

Deformation mechanism of nano-polycrystalline diamond on nanoindentation based on molecular dynamics analysis

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Abstract

To clarify the fundamental deformation mechanism of nano-polycrystalline diamond, molecular dynamics simulations of nanoindentation were carried out and compared with that of monocrystalline diamond. The results showed that the deformation mechanism of polycrystalline diamond was different from that of monocrystalline diamond: slipping was observed in polycrystalline diamond, while fracture was observed in monocrystalline diamond. The deformation mechanism of polycrystalline diamond depended on the grain size. The transgranular slipping mode was dominant when the grain size was larger than 3.6 nm, whereas the intergranular slipping mode was dominant when the grain size was smaller than 2.8 nm. The thermal stability of both types of diamond was analyzed at a high temperature of 1100 K. The results showed that the contact pressure of polycrystalline diamond decreased by 1.6 % when plastic deformation took place, while the contact pressure of monocrystalline diamond on crack initiation decreased by 15 %. In addition, stress analysis suggested that the compressive stresses at the grain boundaries prevented crack initiation and extension in the polycrystalline diamond. As a result, the molecular dynamics simulations clarified the effect of the grain size on both the hardness and the deformation mechanism, as well as the excellent thermal stability of polycrystalline diamond.

Nano-polycrystalline diamond, Molecular dynamics simulation

1. Introduction

Diamond has excellent mechanical properties such as the highest known hardness. However, monocrystalline diamond has anisotropic mechanical properties and cleavage planes. These features have caused serious problems when using diamond tools, particularly cutting edge chipping. Recently, nano-polycrystalline diamond has been synthesized by the direct conversion of graphite [1, 2] and may have higher toughness and more isotropic mechanical properties than monocrystalline diamond. However, the deformation mechanism and the factors contributing to the hardness, fracture toughness and thermal stability of nano-polycrystalline diamond are not fully understood.

In this paper, to clarify the fundamental deformation mechanism, molecular dynamics simulations of the nano-indentation of nano-polycrystalline diamond were carried out at both 293 K and 1100 K and compared with that of monocrystalline diamond [3].

2. Molecular dynamics simulations

The model used in the simulations consisted of a 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 4.5 nm. The Tersoff potential [4] was used to express the diamond structure, while the Morse potential was employed to express the interaction between the diamond specimen and the indenter. Periodic boundary conditions were applied in the thickness direction. Nanoindentation was performed to a

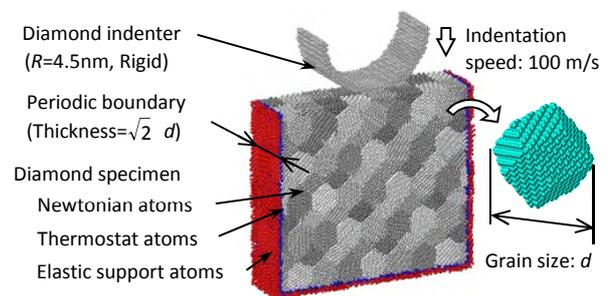


Figure 1. Initial model for nano-indentation and single grain with a rhombic dodecahedral shape and random crystallographic orientation

maximum depth of 6.5 nm with an indentation speed of 100 m/s. The nano-polycrystalline diamond specimens consisted of grains of size 1.4 nm to 10 nm, with a rhombic dodecahedral shape and random crystallographic orientations.

3. Simulation results

According to the results of the molecular dynamics simulations, no cracks formed during the nanoindentation of nano-polycrystalline diamond, while cracks initiated and extended in the monocrystalline diamond as shown in Figure 2. Generally speaking, the hardness and yield stress of a material typically increase with decreasing grain size. This phenomenon is likely known as the Hall-Petch effect [5]. However, softening was observed as the grain size was reduced to single nanosize grains, likely known as the reverse Hall-Petch effect [5] as shown in Figure 3. A larger fraction of the atoms belonged to

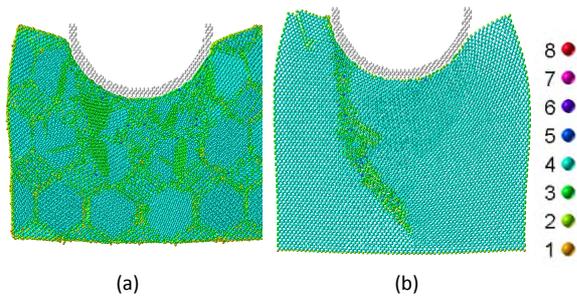


Figure 2. Different deformation mechanism (a) No cracks in nano-polycrystalline diamond with the grain size of 4.3 nm (b) Crack initiation and extension in monocrystalline diamond. Color scales of atoms represent the number of nearest neighbours

