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Graphitization Behavior of Single Crystal Diamond for the Application in Nano-Metric Cutting

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Abstract: Background: Graphitization behavior of diamond has received an increasing interest in nanoscale machining of some hard and brittle materials. Diamond has always been an important and excellent tool material in cutting area. However, the graphitization of the diamond tool is inevitable when it was used in special conditions. It is indicated that the graphitization of diamond crystal has great influence on the wear resistance of diamond cutting tool. The graphitization behavior needs to be investigated extensively in nanoscale with an atomic view. Molecular dynamics simulation provides a useful tool for understanding of the graphitization mechanism of diamond. The investigation on graphitization behavior of single crystal diamond can also provide a useful reference for the application of diamond cutting tool.

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Materials and Methods: In this paper, a molecular dynamics (MD) diamond crystal model is built to examine the graphitization behavior of diamond under various conditions. The sixfold ring method was employed to identify the structural characteristics of graphite and diamond. The effects of temperature and crystal orientation on the graphitization of diamond have been revealed. Considering the effect of temperature, the anisotropy of diamond graphitization against various crystal planes is presented and discussed carefully. The nano-metric cutting model of diamond tool evaluated by the sixfold ring method also proves the graphitization mechanisms in atomic view.

Results: Results indicate that the sixfold ring method is a reliable method to evaluate the graphitization behavior of diamond crystal. There exists a critical temperature of the graphitization of diamond. The results also show that {111} plane is more easy to get graphitization as compared with other crystal planes. However, {100} plane of diamond model presents the highest anti-graphitization property.

Conclusion: The obtained results have provided the in-depth understanding on the wear of diamond tool in nano-metric machining and underpin the development of diamond cutting tool.

Keywords: Graphitization, sixfold ring, crystallographic orientation, molecular dynamics, nano-metric cutting, crystal diamond.

1. INTRODUCTION

Since the graphitization of diamond was firstly noticed in the early stage of last century, it has generated considerably great interest in many diamond related applications [1]. The original theoretical model considered that ripple-like diamond (111) plane transformed into hexagon plane and the distance between two crystal planes can increase by adjusting atomic positions. Eventually, the tridimensional netlike structure of diamond could change to layer-like structure of graphite. Besides theoretical investigation, the activation energy and activation volume of diamond graphitization were also calculated to examine the

graphitization behavior during the heating process of diamond crystal. In 1972, according to the results of the activation volume for graphitization of diamond in high temperature and high pressure (HTHP), Davies *et al.* presented the two-step mechanism of diamond graphitization, in which the single carbon atoms escaped from diamond surface in an intermediate activated state and then cohered to graphite [2]. Fedoseev found that the activation energy of diamond was different in various temperature ranges in 1986 [3]. Butenko further calculated the activation energy of graphitization, which is 188 kJ/mol in the range of 1370-1860K [4]. Due to the great difference of the activation energy of diamond graphitization in high and low temperature conditions, Fedoseev indicated that there were two different graphitization mechanisms in the two temperature ranges divided by Deby temperature [3].

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Diamond has always been an important and excellent tool material in cutting area [5]. Unfortunately, the graphitization of the diamond tool, which is attributed to the atomic reaction between carbon and iron, is inevitable when it was used for cutting iron or low-carbon steel [6, 7]. Kuznetsov investigated the anisotropic effects of diamond in lower temperature [8]. The graphitization behavior of diamond was analyzed in terms of crystal structure and activation energy. Narulkar *et al.* simulated the cutting of pure iron using diamond tool and investigated the graphitic structure of diamond tool [9]. The anti-graphitization of (100) plane was analyzed in their research. With the experiments of ultra-precision cutting of SiC reinforced composites, Ge *et al.* pointed out that the graphitization of diamond occurred under the catalyzing of both copper and oxygen in the matrix [10]. Jia examined the wear of diamond tool after the ultra-precision cutting of optical glass with Raman spectra and the peak of graphite was found in the experiments [11]. These studies indicated that the graphitization of diamond crystal had significant influence on the wear resistance of diamond cutting tool. However, most analyses and results were based on the experimental observation. The graphitization behavior needs to be investigated extensively in nanoscale with an atomic view. Presently, there is a lack of reliable method for the evaluation of graphite and diamond in the nanoscale simulation of diamond cutting. With the aid of molecular dynamics simulation, the in-depth understanding of the graphitization mechanism of diamond, especially knowing the graphitization behavior considering its application on cutting tool is of great significance to fully explore the advance of diamond machining technique [12-14].

