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Deformation mechanism of lonsdaleite based on molecular dynamics analysis of nanoindentation

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Abstract

To clarify the fundamental deformation mechanism of lonsdaleite, molecular dynamics simulations of its nanoindentation were carried out and compared with that of diamond. To investigate the effect of the crystal orientation, nanoindentation was performed in the [0001], [1100] and [1120] directions on lonsdaleite and in the [111], [110] and [112] directions on diamond. The molecular dynamics simulations showed that the deformation mechanism of lonsdaleite indented in the [0001] direction was different from that of diamond and lonsdaleite in the other conditions: a phase transformation to the amorphous structure was observed in the bulk of lonsdaleite, while cracks initiated and extended from the surface of diamond and lonsdaleite in the other conditions. The maximum value of the contact pressure immediately before the phase transformation of lonsdaleite indented in the [0001] direction was 607 GPa, which was 63 % higher than that of diamond at the fracture indented in the [111] direction. The thermal stability of both types of diamond was analysed at a high temperature of 1100 K. The maximum value of the contact pressure of lonsdaleite indented in the [0001] direction decreased by 5.4 %, while that of diamond indented in the [111] direction decreased by 8.4 %. In addition, stress analysis showed that the compressive stresses were applied normal to the cleavage planes on (0001) plane. Normal compressive stresses are unable to cleave the plane, which is the only one cleavage plane in lonsdaleite, whereas diamond has octahedral cleavage planes. As a result, the molecular dynamics simulations showed that the effect of the hexagonal structure of lonsdaleite on the hardness indented in the [111] direction due to the deformation mechanism by the phase transformation instead of fracture, as well as the excellent thermal stability.

Lonsdaleite, Nanoindentation, Molecular dynamics simulation

1. Introduction

Diamond has excellent mechanical properties such as the highest known hardness. Recently, however, it has been reported that lonsdaleite (hexagonal diamond) is harder than diamond (cubic diamond), as analysed by first-principles calculations using less than 30 atoms [1, 2]. However, the deformation mechanism and the factors contributing to the hardness and fracture toughness are not yet fully understood.

In this paper, to clarify its fundamental deformation mechanism, molecular dynamics simulations of the nanoindentation of lonsdaleite were carried out at temperatures of 293 K and 1100 K and compared with that of diamond.

2. Molecular dynamics simulations

The model used in the simulations consisted of a hexagonal or cubic diamond specimen and a rigid diamond indenter, as shown in Figure 1. The diamond specimens consisted of Newtonian, thermostat and boundary atoms. The edge radius of the indenter was 2.5 nm. The Tersoff potential [3] was used to express the diamond structure, while the Morse potential was employed to express the interaction between the specimen and the indenter. Periodic boundary conditions were applied in the thickness direction. Nanoindentation was performed to a maximum depth of 4.0 nm with an indentation speed of 100 m/s. To investigate the effect of the crystal orientation and thermal stability, nanoindentations were performed in the [0001], [1100] and [1120] directions on

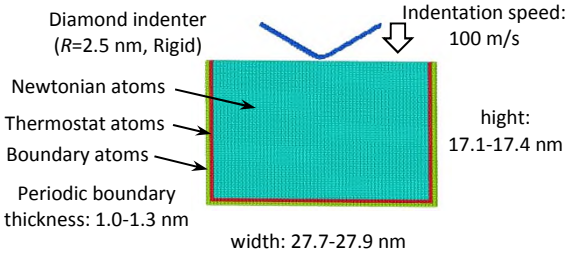

Figure 1. Initial model for nanoindentation.

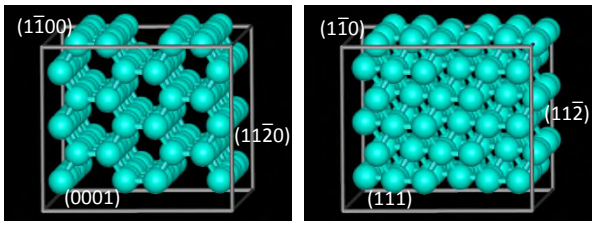

Figure 2. Crystal structure (a) lonsdaleite (hexagonal diamond) (b) diamond (cubic diamond).

lonsdaleite and in the [111], [110] and [112] directions on diamond at temperatures of 293 K and 1100 K, as shown in Figure 2. Einstein's specific heat for diamond was used for the conversion from the kinetic energy of the thermal vibration of atoms to the equivalent temperature. The time step for numerical integration was 0.5 fs for the high temperature and high pressure during the entire simulation process. In this paper, the indentation hardness was defined as the maximum

value of the contact pressure that was observed immediately before the permanent deformation or crack initiation during nanoindentation.

3. Simulation results

According to the results of the molecular dynamics simulations, the deformation mechanism of losdaleite indented in the [0001] direction was different from that of diamond indented in the [111], [110] and [112] directions: a phase transformation to the amorphous structure was observed in the bulk of lonsdaleite, while cracks initiated and extended from the surface of diamond, as shown in Figure 3. The maximum value of the contact pressure of lonsdaleite indented in the [0001] direction was 607 GPa, which was 63 % higher than that of diamond indented in the [111] direction, as shown in Figure 4. However, lonsdaleite indented in the [1120] and [1100] directions had the same deformation mechanism as diamond had: cracks initiated and extended from the surface, as shown in Figure 5, which reduced the indentation hardness of lonsdaleite indented in [1120] and [1100] directions to that of diamond, as shown in Figure 6.

