MD simulation of stress-assisted nanometric cutting mechanism of 3C silicon carbide

Liu, L., Xu, Z., Hartmaier, A., Luo, X., Zhang, J., Nordlund, K. & Rommel, M.

Abstract

Purpose – The paper aims to reveal the underlying mechanism of improvement of ductile machinability of 3C-SiC and associated cutting mechanism in stress-assisted nanometric cutting.

Design/methodology/approach – MD simulation of nanometric cutting of 3C-SiC is carried out in this paper. Two scenarios are considered: (i) normal nanometric cutting of 3C-SiC, (ii) stress-assist nanometric cutting of 3C-SiC for comparison. Chip formation, phase transformation, dislocation activities and shear strain during nanometric cutting are analyzed.

Findings – The results show that in the ductile-brittle transition stage, the deformation mechanism of 3C-SiC is the combination of plastic deformation dominated by dislocation activities and localization of shear deformation. Stress-assisted nanometric cutting can lead to lower cutting resistance and better quality of machined surface indicated by the low subsurface damage depth. But there is a threshold for the applied stress to fully gain advantages offered by stress-assisted nanometric cutting. Furthermore, the stress-assisted nanometric cutting further enhances its plastic deformation ability through the active dislocations' movements.

Originality/value – This work describes a stress-assisted machining method for improving the surface quality, which could improve 3C-SiC ductile machining ability.

Keywords Molecular dynamics simulation, 3C-SiC, Ductile-brittle transition, Pre-stressed machining

Paper type Research paper

1. Introduction

As the third-generation semiconductor materials, silicon carbide (SiC) is widely used in various fields due to its wide energy bandgap, high breakdown electric field, high thermal conductivity, high saturated electron drift velocity (Madar, 2004). However, as a hard and brittle material, it has high hardness and wear resistance, resulting in low removal efficiency and poor surface machining quality, which seriously hinders the application.

In recent years, molecular dynamics (MD) simulation is an effective method to study nanometric cutting. It can systematically and comprehensively study nanometric cutting and reveal the mechanism of nanometric cutting, so as to provide theoretical basis for nanometric cutting experiments. The research shows that hard and brittle materials such as silicon carbide can also achieve ductile removal of the material, so as to obtain good surface integrity. For this reason, many scholars are devoted to study the plastic deformation mechanism of silicon carbide. Gao and Patten successfully achieved ductile removal on single crystal 6H-SiC, and found that the plasticity of silicon carbide was caused by the formation of high pressure phase near the tool edge (Patten et al., 2005). Goel et al. studied atomistic aspects of ductile responses of 3C-SiC during nanometric cutting, it was considered that 3C-SiC undergone sp3-sp2 order-disorder transition resulting in the formation of SiC-graphene-like which caused ductile response (Goel et al., 2011). Wu et al. studied the nanometric cutting deformation mechanism of 6H-SiC by MD simulation. It was believed that with the increase of cutting depth, 6H-SiC experienced the transition from elastic deformation to plastic deformation and then to intermittent cleavage (Wu et al., 2017). Xiao et al. studied the relationship between cutting thickness and stress through MD simulation and concluded that when the cutting depth became small enough, the tensile stress would become lower than the critical tensile stress of brittle fracture, which was not enough to cause brittle fracture (Xiao et al., 2018).

Some methods have been proposed to effectively improve the nanomachining ability of hard and brittle materials, such as ion-implant-assisted machining, surface defect machining and stress-assisted machining. Stress-assisted machining is a method proposed to control the residual stress of machined surface in metal machining. This method refers to applying pre-stress to the material while machining. It has been applied to the experimental machining of brittle materials so as to improve the machining ability. Yoshino et al. conducted single-point diamond turning experiments on silicon under external hydrostatic pressure. It was found that by applying 400 MPa external hydrostatic pressure, both the surface quality and the critical cutting depth of ductile-brittle transition could obviously increase (Yoshino et al., 2005). Jiang et al. conducted stress-assisted scratch tests on SiC ceramics. The results demonstrated that stress-assisted method can contribute to decrease the machining damage (Jiang et al., 2010). Although the above studies have revealed that the stress-assisted machining is indeed helpful to improve the machining ability of brittle materials, the mechanism is still not clear.