In this article, a novel diamond crystal model was built to examine the graphitization behavior of diamond. The sixfold ring method was introduced to identify the structural characteristics of graphite and diamond. Moreover, the temperature and crystallographic orientation has been analyzed in view of the effect of diamond graphitization. At last, the graphitization of diamond tool was examined with sixfold ring method in consideration of the application in nano-metric cutting. The research presents a reliable method for the identification of graphitization and gives a better understanding of the graphitization behavior of diamond cutting tool.

2. THE SIXFOLD RING STRUCTURE IN DIAMOND AND GRAPHITE

As the allotrope of carbon, diamond and graphite can be thought as composition of the minimal spatial sixfold ring structure in the atomic scale. The schematics of sixfold ring structures for diamond and graphite are shown in Fig. (1). For single crystal diamond, each carbon atom is possessed by 12 sixfold rings, which contains 29 carbon atoms in 3 neighbor atom layers as shown in Fig. (1a). In contrast, graphite is composed by layer-like sixfold ring structure, as shown in Fig. (1b).

Fig. (1). The sixfold ring structure in diamond and graphite.

In the atomic structure of graphite, each carbon atom is shared by 3 sixfold rings and the profile of sixfold ring is quite different from that of diamond. The sixfold ring in graphite is planar regular hexagon, whereas the sixfold ring in diamond is ripple-like tridimensional structure. Because of the distinction in the structural characteristics, the atomic sixfold ring structure can be used as a tool to analyze diamond and graphite in the process of graphitization.

3. MATERIALS AND METHODS

3.1. Graphitization Model of Diamond Structure

As to the low indices of diamond crystal (100), (110) and (111) planes, there is no sixfold ring on (100) plane. The graphitization on the (100) plane of diamond needs complex reconstruction greatly, whereas (110) and (111) planes with sixfold rings can change to graphite directly [7]. Hence, the graphitization behavior on (111) and (110) plane is analyzed in the paper in view of the structure property of the diamond.

Fig. (2) shows the (111) and (110) planes of diamond crystal contrasting to the corresponding (001) plane of graphite after graphitization. There are 10 sixfold ring structures along horizontal and vertical directions for both (111) and (110) planes. The original low indices faces of diamond crystal (110) and (111) planes are shown in red color and the (001) plane of graphite is denoted in black color. Under the condition of low temperature, the C-C bonds can be broken out along the dash line in Fig. (2). The shrinking and peeling layer can become planar and eventually change the (111) and (110) planes of diamond crystal to the (001) plane of graphite.

Fig. (2). The (111) and (110) planes of diamond.

The graphitization property is different according to various diamond crystal planes. As shown in Fig. (2a), the projection of (111) plane along crystal direction is 0.063 nm longer than graphite piece, which means the graphitization on the (111) plane of diamond is a shrinking process. If the graphitization behavior occurs on the (111) plane of diamond, the shrinking of graphite piece may produce internal tensile stress and then accelerate the process of graphitization. In some cases, the internal tensile stress can be enough to peel off the graphite piece. Evans found some discontinuous graphite pieces with lengths of 10~15 nm while the (111) face of diamond graphitized [15]. As shown in Fig. (2b), the projection of (110) face along crystal direction is 0.063 nm longer than graphite piece, whereas the projection along [100] is 0.347 nm shorter than graphite piece. This means the (110) face of diamond shrinks along crystal direction and expands along [100] crystal direction in graphitization. The crystal structure denotes that the (110) face of diamond suffers from higher compressive stress, which can restrain the peeling of the (110) face. Generally, the graphitization on the (110) plane of diamond requires more energy. Therefore, it can be concluded that the (111) plane of diamond can be graphitized more easily as compared with the (110) plane.

3.2. MD Simulation Conditions for Diamond Nanoparticle

A nanoscale particle model of diamond was built to examine the anisotropic effects on the graphitization of diamond. Based on the octahedron structure of diamond, the model is adapted for two (100) faces, four (110) faces and four (111) faces. As shown in Fig. (3), the x and z axes of the model are along [110] crystal direction and the y axis is along [100] crystal direction. The geometrical parameters and simulation conditions of the model are listed in Table 1. Tersoff potential function was adopted to describe the interactions among carbon atoms [16]. In order to analyze the effects of temperature on diamond particle, the model was kept separately at each temperature of 750°C, 1000°C, 1500°C and 2000°C for one nanosecond. Energy minimization technique was applied on the simulation results to decrease the effect of thermal vibration on bond length and bond angle.

Fig. (3). Nanoparticle model of single crystal diamond.

Table 1. The parameters and conditions for the simulation of diamond particle.