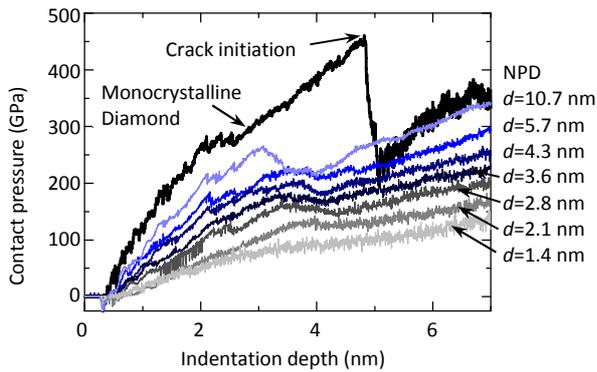


Figure 3. Softening of the nano-polycrystalline diamond (NPD) with decreasing grain size d , known as the reverse Hall-Petch effect

the grain boundaries and grain boundary slipping became easier as the grain size decreased. This led to the softening of the nano-polycrystalline diamond with decreasing grain size. The deformation mechanism of the nano-polycrystalline diamond depended on the grain size. As the grain size decreased, the deformation mechanism changed from an intragranular process to an intergranular process as shown in Figure 4. The transgranular slipping mode was dominant when the grain size was larger than 3.6 nm. In contrast the intergranular slipping mode was dominant when the grain size was smaller than 2.8 nm. Figure 5 shows that the thermal stability of both types of diamond at a high temperature of 1100 K and that the contact pressure of nano-polycrystalline diamond decreased by 1.6 % when plastic deformation took place, while the contact pressure of monocrystalline diamond on crack initiation decreased markedly by 15 %. In addition, stress analysis showed that crack initiation took place when the

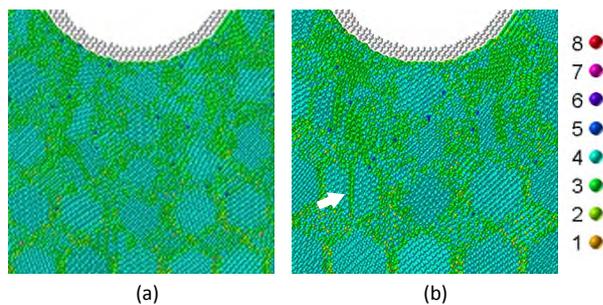


Figure 4. Deformation mechanism of the nano-polycrystalline diamond depending on the grain size (a) Intergranular slipping ($d=2.8$ nm) (b) Transgranular slipping ($d=3.6$ nm)

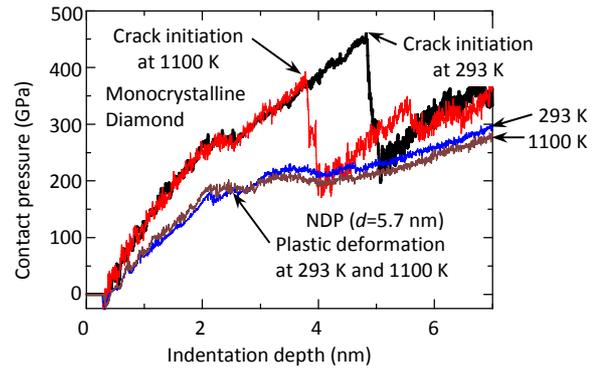


Figure 5. Thermal stability of both types of diamond at a high temperature of 1100 K

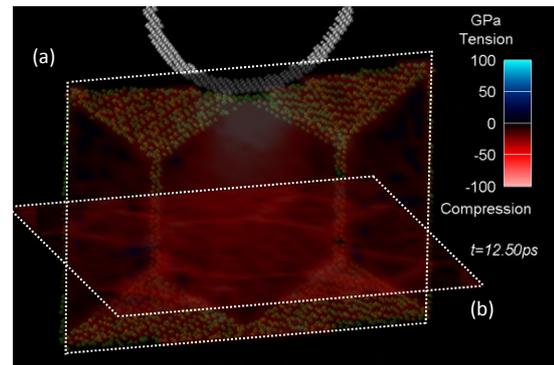


Figure 6. Compressive stresses at the grain boundaries in the nano-polycrystalline diamond consisted of grains of size 10.7 nm on (a) vertical central cross section and (b) horizontal cross section

tensile stress in the monocrystalline diamond exceeded a certain critical value. On the other hand, the stress analysis suggested that the compressive stresses at the grain boundaries prevented crack initiation and extension in the nano-polycrystalline diamond as shown in Figure 6. As a result, the molecular dynamics simulations showed the effect of the grain size on both softening and the deformation mechanism as well as the excellent thermal stability of nano-polycrystalline diamond at high temperatures.

4. Conclusions

Molecular dynamics simulations of nano-polycrystalline diamond showed that the deformation mechanism depended on the grain size, as well as the high toughness of nano-polycrystalline diamond to crack initiation and extension and its excellent thermal stability. These results suggest that nano-polycrystalline diamond has high potential for use as ultraprecision cutting tools.

References

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