In this paper, MD simulation is used to study the material removal mechanism of the ductile-brittle transition and the deformation mechanism of silicon carbide under stress-assisted nanometric cutting.

2. MD simulation details

MD simulation of nanometric cutting of 3C-SiC is carried out in this paper. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code (Plimpton, 1995) is used to simulate nanometric cutting of 3C-SiC. The results are visualized and analyzed by using Open Visualization Tool (OVITO) (Stukowski, 2009). Dislocation Extraction Algorithm (DXA) is adopted in order to analyze dislocations in the material. Fig. 1(a) shows the MD model for nanometric cutting of 3C-SiC where the cutting orientation is (001) [-100]. The model consists of a boundary layer, a thermostatic layer and a newton layer. The boundary layer is adopted to fix the workpiece, the atoms in the thermostatic layer are used to dissipate the heat generated during the cutting and the newton layer satisfies the second newton's law. Periodic boundary condition is applied along the y direction and the timestep is 0.5 fs. The simulated cutting temperature is kept at 293 K with a Nose-Hoover thermostat (Nose, 1984; Hoover, 1985). The diamond tool is set as a rigid body. A tool edge radius of 5 nm is adopted and tool rake and clearance angle are 0° and 10°, respectively. A high cutting speed of 50 m/s is adopted to reduce the computation demand. The analytical bond order potential (Erhart et al., 2005) is used to describe the interactions between Si-Si, Si-C, C-C in the tool and silicon carbide and among them. In the model of stress-assisted nanometric cutting, uniaxial compression with stress of 1, 5, 10 GPa within the elastic region are applied to the 3C-SiC along -x-axis, respectively, as shown in Fig. 1(b).

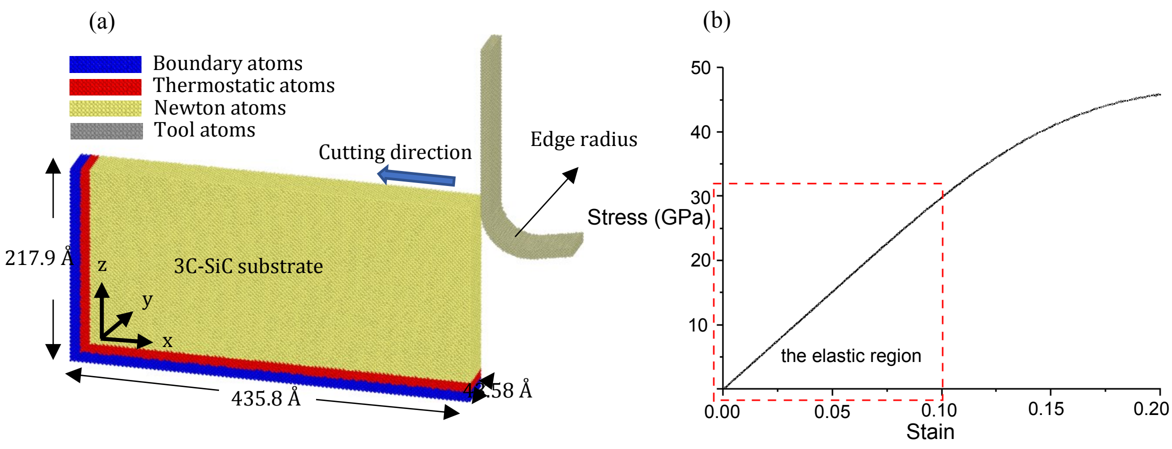

Figure 1. Schematic of the nanometric cutting simulation model (a) and stress-strain curves from uniaxial compression simulation (b).