Parameters	Value
Top length L_1 / nm	7
Bottom length L_2 / nm	13.5
Height H / nm	10
Potential	Tersoff
Time step / fs	1

4. RESULTS AND DISCUSSION

4.1. Evaluation for the Graphitization Behavior in Diamond

Fig. (4) shows the extracted atoms by the methods of coordination number (CN) and sixfold ring. The CN method was used as reference because it is one of the most popular tools for denoting the carbon atom structure [17-19]. The purple atoms in the Figure represent the CN or sixfold ring is three and the cyan represents the atom that the number is less than three. The inner carbon atom in diamond crystal with a coordination number of four represents the sp^3 structure. The coordination number of surface carbon atom is usually lesser for the reason of inherent structure defects on the surface. Generally, the surface carbon atoms on the {110} and {111} faces with CN 3 are sp^2 bonding structure, whereas the surface carbon atoms on the {100} planes with CN 2 are sp bonding. The coordination number of most carbon atoms in graphite crystal is 3 except for a few edge atoms. As shown in Fig. (4a), though the atoms changing from sp^3 to sp^2 can be extracted by using the tool of coordination number, the surface carbon atoms without any structural change are also extracted. So the coordination number method is quite hard to distinguish these two kinds of atoms.

If the sixfold ring method is used to distinguish diamond and graphite, it can work properly on the {110} and {111} faces. The maximum sixfold ring number for the inner carbon atom in diamond crystal is 12. The sixfold ring number for the surface carbon atoms on the {110} and {111} faces is greater than 4. However, the sixfold ring number for the

surface and edge carbon atoms on the $\{100\}$ is less than 4. The sixfold ring number of graphite is also less than 4. As shown in Fig. (4b), since the sixfold ring numbers for diamond particle and graphite atoms are not in the same range, the atoms extracted on the $\{110\}$ and $\{111\}$ faces are the changing atoms from sp^3 to sp^2 and a few of edge atoms without structure changing. Because the sixfold ring numbers for diamond particle and graphite atoms on the $\{100\}$ faces are in the same range, all the atoms can be extracted except some reconstructed atoms. Compared with the coordinate number, the sixfold ring can be useful to extract the structure changing atoms on the $\{110\}$ and $\{111\}$ faces, so it is adopted to distinguish the diamond and graphite atoms, even the graphitization status of diamond nano-particle. It is shown in Fig. (4b) that the sixfold ring method can be used to identify the graphitized atom when the temperature reaches 750°C. The result of sixfold ring also indicates that the atoms with structure defects or located in $\{111\}$ faces are easier to be graphitized than the atoms in the other two low lattice faces.

Fig. (4). Extraction results of carbon atoms on diamond surface by using various identification methods.

4.2. The Effect of Temperature on the Graphitization of Diamond Nanoparticle

It was proved that nanoscale diamond particle could be graphitized when the critical temperature increases to 640°C [20]. However, so far the effect of temperature variation on the graphitization behavior has not been fully understood in terms of atomic point view. With the MD nanoparticle model of single crystal diamond, the effect of temperature on diamond graphitization has been analyzed. Fig. (5) shows the results of radial distribution function (RDF) and angular distribution function (ADF) of diamond nanoparticle in various temperatures. As shown in Fig. (5), the first peak of RDF and ADF centered at 0.1545 and 109.5° can be found respectively before relaxation. These results including the bond length and bond angle are in good agreement with the ideal diamond structure. When the particles are relaxed at 750°C and 1000°C, respectively, the RDF and ADF coincide with those of the ideal diamond structure approximately. In this stage, the diamond peak values decline slightly and smaller new peaks appear at bond length of 0.148 nm and bond angle of 120°. The new bond angle is the same as that of graphite. Correspondingly, the new-born bond length between diamond and graphite bond lengths is slightly larger than the carbon onion of 0.146 nm [21]. This characterized effect indicates a mixture status of diamond and graphite that can be seen as a clear evidence of the slightly graphitization of diamond nanoparticle at this stage. Thereafter, 1000°C can be

considered as the critical temperature for graphitization. These results agree with previous experimental results, where the graphitization of diamond can only be seen above 900°C [22]. Because the relaxation temperature is slightly higher than the initial temperature of the diamond graphitization, the graphitization is not obvious, which makes the peak values of graphite carbon much lower.

a) Bond length

b) Bond angle

Fig. (5). RDF and ADF of diamond nanoparticle in various temperatures.

At temperature of 1500°C, the graphite peak increases while the decrease of diamond peak can be found. However, the peak value of diamond is still larger than that of graphite. When temperature reaches 2000°C, the diamond peak completely disappears. The diamond nanoparticle is fully graphitized at 2000°C and the bond length of graphite also drops to 0.147 nm, which is also in close agreement with the previous simulation results.