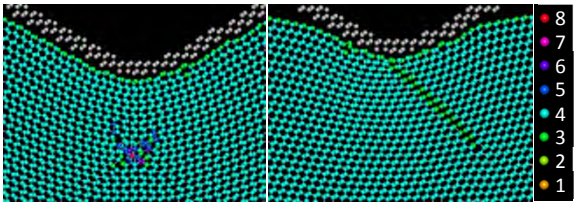

Figure 3. Different deformation mechanism (a) Phase transformation of lonsdaleite in [0001] direction (b) Crack initiation and extension of diamond in [111] direction.

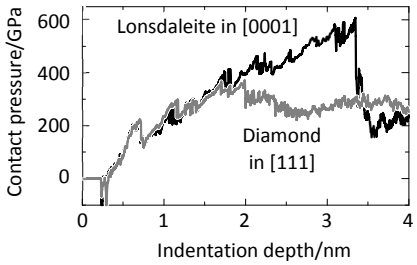

Figure 4. Contact pressure of lonsdaleite in [0001] direction and diamond in [111] direction.

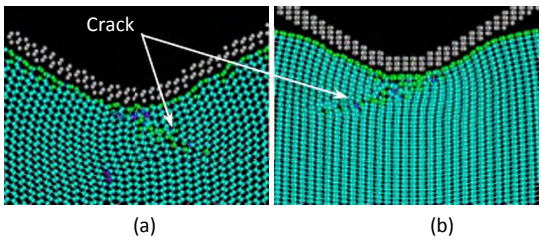

Figure 5. Effect of the crystal orientation of lonsdaleite (a) in [1120] direction (b) in [1100] direction

The thermal stability of both types of diamond was analysed at the high temperature of 1100 K. The maximum value of the contact pressure of lonsdaleite indented in the [0001] direction decreased by 5.4 %, while that of diamond indented in the [111] direction decreased by 8.4 %, as shown in Figure 7.

In addition, the stress analysis suggested that the compressive stresses normal to the cleavage planes on the (0001) planes prevented crack initiation and extension in lonsdaleite in the [0001] direction, as shown in Figure 8.

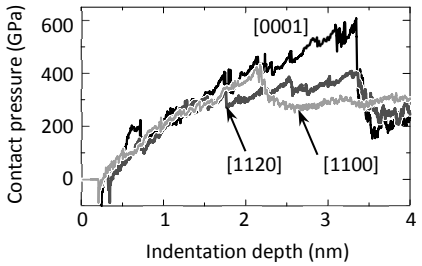

Figure 6. Effect of crystal orientation of lonsdaleite on contact pressure indented in [0001], [1120] and [1100] direction.

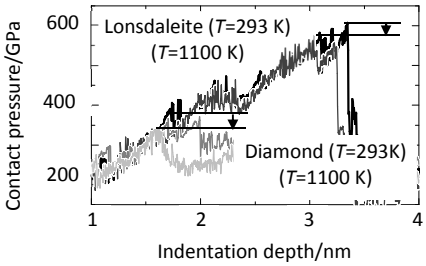

Figure 7. Thermal stability of lonsdaleite in [0001] direction and diamond in [111] direction at temperatures of 293 K and 1100 K.

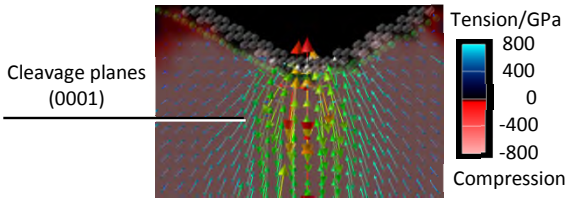

Figure 8. Stress distribution of maximum principal stress in lonsdaleite at the maximum contact pressure.

4. Conclusions

Molecular dynamics simulations of lonsdaleite showed that the deformation mechanism of lonsdaleite in the [0001] direction was different from that of diamond indented in the [111], [110] and [112] directions and from that of lonsdaleite indented in the [1120] and [1100] directions: a phase transformation to the amorphous structure was observed in the bulk of lonsdaleite. The maximum value of the contact pressure of lonsdaleite indented in the [0001] direction was 607 GPa, which was 63 % higher than that of diamond indented in the [111] direction at 293 K. According to the thermal stability of lonsdaleite, the maximum contact pressure of lonsdaleite indented in the [0001] direction decreased by 5.4 %, while that of diamond indented in the [111] direction decreased by 8.4 % at a high temperature of 1100 K. In addition stress analysis showed that the compressive stresses were applied normal to the cleavage planes on (0001) plane. Normal compressive stresses do not cause to cleave the plane, which is the only one cleavage plane lonsdaleite has, whereas diamond has octahedral cleavage. In conclusion the hexagonal structure of the lonsdaleite contributes to the hardness due to the deformation mechanism by the phase transformation instead of fracture indented in the [0001] direction, as well as the excellent thermal stability. These results suggest that lonsdaleite has high potential for use as ultraprecision cutting tools. Future work will focus on the wear resistance of the lonsdaleite.

References

[1] Pan Z, Sum H, Zhang Y and Chen C 2009 Physical Review Letters **102** 055503 (4)

[2] Qingkun L, Yi S and Yu Z 2011 Scripta Materialia **65** 229-32

[3] Tersoff J 1989 Phy. Rev. B **37**/8 5566-68