3. Results and discussions

3.1 Analysis of material removal in ductile-brittle transition

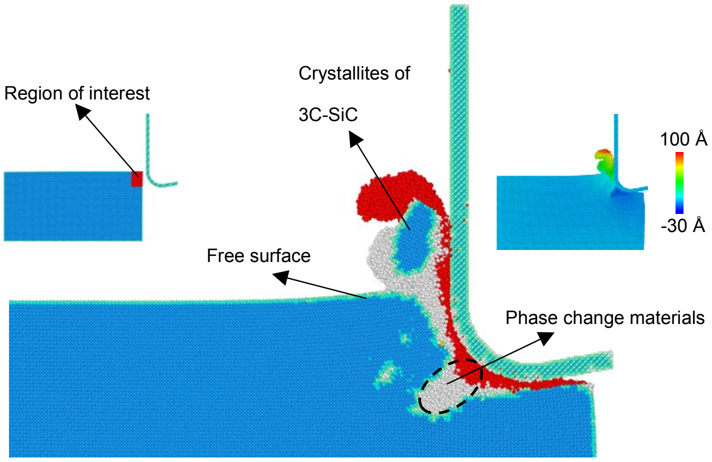

Figure 2. A snapshot of chip formation at 200 ps under normal nanometric cutting. A snapshot at 0 ps is at the top left and the top right is the z-direction displacement vector at 200 ps.

As can be seen from Fig. 2, when the tool cuts the material in the region of interest, some atoms in the region are pushed by the tool so that they move upward along rake face to form chips, and the others move downward to form the machined surface after being machined by the tool (the atomic z-direction displacement in the chip is positive, and the value below the tool edge is negative as shown in the top right of Fig. 2). During this process, it is interesting to find that a tiny amount of atoms still retain original lattice structure in the chips. This phenomenon is attributed to the fact that some phase change materials exist in the bottom left of the tool edge and the boundary of these phase change materials is distinguished from the free surface. Materials without phase change can be observed between these phase change region and the free surface. So some 3C-SiC crystallites are taken away when these phase change materials form chips in the way of plastic flow. The mechanism of this phenomenon is discussed in detail in Sec. 3.2.

Subsurface deformation is of critical importance because they govern the obtainable surface finish and form accuracy (Luo et al., 2012). Fig. 3 shows the comparison of the subsurface deformation depth under normal nanomachining and stress-assisted nanomachining with different stress value. It is obvious that the external stress value has a large effect on the subsurface damage depth. Among the pre-stress setup of 1 Gpa, 5 Gpa and 10 GPa, the stress-assisted machining with 5 GPa external stress will obtain the best quality of the finished surface indicated by the result of subsurface damage depth. So the results indicate that there will be a threshold for the pre-stress setup. The cutting force mainly derives from the interaction force between the tool atoms and the workpiece atoms in the nanometric cutting (Lai et al., 2013). Table 1 summarizes the average cutting force obtained from different machining conditions. The results indicated that the maximum reduction of 10.4% in average cutting force is achieved under 5 GPa stress-assisted machining. So the stress-assisted machining with an external stress of 5 GPa can obtain the best quality of the finished surface with lowest cutting resistance. Therefore, an external stress value of 5 GPa is adopted in the ductile-brittle transition stage.

Table 1 Comparison of the average cutting force with 5 nm depth of cut.

Machining condition	Normal nanometric cutting	Stress-assisted nanometric cutting		
		1 GPa	5 GPa	10 GPa
Average cutting force	1738.05 nN	1582.63 nN	1557.10 nN	1605.80 nN
Percentage of reduction in average cutting force		8.9%	10.4%	7.6%