4.3. The Effect of Crystallographic Orientation on the Graphitization of Diamond Nanoparticle

Besides the temperature factor, the effect of diamond anisotropy on its graphitization is so important that the anti-

wear and hardness in various crystallographic orientations must be considered as it is used as a cutting tool. In order to examine the graphitization behavior of the nano-particle, a slice with thickness of 1 nm is extracted in the middle of the nanoparticle paralleling to its $\{110\}$ crystal plane. The anisotropy effects on graphitization of the diamond nanoparticle at various temperatures are shown in Fig. (6).

It is shown in Fig. (6a) that slight delamination can be noticed on the nanoparticle surface due to the rupture of C-C bonds between the two outermost layers at temperature of 750°C. The delamination indicates that the nanoparticle has been graphitized, which also further verifies the previous results of the RDF and ADF. The delamination is observed on the $\{111\}$ plane, whereas little delamination are found on the $\{100\}$ and $\{110\}$ planes. The graphitization mode of the $\{111\}$ plane is in agreement with that in Fig. (2a), i.e., the $\{111\}$ plane can be transformed into graphite fragments with interlayer C-C bonds broken between the $\{111\}$ planes. Due to more dangling bonds on $\{110\}$ plane, the bond reconstructions are easily to occur on these surfaces. The new C-C bonds formed between the dangling bonds can make the surface thermodynamic property much stable. However, no delamination and reconstructions are found on the $\{110\}$ plane. The results agree well with the simulation of previous researchers by using density functional theory [23].

At 1000°C, the delamination on the nanoparticle surface is a little bit obvious, which can be observed in the sub-surface as shown in Fig. (6b). Some larger pieces of graphite fragments are formed on the $\{111\}$ surface, without full exfoliating from the nano-particle. The level of reconstruction on the $\{100\}$ surface is higher than that at lower temperature. A thin reconstruction layer has already formed. However, there is still no deformation on the $\{110\}$ surface.

More sp^3 -bonded carbon atoms are transformed into graphite structure at 1500°C, as shown in Fig. (6c). Except the $\{100\}$ surface, the graphitization appears on both the $\{111\}$ and $\{110\}$ surfaces. However, the level of graphitization on the $\{111\}$ surface is much higher than that on the $\{110\}$ surface. The outermost layers on the $\{111\}$ surface nearly exfoliate fully from the nanoparticle and transform to layered graphite fragments. The size of the delamination on the $\{110\}$ surface are much smaller than on the $\{111\}$ surface. The graphitization takes place on the $\{110\}$ surface along $\langle 110 \rangle$ direction. The graphitization mode of the $\{110\}$ surface is also in agreement with that in Fig. (2b), i.e., the breaking of C-C bonds between the outermost layers along the dashed line makes the graphitization occurred on the $\{110\}$ surface. It can be noticed that the graphite fragments on the $\{110\}$ surface protrude out of the original boundary of nano-particle.

When the temperature reached 2000°C, the nanoparticle almost fully graphitizes. As shown in Fig. (6d), most diamond atoms change from sp^3 to sp^2 bonding, leaving a small quantity of sp^3 carbon marked in purple color in Fig. (6d). Kuznetsov proposed that the complicated construction was necessary to make the $\{100\}$ surface transform into graphite fragments [8]. The graphitization of the upper and lower parts of the nanoparticle are along different $\langle 111 \rangle$ lines. The dashed line in Fig. (6d) between the two middle points

Fig. (6). Effect of diamond anisotropy on graphitization of diamond nanoparticle at various temperatures.

on the projection lines of $\{110\}$ surface can be thought as the boundary of the different graphitization directions.

The graphitization of upper and lower parts of the nanoparticle takes place along two $\langle 111 \rangle$ directions with an angle of 70.52° and forms graphite fragments with two different directions at the same time [24]. The neighboring $\{111\}$ planes were connected by the reconstructions of the carbon atoms on the $\{100\}$ surface, which formed various U-shaped

structures. During the graphitization process, the structures were transformed into U-shaped graphite shell. The average interlayer spacing is calculated along the calculation line in Fig. (6d). It is 0.265 nm from the calculation, whereas it is 0.206 nm for two adjacent diamond $\{111\}$ planes and 0.35 nm for graphite. The average interlayer spacing lies between those of diamond and graphite. This is because the two ends of the graphite fragments still connected to the nanoparticle and the graphite fragments don't fully exfoliated from the particle. From the simulation, it is shown that $\{111\}$ plane is apt to graphitize and $\{110\}$ plane is the next one at temperature ranging from 750°C to 2000°C. The $\{100\}$ surface has the strongest capability for anti-graphitization in this temperature range. The simulation result is in agreement with experimental report from Ref. [8].

