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Superiority of lonsdaleite to diamond in wear resistance as abrasive grain based on molecular dynamics analysis of grinding silicon carbide

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Abstract

Lonsdaleite (hexagonal diamond) was discovered from the meteorite and has been synthesized from graphite or diamond (cubic diamond). Recently, it was reported by the authors that lonsdaleite in the <0001> direction was harder than diamond in the <111> direction by 63 % and lonsdaleite was tougher than diamond by 32 % based on molecular dynamics analysis of nano-indentation and three-point bending, respectively. However, the wear resistance and mechanism have not been fully understood.

In this paper, to clarify the fundamental wear mechanism of lonsdaleite, molecular dynamics (MD) simulations of grinding silicon carbide by an abrasive grain of lonsdaleite were carried out and compared with that of diamond. The model used in the simulations consisted of a hexagonal or a cubic diamond and a silicon carbide. In general, hexagonal structures have lower friction and wear than cubic structures. To understand the effect of crystal structure on the wear resistance, especially hexagonal structure of lonsdaleite, grinding silicon carbide by lonsdaleite and diamond abrasive grains were performed.

The results showed that the wear mechanism of lonsdaleite was the abrasion subsequent to the graphitization. This was the same wear mechanism as that of diamond. However, the volumetric wear of lonsdaleite was smaller than that of diamond by 34 % at the grinding speed of 200 m/s because of higher resistance for graphitization of lonsdaleite. Furthermore, wear resistance of lonsdaleite was also higher than that of diamond at the higher grinding speed of 400 m/s. As a result, the molecular dynamics simulations clarified the superiority of hexagonal diamonds to cubic diamonds in the wear resistance, as well as high resistance at the higher temperature. These results suggest that lonsdaleite has high potential for use as ultraprecision cutting tools.

Lonsdaleite, Diamond, Wear, Molecular dynamics simulation

1. Introduction

Diamond (cubic diamond) has excellent mechanical properties such as the highest known hardness. On the other hand, lonsdaleite (hexagonal diamond) was discovered from the meteorite and has been synthesized from graphite or diamond (cubic diamond) in a small quantity [1]. Therefore, pcactical application and experiment using lonsdaleite are not yet feasible. However, recently, it was reported by the authors that the maximum contact pressure of lonsdaleite in the <0001> direction was superior to that of diamond in the <111> direction by 63 % and the maximum tensile stress of lonsdaleite in the <0001> direction superior to that of diamond in the <111> direction by 32 % based on molecular dynamics analysis of nano-indentation and three-point bending, respectively [2,3]. However, the wear resistance and mechanism have not been fully understood.

In this paper, to clarify the fundamental wear mechanism of lonsdaleite, MD simulations of grinding silicon carbide by an abrasive grain of lonsdaleite were carried out and compared with that of diamond.

In section 2, simulation methods of MD are described. In section 3, simulation results and discussions are described. Finally in section 4, conclusions of this paper are presented.

2. Molecular dynamics simulations

In general, hexagonal structures have lower friction and wear than cubic structures. To understand the effect of the crystal structure on the wear resistance of lonsdaleite, MD simulations of grinding silicon carbrbide by lonsdaleite (hexagonal) and diamond (cubic) abrasive grains were carried out. The edge radius of the abrasive grain was 4.0 nm with the rake and clearance angle of -45° and 45°, respectively, as shown in Figure 1. The loading and grinding directions of lonsdaleite were <0001> and <1120> and those of diamond were <111> and <112>, respectively.

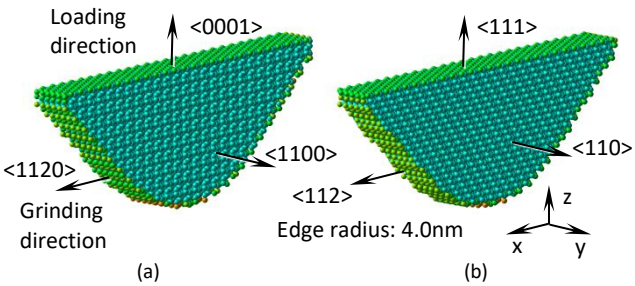

Figure 1. Crystal orientation of grains (a) Lonsdalite (b) Diamond

The model used in the simulations consisted of a hexagonal or a cubic diamond grain and a silicon carbide workpiece, as shown in Figure 2. The both of diamonds abrasive grains and silicon carbide workpiece consisted of Newtonian, thermostat and fixed boundary atoms. The workpiece had the dimensions 17.3 nm × 3.0 nm × 5.4 nm. The Tersoff potential [4] was used to express the diamond structure of lonsdaleite, diamond and silicon carbide, while the Morse potential was employed to express the interaction between both diamonds and silicon carbide. Periodic boundary conditions were applied in the y direction. For the conversion of the kinetic energy of atoms into

an equivalent temperature, the thermal energy derived from the equation of specific heat proposed by Einstein and Debye were used for both diamonds and silicon carbide, respectively. In the thermostat layers which absorb the heat outwards in the model, the kinetic energy of atoms was adjusted for every computational time step so as to maintain the equivalent average temperature at 293 K. The grinding speeds (*Vc*) were 200 m/s and 400 m/s in the x direction with the loading speed of 10 m/s in the z direction.