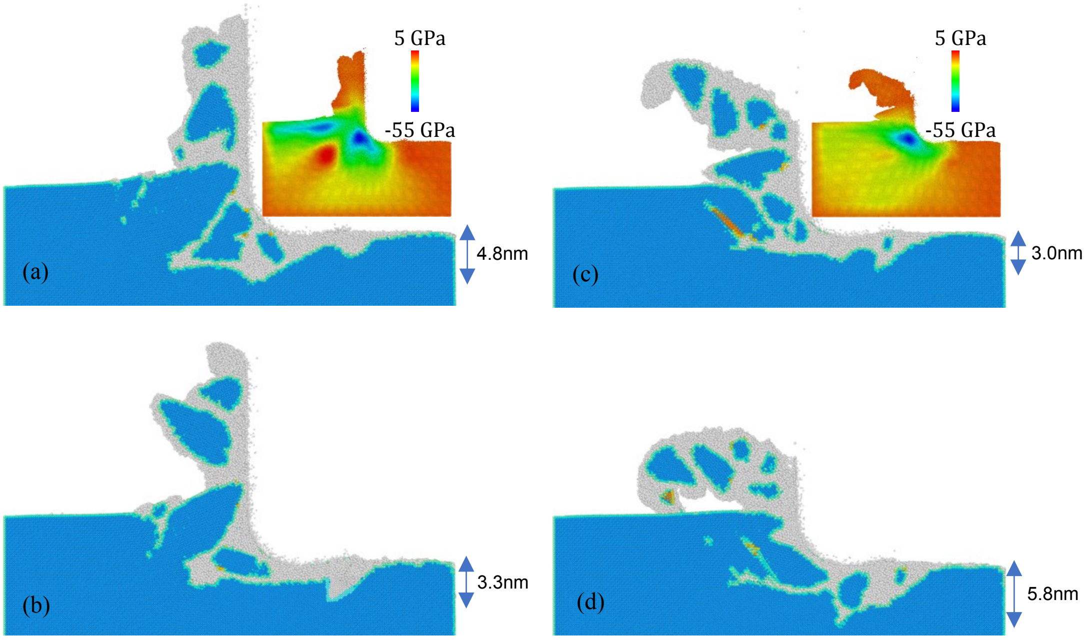

Figure 3. Snapshots from the different nanometric cutting simulation at 425 ps. The top right is the hydrostatic pressure distribution at the corresponding time. (a) Normal nanometric cutting. (b) Stress-assisted nanometric cutting with a stress of 1 GPa. (c) Stress-assisted nanometric cutting with a stress of 5 GPa. (d) Stress-assisted nanometric cutting with a stress of 10 GPa.

3.2 Phase transformation and analysis of dislocations

As mentioned in Sec. 3.1, some 3C-SiC crystallites are taken away when the phase change materials form chips in the way of plastic flow. However, it is not clear whether this plastic flow is caused by high pressure phase transformation (HPPT) or dislocation activities. In addition, MD results show that stress-assisted machining is indeed helpful to enhance plastic deformation ability of 3C-SiC, but the mechanism of stress-assisted machining is still unclear. Therefore, it is necessary to analyze the phase transformation and dislocation activities of the ductile-brittle transition for the stress-assisted nanomachining. Some scholars believe that the high pressure phase transformation caused by high hydrostatic stress in front of the tool is a major reason for the plastic deformation of silicon carbide (Patten et al., 2005; Goel et al., 2013). It is worth noting that simulations have revealed that the rocksalt structural transformation in 3C-SiC requires a pressure of 64.9 GPa (Tang, 1995) and 66 GPa (Chang et al., 1987). The hydrostatic stress distribution under normal and stress-assisted nanometric cutting are shown in Fig. 3 (a) and (c). High hydrostatic stress occurs in front of and beneath the tool edge and the peak hydrostatic stress is only -55 GPa (negative value represents compressive stress). Therefore, the hydrostatic stress is not enough to induce the high pressure phase transformation in nanometric cutting 3C-SiC at a cutting depth of 5 nm whether under normal or stress-assisted nanometric cutting.

