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Fracture mechanism of lonsdaleite based on molecular dynamics analysis of three-point bending

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Abstract
To clarify the fundamental fracture mechanism of lonsdaleite, molecular dynamics simulations of three-point bending were carried out and compared with that of diamond. The model used in the simulations consisted of a hexagonal or a cubic diamond specimen and three rigid diamond indenters. The Tersoff potential was used to express the diamond structure, while the Morse potential was employed to express the interaction between the atoms in the specimen and the indenters. To understand the effect of crystal orientation especially hexagonal structure of lonsdaleite, three-point bendings were performed in the [0001] direction on lonsdaleite and in the [111] direction on diamond. The results showed that the fracture mechanism of lonsdaleite was different from that of diamond: an amorphous phase transformation from the surface was observed in lonsdaleite, while a slip on the (100) plane in the bulk was observed in diamond. Then the cracks extended toward to the inside of the specimen. The maximum tensile stress of lonsdaleite was 412 GPa, which was superior than that of diamond by 32 %. No activated cleavage plane makes lonsdaleite tougher than diamond. The thermal stability of both types of diamond was analysed at a high temperature of 1100 K. The maximum tensile stress of lonsdaleite decreased to 320 GPa, while that of diamond decreased to 282 GPa. As a result, the molecular dynamics simulations clarified the effect of the hexagonal structure on both the fracture toughness and the fracture mechanism, as well as the excellent thermal stability of lonsdaleite.

Lonsdaleite, Three-point bending, Molecular dynamics simulation

1. Introduction

Lonsdaleite (hexagonal diamond) was discovered from the meteorite and has been synthesized from graphite or diamond (cubic diamond) in a small quantity [1]. Recently, it was reported that lonsdaleite was harder than diamond using the analyses by first-principles calculations [2]. However, the fracture mechanism and factors contributing to the fracture toughness have not been fully understood. In this paper, to clarify the fundamental fracture mechanism of lonsdaleite, molecular dynamics simulations of three-point bending were carried out and compared with that of diamond.

2. Molecular dynamics simulation

The model used in the simulations consisted of a hexagonal or a cubic diamond specimen and three rigid diamond indenters, as shown in Figure 1. The diamond specimens consisted of Newtonian and thermostat atoms that were arranged in 8 layers at both end of the specimen. The specimen had the dimensions 80 nm × 1.0 nm × 9.9 nm. The radius of the rigid indenters were 5.0 nm. The Tersoff potential [3] was used to express the diamond structure, while the Morse potential was employed to express the interaction between the atoms in the specimen and the indenters. Periodic boundary conditions were applied in the *y* direction. For the conversion of the kinetic energy of carbon atoms into an equivalent temperature, the thermal energy derived from the equation of specific heat proposed by Einstein was used. In the thermostat layers which absorb the heat outward in the model, the kinetic energy of atoms was adjusted for every computation time step so as to maintain the equivalent average temperatures at 293 K or 1100 K. Three-point bending was performed by an upward movement of the supporting indenters at both end of the specimen and a downward movement of the central indenter with a speed of 100 m/s. To understand the effect of crystal orientation especially hexagonal structure of lonsdaleite, three-point bendings were performed in the [0001] direction on lonsdaleite and in the [111] direction on diamond. The stress of the atomic model was defined and calculated from the resultant interatomic force between the atoms on both sides of a small interface plane, the area of which was $2L_c$ x $2L_c$ [4]. Here, L_c=0.356 nm was the lattice constant of diamond. Equation 1 was used for the flexural strain.

$$\varepsilon = \frac{6Dt}{L^2} \quad (1)$$

Here, *D* is the maximum deflection of the center of the beam, *t* is the thickness of the beam and *L* is the support span.

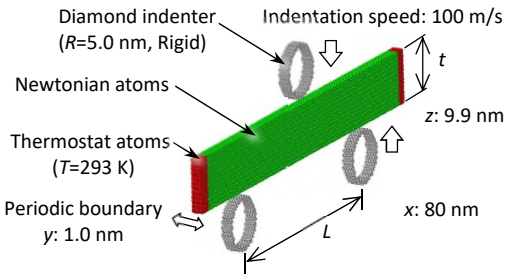
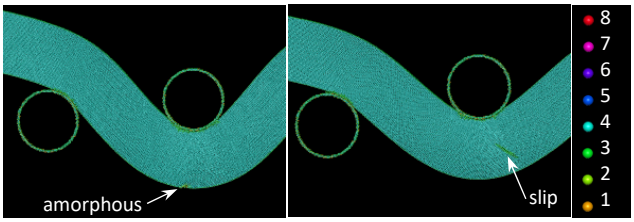


