Born-Oppenheimer Molecular Dynamics of OH Radical in the SiC Grains in the Reaction-Sintered Silicon Carbide

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Abstract. Born-oppenheimer molecular dynamics is an effective method to analyze machining mechanism of some advanced manufacturing techniques, which was introduced to investigate the absorption of OH radical on different β-SiC surfaces in the reaction-sintered silicon carbide. During the plasma oxidation-assisted polishing of reaction-sintered silicon carbide, absorption of the OH radical in the SiC grains was one of the most important process, because hardness of the SiC grains was obviously higher than that of the Si grains. The born-oppenheimer molecular dynamics model to investigate the absorption process of the OH radical was constructed firstly, which could form the foundation for the further simulation and analysis. Secondly, absorption of the OH radicals in the Si-face, those in the C-face, and those in the asymmetric face were investigated successively, which included the absorption process and the oxide product. Finally, comparisons of the absorption of the OH radical in the different faces were conducted, which aimed to further understand the plasma oxidation-assisted polishing of reaction-sintered silicon carbide. Simulation result of born-oppenheimer molecular dynamics was propitious to promote the machining level of reaction-sintered silicon carbide and promote its practical application.

1. Introduction
Born-oppenheimer molecular dynamics is an effective method to analyze the machining mechanism of some advanced manufacturing technique, which could be propitious to improve width, thickness, and accuracy of the computer simulation. Bui et al. [1] had utilized born-oppenheimer molecular dynamics to analyze absorption process of the hydrogen fluoride (HF) on single crystal silicon carbide surface in the catalyst-referred etching. Born-oppenheimer molecular dynamics model of machining of the single crystal copper (Cu) had been constructed by Gao et al. [2] based on the massively parallel algorithm, and temperature distribution of the system and influences of its thermal effect in the nano-machining process were investigated. Du et al. [3] had applied born-oppenheimer molecular dynamics to simulate the femtosecond laser processing process of the single crystal silicon, which could study influence of the ablation phenomena and laser characteristic parameters to the manufacturing object. Therefore, the born-oppenheimer molecular dynamics of OH radical in the SiC grains in the reaction-sintered silicon carbide was conducted in this study, which aimed to improve its machining level.

Reaction-sintered silicon carbide surface with high accuracy could be obtained by novel oxidation-assisted polishing method [4-11], which was combination of oxidation of the original ultra-hard silicon carbide and further polishing of the soft oxide layer. During the plasma oxidation-assisted polishing of reaction-sintered silicon carbide, absorption of the OH radical in the SiC grains was one of the most important process, because hardness of the SiC grains was obviously higher than that of the Si grains in the reaction-sintered silicon carbide. However, these SiC grains in reaction-sintered silicon carbide
were not uniform, and the major component was $\beta$-SiC. Therefore, absorption characteristics of the OH radical on different $\beta$-SiC surfaces were investigated in this research.

Firstly, the born-oppenheimer molecular dynamics model to investigate absorption process of the OH radical was constructed, which could form the foundation for the further simulation and analysis. Secondly, absorption of the OH radical in the Si-face, that in the C-face, and that in the asymmetric face were investigated successively, which included the absorption process and the products. Finally, comparisons of the absorption of the OH radical in the different faces were conducted, which aimed to further understand and master plasma oxidation-assisted polishing of reaction-sintered silicon carbide.

2. Absorption in the Si-face
Schematic diagram of the absorption of the OH radical in the Si-face by born-oppenheimer molecular dynamics at 373K is shown in Figure 1, and the corresponding simulation times were 0fs, 30fs, 206fs, 355fs, 419fs, 701fs, 758fs, 2024fs, and 4999fs respectively.