5. APPLICATION OF GRAPHITIZATION ANALYSIS FOR DIAMOND CUTTING TOOL

A new simulation was performed with cutting single crystal silicon with the diamond cutting tool. MD model of diamond cutting tool is shown in Fig. (7), in which single crystal silicon acts as the workpiece material. The tool model includes the rigid atoms, which are marked in purple color in the fixed layer, and the rest parts are the non-rigid atoms. According to the analysis above, $\{111\}$ planes of diamond crystal are prone to graphitization, so (111) plane is chosen as the rake face and $(11\bar{2})$ plane acts as the flank face of the tool separately. The $(11\bar{2})$ plane is composed of several step-like (111) planes. In the geometrical model, there is an (001) plane facet in the middle of cutting edge, forming 'round' cutting edge with radius of 3 nm. The rake angle is set as -7° and the flank angle is 7° in the model.

The graphitization status of diamond tool is presented in Fig. (8). The purple balls represent the fixed layer. The black balls represent the atoms with sixfold ring number of 1 ~ 3 and the sixfold ring number of other atoms are ranged from 4 ~ 12. It is shown in Fig. (8a) that there are some atomic rings on the rake face and cutting edge. Especially the atoms in the sixfold ring structure are shared only by about one to three sixfold rings, which means graphitization wear occurs on the area. The atoms in regions A and B denote the severe graphitization wear in nanometric cutting. In region A, the atoms evolve into a graphite scrap with seven rings in multiple lines and a single line graphite scrap can be found in region B. It is hard to distinguish the graphitization status of region C in the angle of view in Fig. (8a). The local enlarged view of region C is shown in Fig. (8b). The C-C bonds on the last three step-like (111) planes on the flank face are broken out completely. Delamination can be noticed on the surface, indicating the severe graphitization in this region. Compared with the status on the rake face and the 'round' cutting edge, the graphitization behavior is much distinct on the flank face.

According to the compared results, it is denoted that the most severe graphitization occurs on the $(11\bar{2})$ plane and the next is (111) plane. The $(1\bar{1}0)$ and (001) planes are hard to be graphitized under this cutting condition. In the simulation, $(11\bar{2})$ and (111) planes are composed with $\{111\}$ plane, in which the graphitization is caused by the direct

Fig. (7). MD model for diamond cutting tool.

Fig. (8). Graphitization behavior of diamond tool.

change of diamond to graphite. So the $\{111\}$ plane of diamond can cause the graphitization of cutting tool, which is consistent with the previous analysis of diamond particle. The sixfold ring method is also confirmed to be reliable in describing the graphitization wear of diamond tool in the nanometric cutting.

CONCLUSION

In this paper, the sixfold ring method is presented to evaluate the graphitization of single crystal diamond. With the analysis of diamond structure and nanoparticle of MD model, the validity for evaluating the graphitized diamond using sixfold ring is investigated in order to obtain the key property of the graphitization behavior. Meanwhile, the temperature effect on graphitization is investigated with the model. The results show that the $\{110\}$ and $\{111\}$ surfaces including sixfold ring can be transformed directly into graphite fragments by delamination, however, the $\{100\}$ surface cannot be changed directly due to the lack of sixfold ring structure. Among the three low index planes, the $\{111\}$ plane can be graphitized easily and the $\{100\}$ plane is the most difficult at temperature ranging from 750°C to 2000°C. At 2000°C, the severe change on the $\{100\}$ plane can cause full graphitization of the nanoparticle. The effect of graphitization behaviors of diamond cutting tool are also revealed with

the aid of sixfold ring method. It is also denoted that {111} plane tends to be graphitized easily, which can provide a useful reference for the application of diamond cutting tool.

LIST OF ABBREVIATIONS

ADF	=	Angular Distribution Function
C-C	=	Carbon - Carbon
CN	=	Coordination Number
HTHP	=	High Temperature and High Pressure
MD	=	Molecular Dynamics
RDF	=	Radial Distribution Function

ETHICS APPROVAL AND CONSENT TO PARTICIPATE

Not applicable.

HUMAN AND ANIMAL RIGHTS

No Animals/Humans were used for studies that are the basis of this research.

CONSENT FOR PUBLICATION

Not applicable.

CONFLICT OF INTEREST

The authors declare no conflict of interest, financial or otherwise.

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