Figure 1. Initial model for three-point bending

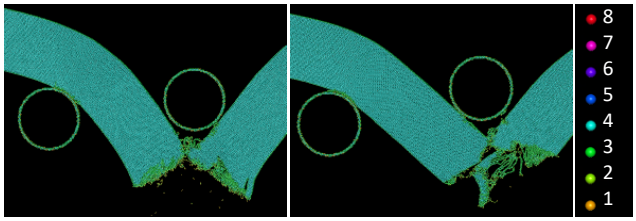
3. Simulation results

The results showed that the fracture mechanism of lonsdaleite was different from that of diamond: an amorphous phase transformation from the surface was observed in lonsdaleite, while a slip on the (100) plane in the bulk was observed in diamond, as shown in Figure 2. Then the cracks extended toward to the inside of lonsdaleite and toward to the surface of diamond, as shown in Figure 3. The crack extended spontaneously by releasing the elastic strain energy without any extra external force after the beginning of crack extension. The maximum tensile stress of lonsdaleite was 412 GPa, which was superior than that of diamond by 32 %, as shown in Figure 4. No activated cleavage plane makes lonsdaleite tougher than diamond.



(a) (b)

Figure 2. Different fracture mechanism (a) an amorphous phase transformation from the surface in lonsdaleite (b) a slip on the (100) plane in the bulk in diamond



(a) (b)

Figure 3. After crack extension (a) lonsdaleite (b) diamond

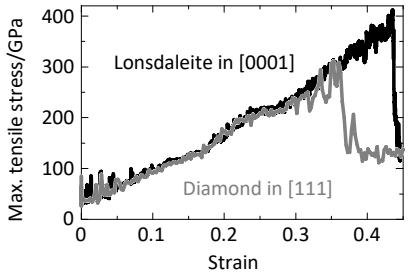


Figure 4. The maximum tensile stress of lonsdaleite in the [0001] direction and diamond in the [111] direction

The thermal stability of both types of diamond was analysed at a high temperature of 1100 K. The maximum tensile stress of lonsdaleite decreased to 320 GPa, while that of diamond decreased to 282 GPa, as shown in Figure 5.

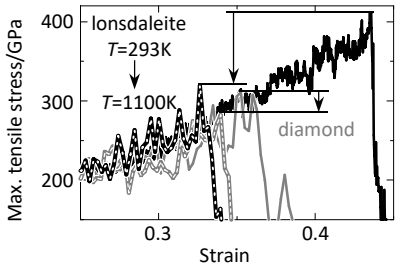


Figure 5. Thermal stability of lonsdaleite in the [0001] direction and diamond in the [111] direction at temperatures of 293 K and 1100 K

In addition three-point bending of lonsdaleite in the [1100] and [1120] directions had the same fracture mechanism as diamond had in the [110] and [112] directions: cracks initiated from the surface and extended toward to the inside of the specimens. Their stress-strain curves had the similar results, as shown in Figure 6 and 7.

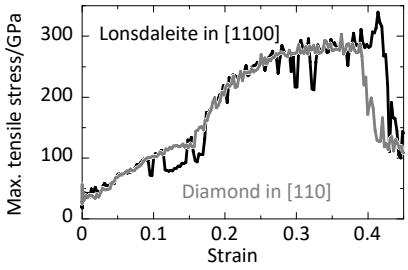


Figure 6. The maximum tensile stress of lonsdaleite in the [1100] direction and diamond in the [110] direction

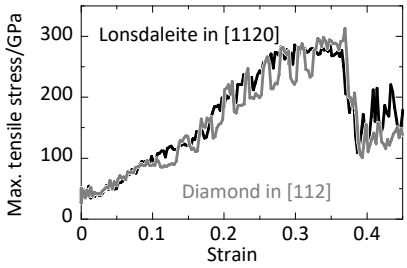


Figure 7. The maximum tensile stress of lonsdaleite in the [1120] direction and diamond in the [112] direction

As a result, the molecular dynamics simulations clarified the effect of the hexagonal structure on both the fracture toughness and the fracture mechanism, as well as the excellent thermal stability of lonsdaleite.

4. Conclusion

The results showed that the fracture mechanism of lonsdaleite in the [0001] direction was different from that of diamond in the [111] direction: an amorphous phase transformation from the surface was observed in lonsdaleite, while a slip on the (100) plane in the bulk was observed in diamond. Then the cracks extended toward to the inside of the specimen. The maximum tensile stress of lonsdaleite was 412 GPa, which was superior than that of diamond by 32 %. No activated cleavage plane makes lonsdaleite tougher than diamond. The thermal stability of both types of diamond was analysed at a high temperature of 1100 K. The maximum tensile stress of lonsdaleite decreased to 320 GPa, while that of diamond decreased to 282 GPa. As a result, the molecular dynamics simulations clarified the effect of the hexagonal structure on both the fracture toughness and the fracture mechanism, as well as the excellent thermal stability of lonsdaleite. These results suggest that lonsdaleite has high potential for use as ultraprecision cutting tools. Future work will be focused on the wear resistance of the lonsdaleite.

References

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