![Figure 1. Absorption of OH radical in the Si-face by born-oppenheimer molecular dynamics at 373K.](image)

In order to evaluate influence of the experimental temperature to the simulation results in the born-oppenheimer molecular dynamics model, absorption process of OH radical in the Si-face at 353K was conducted, which could be treated as a contrast with that at 373K. Before the simulation time of 710fs, the simulation process in the Figures 1(a) to 1(f) was almost consistent with that in the Figures 2(a) to 2(f). However, after the 758fs, the water molecule absorbed in the upper surface rose suddenly, and it was finally absorbed by the lower surface at 1650fs. Meanwhile, this water molecule was completely
absorbed and decomposed in the lower surface. At this moment, both the upper surface and the lower surface absorbed three O atoms. For the experimental temperature 373K in Figure 1, two OH radicals were generated when the water molecule was absorbed completely, because there was only one O atom on the original surface. On the contrast, there was one H atom absorbed on the Si atom alone at the lower surface, because two OH radical had already been absorbed on the lower surface when the water molecule was absorbed, which was consistent with the simulation results in the Figure 2. Thus, it could be found that experimental simulation temperature had little influence to the simulation result, which indicated that the further simulation temperature could be set 353K.
3. Absorption in the C-face

Absorption simulation of the OH radical in the C-face by born-oppenheimer molecular dynamics was conducted, and the simulation results were shown in the Figure 3. It could be found that the reaction was occurred among the two OH radicals and the lower surface at the time of 585fs. In this process, One O atom was absorbed on the surface, and the other atoms formed one water molecule. Meanwhile, the other OH radicals formed the H$_2$O$_2$ molecule, and this H$_2$O$_2$ molecule was not absorbed, although it approached the surface for several times. The simulation result at 585fs proved that the C-face also had some potential to absorb and decompose the OH radical. The lower surface absorbed with O atom still kept in good order, which indicated that the inner structure was not destroyed and there was no further decomposition reaction. The simulation results proved that absorption of the OH radical in the C-face was obviously poor relative to that in the Si-face. The major reason for this phenomenon was that the C-face was more steady resulted from recombination of the C atoms.
4. Absorption in the asymmetric face
Absorption process of the OH radical in asymmetric face by born-oppenheimer molecular dynamics was conducted, and the simulation results were summarized in the Figure 4. The corresponding times were 0fs, 240fs, 383fs, 540fs, 576fs, 3400fs, 4999fs, 6284fs, 7500fs and 10000fs respectively. It could be observed that the simulation result for the asymmetric face in the Figure 4 was quite different from that for the Si-face in the Figure 1 and that for the C-face in the Figure 3. Both C atoms and Si atoms existed in the asymmetric face, which caused the differences among the simulation results. The lower Si atoms could absorb two OH radicals, and there was no H atom generated when the water molecule joined. Meanwhile, three OH radicals generated two water molecules and one O atom in intermediate reaction, and the O atom was not decomposed when it was absorbed by the upper surface. The original C atom was squeezed to the side when the O atom was absorbed, and the structure kept steady. What’s more, the OH radical absorbed on the lower surface could always absorb two water molecules.

5. Conclusions
For the absorption of the OH radical in the Si-face by born-oppenheimer molecular dynamics, the MD simulation time was 10Ps, and the products were Si-O-H, Si-O-Si, and Si-H. Firstly, the OH radical is
absorbed; secondly, water molecule was produced, and further decomposition reaction was generated when the water molecule moved to the surface absorbed with OH radical. Moreover, for absorption of the OH radical in the C-face by Born-Oppenheimer molecular dynamics, the MD simulation time was 5Ps, and the oxidation products were C-O, H2O, and H2O2. When the OH radical was absorbed, the O atom connected with the C atom, and the H atom could change to water molecule by the combination with the other OH radical. Meanwhile, the other OH radicals generated the water molecule and H2O2 molecule. Furthermore, for absorption of the OH radical in the asymmetric face by Born-Oppenheimer molecular dynamics, the MD simulation time was 10Ps, and the products were Si-O-O-Si, Si-C-C, H2O, and Si-O-H. The lower Si-face could absorb the OH radicals. However, the further absorbed water molecule was not decomposed any more after the absorption of two OH radicals. The research achievement could be favorable to further understand and master plasma oxidation-assisted polishing of reaction-sintered silicon carbide.

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