Results of molecular dynamics analysis of nanoindentation in monocrystalline and amorphous silicon carbide compared with experimental results

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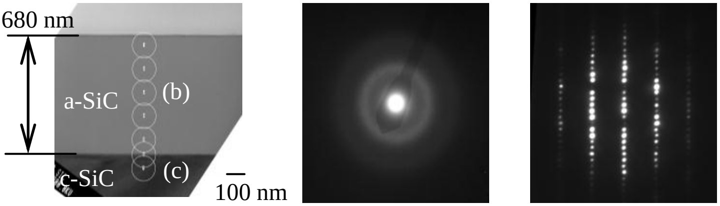
Abstract

Molecular dynamics (MD) simulations of nanoindentations of both monocrystalline and surface-modified amorphous SiC are carried out and the results are compared with experimental results to understand the difference in fundamental mechanical properties, especially those regarding the machining process, between both SiC. Firstly, experimental results of nanoindentation tests showed that the hardnesses were 52.5 and 32.5 GPa and the elastic moduli were 458 and 430 GPa for c-SiC and a-SiC, respectively. Secondly, MD simulations showed that an inelastic deformation occurred accompanied by phase transformation in c-SiC during loading. On the other hand, the density of a-SiC beneath the indenter increased as the indentation depth increased. The size of the amorphous zone in c-SiC decreased during unloading because of the continuous recrystallization. As a result, MD simulation revealed that the surface modification of the amorphous structure reduced the hardness and stiffness of c-SiC. These results are in good agreement with the experimental results.

1. Introduction

The performance of silicon semiconductors has almost reached its limit. Therefore, silicon carbide (SiC) is expected to become the next-generation semiconductor material, because of its higher output power than silicon and highly reliable use in extreme environments. However, it is difficult to manufacture SiC because of its hardness and brittleness.

The authors have reported that amorphous SiC (a-SiC) should have a higher machinability than monocrystalline SiC (c-SiC) and that the damage-free machining



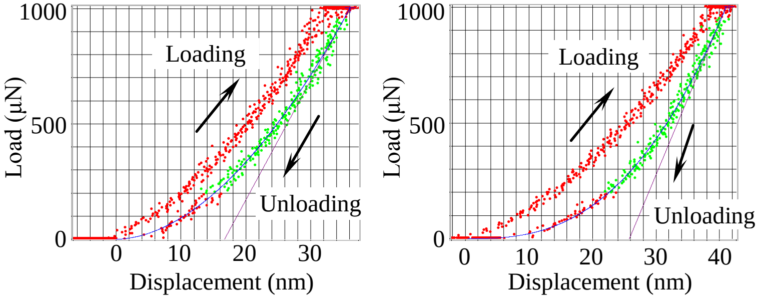
(a) TEM image (b) Middle layer (c) 6H-SiC substrate

Figure 1: TEM image and electron diffraction patterns after ion implantation on crystalline 6H-SiC with surface orientation of (0001) exposed to carbon ions accelerated by 350 keV

of c-SiC is possible with surface modification to the amorphous structure [1]. However, the differences in the machining process between c-SiC and a-SiC are not yet fully understood. In this study, to understand the difference in fundamental mechanical properties between c-SiC and a-SiC, molecular dynamics (MD) simulations of nanoindentations of both SiC are carried out and the results are compared with experimental results.

2. Nanoindentation tests of monocrystalline and surface-modified SiC

Nanoindentation tests were carried out using a commercial nanoindentation instrument equipped with a Berkovich pyramidal indenter associated with an atomic force microscope. For each sample, a series of 10 indentations were performed under a maximum load of 1 mN. The periods of loading, holding, and unloading were 5 s each. For surface modification, ion implantation was performed on c-SiC with the



(a) c-SiC (b) a-SiC

Figure 2: Load displacement curves for crystalline SiC and surface-modified SiC

surface orientation of (0001) exposed to carbon ions accelerated by 350 keV. The surface of 680 nm thickness was modified to the amorphous structure, as shown in Figure 1. Nanoindentation tests showed that the hardnesses were 52.5 and 32.5 GPa and the elastic moduli were 458 and 430 GPa for c-SiC and a-SiC, respectively, as shown in Figure 2.

