Influence of nanoparticle coolant and crystal structure of the workpiece during nanometric cutting of silicon carbide.

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Abstract

Silicon carbide (SiC) is a suitable candidate for MEMS, NEMS, optoelectronic and nanotribological applications e.g. airborne laser devices, laser radar systems, vacuum ultraviolet (VUV) telescopes and space based laser mirrors. In-depth understanding of the influence of coolant and crystal structure of the work material on the nanometric cutting process of SiC could help in cost saving operations. Therefore, nanoscratching trials were carried out on single crystal 6H-SiC involving four pre-selected coolants to emulate nanometric cutting. A specific coolant was found to improve the cutting conditions tremendously and hence recommended. Moreover, a molecular dynamics (MD) simulation model was developed to simulate nanometric cutting of polycrystalline (PC) 3C-SiC and single crystal (SC) 3C-SiC. Besides explaining the reasons for the ease of machinability of chemically vapour deposited (CVD) 3C-SiC compared to SC-3C-SiC, simulation results also explains why SC-SiC provides a better measure of attainable surface roughness in comparison to CVD-SiC and reaction bonded (RB)-SiC.

1 Introduction

It is due to its superior properties that SiC is being actively explored as a material for advanced semiconductor electronic device applications, leading to a potential demand for complex optical components with mirror finish. Single point diamond turning (SPDT) offers highest efficiency compared to any other ultra-precision manufacturing process for generating optics surface in complex shapes on a range of brittle materials including SiC [1]. However, rapid wear of diamond tool due to abrasion leading to interfacial graphitization is a precursor to tool life and thus for significant exploitation of SiC [2]. Hence, exploring insights of the SPDT process of SiC is both scientifically

and technologically relevant. Accordingly, a nano-scratching test on SC-6H-SiC was done to emulate nanometric cutting involving four pre-selected coolants. Coolants were selected based on their capability to improve the tribological properties of diamond under frictional contact [3]. Besides nanoscratching trials, molecular dynamics (MD) simulation results comparing nanometric cutting of polycrystalline 3C-SiC and single crystal 3C-SiC have been presented and discussed in the subsequent sections.

2 Experimental setup

Hysitron Triboindenter having three-sided pyramidal Berkovich probe (negative tool rake angle of 65.35°, clearance angle of 13° with a cutting edge radius of 150 nm) was used for experiment. Load control (LC) feedback system with a constant normal load of 11,000 μN was used. 6H-SiC wafer with orientation (001) of size 5x5x0.33 mm were used. Coolants used were graphite nanoparticles, copper nanoparticles, MoS_2 nanoparticles and 3-amino propyl (diethoxyl) methyl silane [4].

3 Results and discussions

3.1 Variation in the cutting forces

Since, load control feedback system was used, only cutting forces (F_c) varied during the scratch process as per the individual coolant. A comparison of the variation in the cutting forces has been shown in Figure 1 suggesting copper nanoparticles as the superior coolant on account of overall lower cutting forces and least fluctuations, which is in accord with a realistic SPDT operation on RB-SiC [5].

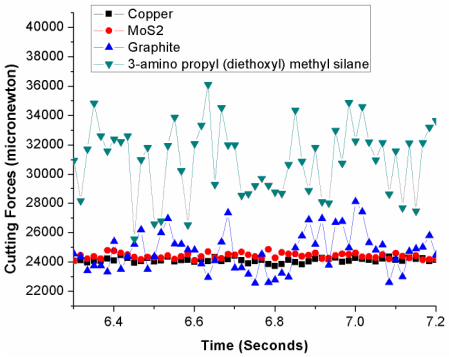
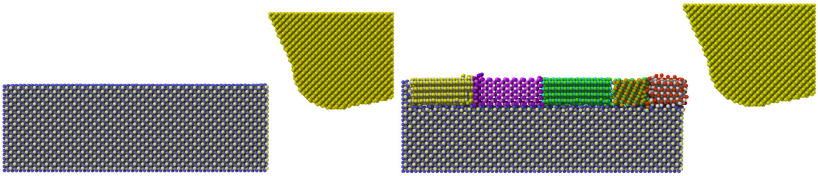


Figure 1: Comparison of cutting forces with various coolants.