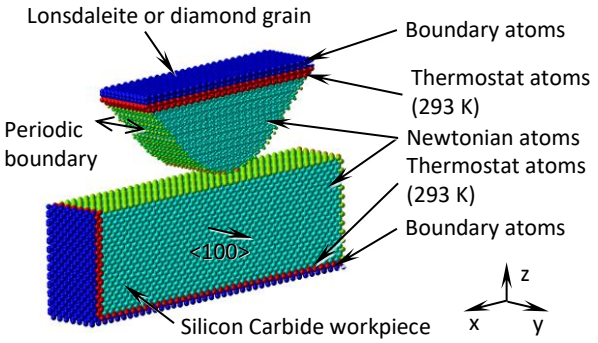

Figure 2. Initial model for grinding of silicon carbide by lonsdaleite or diamond grain

3. Simulation results

Figure 3 shows the difference in amount of material removal between lonsdaleite and diamond. High wear resistance of lonsdaleite resulted in large amount of material removal.

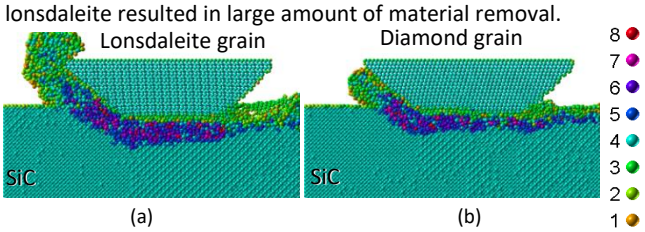

Figure 3. Effect of wear of grain on chip removal at a grinding distance of 50 nm (a) Lonsdaleite (b) Diamond

The results showed that the wear mechanism of lonsdaleite was the abrasion subsequent to the graphitization, as shown in Figure 4. This was the same wear mechanism as that of diamond. However, the volumetric wear of lonsdaleite was smaller than that of diamond by 34 % at the grinding speed of 200 m/s because of higher resistance for graphitization of lonsdaleite, as shown in Figure 5. Step-like graphitizations of lonsdaleite grain showed higher resistance for graphitization. On the other hand, gradual graphitizations of diamond grain showed lower resistance for graphitization.

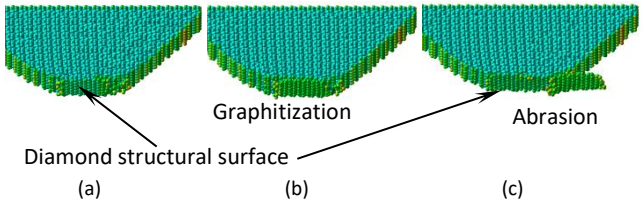

Figure 4. Wear mechanism of lonsdaleite at a grinding distance of (a) 22.5 nm (b) 23.5 nm (c) 26.0 nm

Furthermore, wear resistance of lonsdaleite was also higher than that of diamond at the higher grinding speed of 400 m/s, as shown in Figure 5. The grinding speeds became the higher, the higher temperature were observed at the interface between grain and workpiece, as shown in Figure 6. It showed the excellent wear resistance at the higher temperature.

As a result, the MD simulations clarified the superiority of lonsdaleite to diamond in the wear resistance, as well as high resistance at the higher temperature. These results suggest that lonsdaleite has high potential for use as ultraprecision cutting tools.

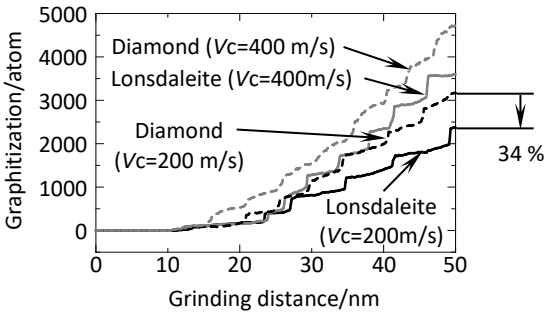

Figure 5. Comparison of number of graphitization atoms between lonsdaleite and diamond at the grinding speed of 200 m/s and 400 m/s

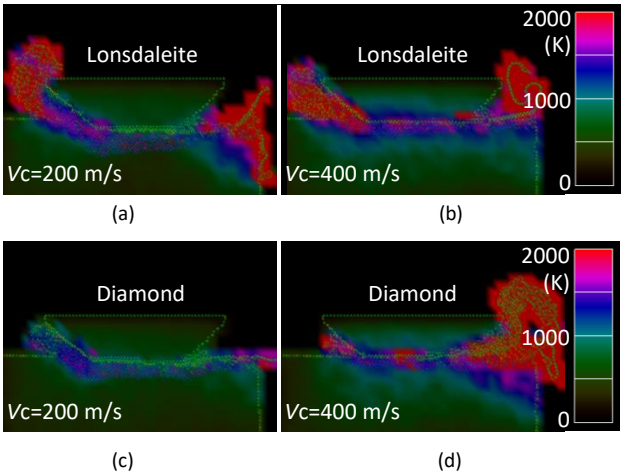

Figure 6. Temperature distribution at a grinding distance of 50 nm (a) Lonsdalite, *Vc*=200 m/s (b) Lonsdaleite, *Vc*=400 m/s (c) Diamod, *Vc*=200 m/s (d) Diamond, *Vc*=400 m/s

4. Conclusions

The results showed that the wear mechanism of lonsdaleite was the abrasion subsequent to the graphitization. This was the same wear mechanism as that of diamond. However, the volumetric wear of lonsdaleite was smaller than that of diamond by 34 % at the grinding speed of 200 m/s because of higher resistance for graphitization of lonsdaleite. Furthermore, wear resistance of lonsdaleite was also higher than that of diamond at the higher grinding speed of 400 m/s. As a result, the MD simulations clarified the superiority of lonsdaleite to diamond in the wear resistance, as well as high resistance at the higher temperature. These results suggest that lonsdaleite has high potential for use as ultraprecision cutting tools. Future work will be forcused on the effect of crystal orientations on the wear resistance of lonsdaleite and compared with that of diamond.

References

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