3. Molecular dynamics simulation

Secondly, MD simulations of nanoindentation in crystalline and surface-modified SiC were carried out. The model used consists of a SiC specimen and a dynamic diamond indenter, as shown in Figures 3 and 4. The SiC and diamond consist of Newtonian, thermostat, and boundary atoms. The edge radius of the indenter was 4.0 nm with a half-angle of 45 deg. Tersoff potential [2] was used for SiC and diamond, while Morse potential was employed to express the interaction between SiC and diamond. Periodic boundary conditions were applied in the thickness direction. For surface modification, the surface was exposed to 10 silicon ions accelerated by 3 keV. Nanoindentations were performed under the conditions of a maximum depth of 1.5 nm with an indentation speed of 50 m/s.

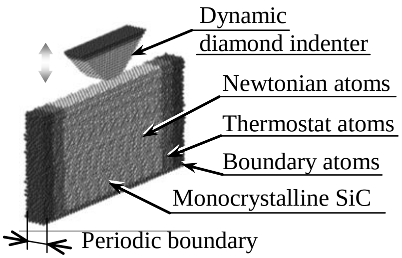


Figure 3: Initial model of nano-indentation of monocrystalline SiC with a dynamic diamond indenter

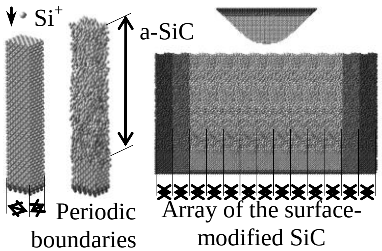
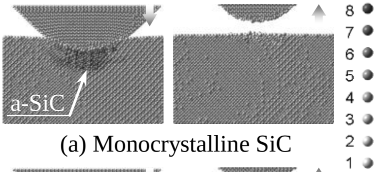


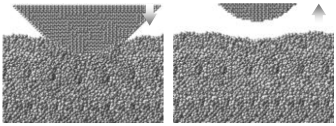
Figure 4: Surface preformed by ion implantation and initial model of nano-indentation of surface-modified SiC

4. Simulation results

The MD simuations showed that an inelastic deformation occurred accompanied by phase transformation beneath the indenter in c-SiC during loading, as shown in Figure 5. On the other hand, the density of a-SiC beneath the indenter increased as the indentation depth increased. Throughout the entire indentation process, dislocations did not appear and purely elastic deformation was observed only in an extremely narrow regime. The size of the amorphous zone in c-SiC decreased during unloading because of continuous recrystallization. This result explains why the depth of residual impression measured by AFM is much smaller than that of contact impression estimated from the load-displacement curve in c-SiC. MD simulations also showed that surface modification of the amorphous structure reduced the hardness and stiffness of c-SiC, as shown in Figure 6.



(a) Monocrystalline SiC



(b) Surface-modified SiC

Figure 5: Nanoindentation of monocrystalline and surface-modified SiC at a maximum indentation depth of 1.5 nm and after unloading

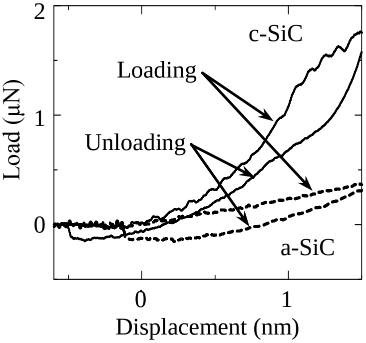


Figure 6: Load displacement curve for crystalline SiC and surface-modified SiC

5. Conclusions

MD simulations showed that surface modification of the amorphous structure reduced the hardness and stiffness of c-SiC. These results are in good agreement with the experimental results. Therefore, a-SiC has a higher machinability than c-SiC and the damage-free machining of c-SiC is possible with surface modification of the amorphous structure.

References:

[1] H. Tanaka, S. Shimada: Annals of CIRP, **62** (2013) 55-58.

[2] J. Tersoff: Physical Review B, **39**/8 (1989) 5566-5568.