3.2 Molecular dynamics simulation

MD simulation model for the nanometric cutting with a tool cutting speed of 5 m/sec, uncut chip thickness of 1.31 nm, negative rake diamond tool having cutting edge radius as 2.3 nm and total included angle as 105° was developed [2]. For the purpose of brevity, results are directly presented here. Figure 2 and figure 3 shows the comparison of the responses of SC-SiC and PC-SiC before and during cutting.



(a) Snapshot of SC-3C-SiC (b) Snapshot of sample PC-3C-SiC

Figure 2: Snapshot from simulation after equilibration of both the workpieces.

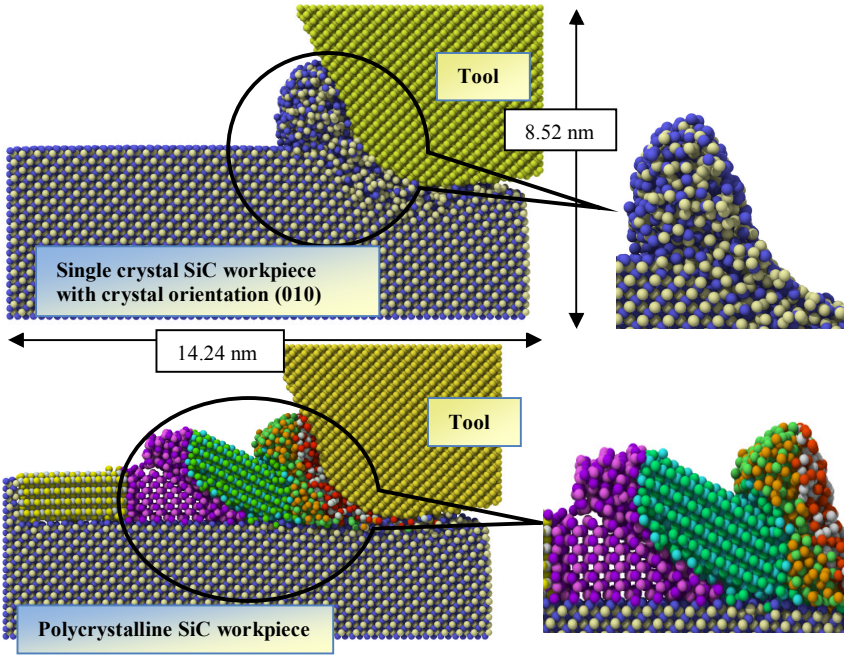


Figure 3: Snapshot from simulation showing response of workpieces during cutting.

As evident from figure 3, uniformity in SC lattice causes the dislocation nucleation to move on a continous slip plane. In PC lattice, however, not only the lattice structure of the adjacent grains may differ in orientation, the grain boundary too remain

disordered. Hence, the cleavage occurs in a random manner depending on the ease of lowest cleavage energy offered by a particular grain. Thus, apart from grain boundary sliding and stacking faults, a phenomenon of cleavage along the easy slip plane also occurs simultaneously. This mechanism is reminiscent to the experimental study on RB-SiC (figure 4) and is also principally responsible for a random and slightly higher observed surface roughness in PC- SiC such as CVD-3C-SiC and RB-SiC.

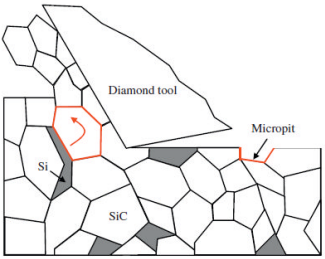


Figure 4: Effect of grain boundaries on the nanometric cutting of SiC [1].

Average specific cutting energy for both the configurations was also computed from the simulation. While the value obtained for PC-3C-SiC was found as 115 GPa, it was relatively higher for SC-3C-SiC as 150 GPa. This is for the fact that sliding along the easily cleavable direction in a non-uniform lattice will require least energy in comparison to cut a continuous and uniform crystal lattice on a relatively harder direction of cut. Moreover, in SC-3C-SiC every individual atom underwent distortion in contrast to PC-3C-SiC where a lump of grain just slides over another grain. The above mechanism explains why in the previous experiments RB-SiC [1] and CVD-3C-SiC [6], despite providing high surface roughness, were observed to be relatively more machinable than the single crystal SiC.

References:

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