Equivalent Von Mises strain is an index of local shear deformation of materials based on shear strain energy, which is a good measure for shear deformation along arbitrary directions (Shimizu et al., 2007). As shown in Fig. 4(a), significant shear bands occur inside the material in front of the tool. As the tool moves, a second shear band is formed which is parallel to the former and both are oriented in the -45° direction. The results are consistent with the conclusions obtained by Xiao et al. in studying the crack propagation direction of silicon carbide (Xiao et al., 2015). The formation of deformed localized shear bands is the precursor of fracture. Once the shear band is formed, the subsequent cutting process will be dominated by the brittle removal mode.

Fig. 5 shows output of the DXA algorithm during nanometric cutting. Before the formation of the shear band shown in Fig. 4(a), a variety of dislocations occur simultaneously, such as perfect dislocations with 1/2<110>

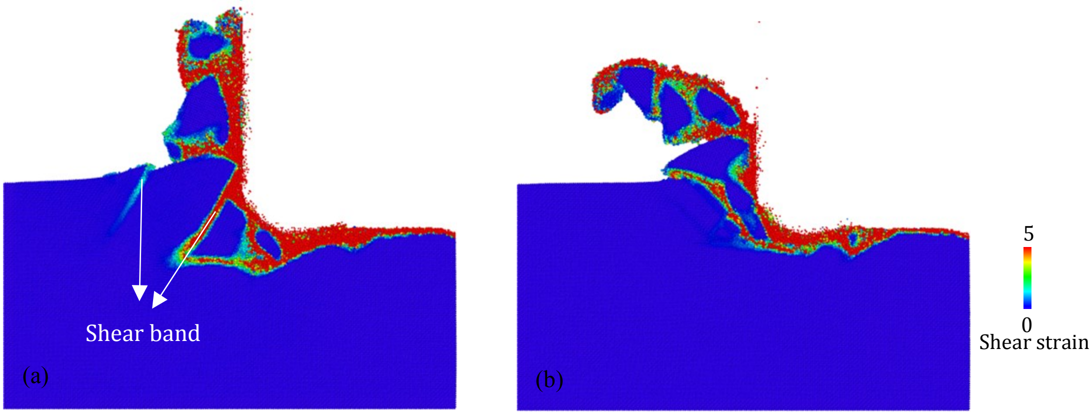

Figure 4. Variation of the shear strain during nanometric cutting of 3C-SiC at 425 ps. (a) Normal nanometric cutting. (b) Stress-assisted nanometric cutting.

