Guideline for Ultra-precision Machining of Silicon Carbide Based on Molecular Dynamics Analysis

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Abstract

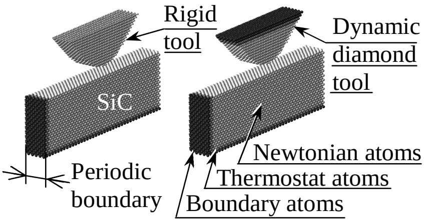
Molecular dynamics (MD) simulations of nano-machining of mono-crystalline silicon carbide (SiC) were carried out to obtain scientific guidelines for ductile-mode machining of SiC. In a cutting simulation, no chip removal was observed due to a severe wear and a cutting edge chipping of diamond tool. In order to reduce cutting force acting on the tool, an amorphous layer was pre-formed on the workpiece surface to be cut. In the simulation, ductile-mode chip removal was observed as a result of a continuous and stable plastic flow by a shearing deformation in the amorphous region without the cutting edge chipping. Furthermore, the wear decreases by applying cutting fluid and slower cutting speed. However, the tool wear is still severe for cutting with single point cutting edge. In practice, to realize effective ductile-mode machining of SiC, it is recommended that mono-crystalline SiC should be pre-formed to amorphous to be cut and ground with lubricant.

1 Introduction

Although silicon is a dominant semiconductor material, the performance of silicon semiconductor almost reaches the limitation. Therefore, as a semiconductor material for the next generation, SiC is expected as a higher-power and higher-frequency device. However, it is difficult to manufacture SiC because of its hardness and brittleness. In this paper, to obtain scientific guidelines for high efficient and low-cost ductile-mode machining of SiC with high accuracy and high quality surface, molecular dynamics (MD) simulations of nano-machining of SiC were carried out.

2 Molecular dynamics simulation

MD simulations of nano-machining of SiC were carried out to obtain scientific guidelines for ductile-mode machining of SiC, using three models with surfaces composed of {100} planes as shown in Figures 1 and 2. The dimensions of the initial model for nano-machining are 17.3nm ×2.2nm×5.4nm. The SiC specimen is machined in the <100> direction with the speed of 200m/s and 10m/s by a diamond tool with an edge radius of 4.0 nm and rake angle of -45 degrees under a depth of cut of 2.5nm. For steady-state chip removal, the moving control volume method [1] is employed. Periodic boundaries are applied in y direction. The Tersoff potential [2] is used for a SiC specimen and a diamond tool, while the Morse potential is used for interaction between specimen and tool. The equivalent average temperature [3] of the thermostat atoms is adjusted at 293K. The number of nearest neighbors, N_n, is used as an index of crystallinity of diamond structure.



(a) Rigid tool (b) Dynamic tool

Figure 1: Initial models for nano-machining of mono-crystalline SiC with a rigid and a dynamic diamond tools

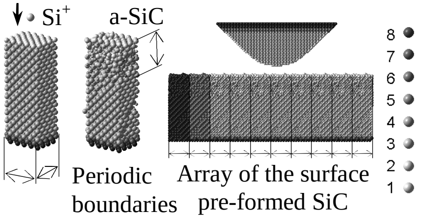
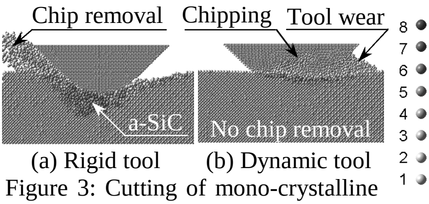


Figure 2: Surface pre-formed by ion implantation and an initial model for nano-machining of surface pre-formed SiC

3 Simulation results

3.1 Nano-machining of mono-crystalline SiC with a rigid tool



(a) Rigid tool (b) Dynamic tool

Figure 3: Cutting of mono-crystalline SiC with a rigid and a dynamic tool for the cutting distance of 10 nm

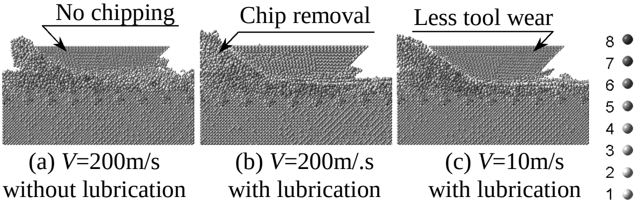
The first model simulates nano-machining of mono-crystalline SiC with a rigid diamond tool to analyze fundamental cutting mechanisms under an ideal cutting condition as shown in Figure 1(a). In the simulation chip removal was observed as a result of a shearing deformation in an amorphous region after phase transformation from mono-crystalline SiC to amorphous silicon carbide (a-SiC) in front of the cutting edge as shown in Figure 3(a). The amorphous phase transformation is inevitable for ductile-mode chip removal of SiC.

