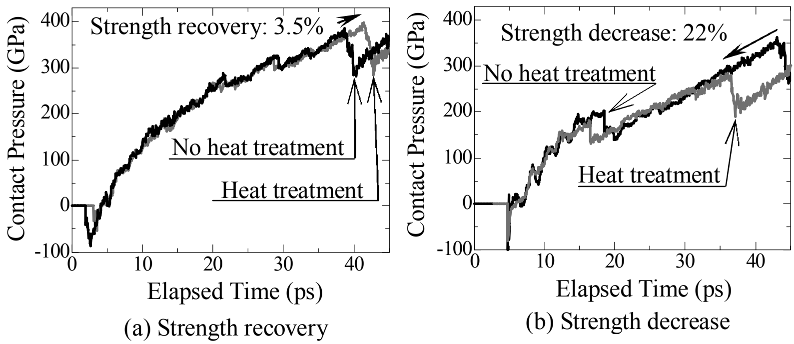


Figure 4: Strength change caused by heat treatment. (a) Strength recovery achieved by complete crack healing of small crack after heat treatment at 1070 K for 55 ps. (b) Strength decrease caused by graphitization of large crack after heat treatment at 1700 K for 2375 ps.

observed around the crack and the area of graphitization gradually increased. As a result, the strength increased by crack healing and decreased by graphitization depending on the heating temperature.

References:

[1] S. Shimada, H. Tanaka, et al.: Annals of CIRP, **49**/1 (2000) 21-24.

[2] H. Tanaka, S. Shimada, et al.: Annals of CIRP, **54**/1/ (2005) 51-54.

[3] H. Tanaka, S. Shimada, L. Anthony: Annals of CIRP, **56**/1 (2007) 53-56.

[4] J.Tersoff : Physical Review B, **39**/8 (1989) 5566-5568.