3.2 Nano-machining of mono-crystalline SiC with a dynamic tool

In practical cutting of SiC, cutting edge chipping immediately takes place when the cutting starts. Therefore, in the second model, to investigate the tool wear and chipping phenomena, the model of the rigid diamond tool was replaced by dynamic one that consists of Newtonian, thermostat and fixed atoms as shown in Figure 1(b). In the simulation no chip removal was observed due to a severe tool wear and a cutting edge chipping as shown in Figure 3(b).

3.3 Nano-machining of pre-formed surface SiC

In order to realize effective ductile-mode machining of SiC, it is important to prevent the cutting edge chipping. Stress analyses reveal that rather higher stress is necessary for the phase transformation than for chip removal by shearing deformation in the amorphous region. For reducing cutting force acting on the tool face, an amorphous layer was pre-formed on a surface to be cut in the third model as shown in Figure 2. For pre-forming SiC on the surface homogeneously, for instance, assuming an ion implantation, a silicon ion was accelerated to collide perpendicularly against the surface of SiC by the kinetic energy of 1keV. Phase transformation is taken place from mono-crystalline SiC to a-SiC on the surface by the ion implantation. In the simulation a flow type chip formation was observed as a result of the continuous and stable plastic flow generated by a shearing deformation in the amorphous region without the cutting edge chipping as shown in Figure 4(a).



(a) V=200m/s without lubrication

(b) V=200m/.s with lubrication

(c) V=10m/s with lubrication

Figure 4: Cutting of pre-formed surface SiC for the cutting distance of 20nm.

3.4 Effect of lubricant and cutting speed on tool wear

Usage of lubricant is effective to reduce a tool wear. Supposing that the lubricant enlarges the gap between the workpiece and the tool atoms, Morse potential parameters are modified to enlarge the inter-atomic distance by 0.1nm. Figure 4(b) shows that chip removal was observed with less tool wear with lubrication. In addition, Figure 4(c) shows results in the case of the slower cutting speed of 10m/s and Figure 5 shows comparisons of tool wear rates under different cutting conditions. As the tool wear rate is still high for cutting SiC with single cutting edge, grinding with multiple cutting edges is recommended.

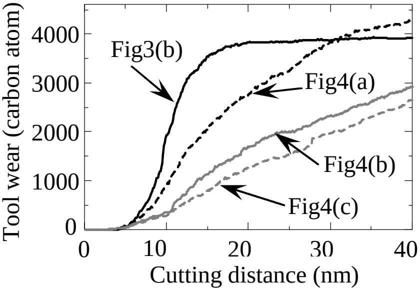


Figure 5: Comparison of tool wear rate under different conditions

4 Conclusions

The followings are the results of the MD simulation for nano-machining of SiC to obtain scientific guidelines for high efficient and low-cost ductile-mode machining of SiC.

1. It is difficult to cut mono-crystalline SiC by single point diamond turning due to a severe tool wear and cutting edge chipping.
2. A flow type chip formation was observed without cutting edge chipping as a result of nano-machining of pre-formed surface SiC.
3. Lubricant decreases the tool wear rate by 40% during the nano-machining of pre-formed surface SiC.
4. Slower cutting speed of 10m/s decreases the tool wear rate by 20% comparing to the case of the cutting speed of 200m/s with lubricant.

In summary, in order to realize effective ductile-mode machining of SiC, it is recommended that mono-crystalline SiC should be pre-formed to a-SiC on the surface to be cut and ground with lubricant.

References:

[1] W.-D. Cheong, L.C. Zhang, H. Tanaka: Key Engineering Materials **196** (2001) 31-42.

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

[3] H. Tanaka, S. Shimada, L. Anthony: Annals of CIRP, **56**/1 (2007) 53-56.