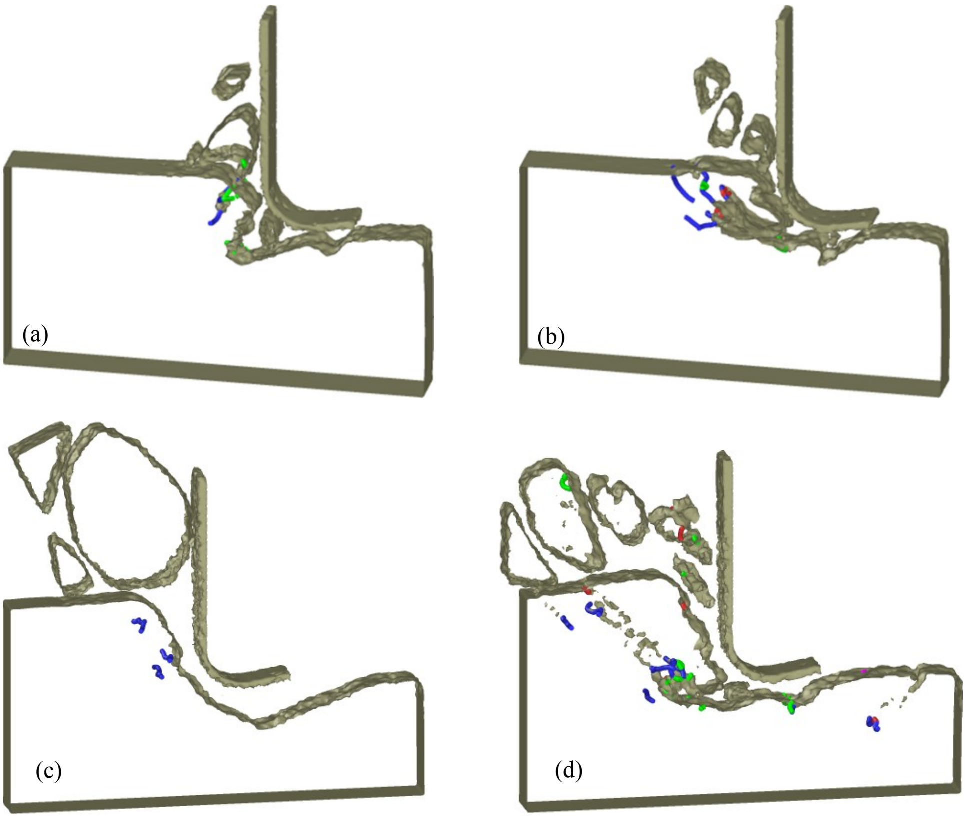

Figure 5. Output of the DXA algorithm showing dislocation lines during nanometric cutting. (a) Normal nanometric cutting with 5 nm depth of cut at 375 ps. (b) Stress-assisted nanometric cutting with 5 nm depth of cut at 375 ps. (c) Normal nanometric cutting with 10 nm depth of cut at 500 ps. (d) Stress-assisted nanometric cutting with 10 nm depth of cut at 500 ps. Blue lines, green lines, red lines represent dislocations with Burgers vector 1/2<110> and 1/6<112> and unidentified dislocations, respectively.

Burgers vectors and Shockley partial dislocations with 1/6<112> Burgers vectors, as seen in Fig. 5(a). The perfect dislocations with 1/2 <110> Burgers vectors and Shockley partial dislocations with 1/6 <112> Burgers vectors are seen to glide on the closely packed {111} planes, which facilitates the plasticity of 3C-SiC (Chavoshi et al., 2016). Thus continuous deformations can occur to form chips in the form of ductile removal. In addition, it can be seen that with the progress of cutting, the position where the dislocation occurs gradually forms a shear band. The reason for the formation of shear band is that silicon carbide cannot absorb a large amount of elastic strain energy through dislocation slip mechanism, so the strain is released to form shear band. It can be inferred that prior to the formation of the shear band, the tool extrusion will form a large number of dislocations inside the silicon carbide, so that the material has certain plastic deformation ability while brittle fracture occurs. So it can be concluded that in the ductile-brittle transition stage, the deformation mechanism of 3C-SiC is the combination of plastic deformation dominated by dislocation activities and shear localization characterized by fracture.

Furthermore, the results of dislocation analysis under stress-assisted nanometric cutting indicate that perfect dislocations with 1/2<110> Burgers vectors increase significantly comparing with the normal nanometric cutting, as shown in Fig. 5(b). Compared with 3C-SiC under normal nanometric cutting, the stress-assisted nanometric cutting further enhances its plastic deformation ability through the active dislocations' movements. Therefore, the stress-assisted machining with an external stress of 5 GPa will obtain the best quality of finished surface indicated by the subsurface damage depth, as shown in Fig. 3(c).

In addition, the nanometric cutting process of 3C-SiC with a larger depth of cut (10 nm) was further studied. From Fig. 6 (a) and (b), it is observed that the fracture occurs along the shear band to form fragmented chips, resulting in pits on the machined surface and poor quality of the machined surface. This phenomenon indicates that brittle fracture is predominant in the material removal process. In other words, nanometric cutting of silicon carbide is in the stage of brittle removal. The results of stress-assisted machining with a stress of 7 GPa are shown in Fig. 6 (c) and (d). In this case, the proportion of amorphous materials in the chips has been significantly increased, which indicates that the plasticity of the material is enhanced under stress-assisted machining. Therefore, the dislocation activities under the above two cutting modes are analyzed, as shown in Fig. 5(c) and (d). It is found that perfect dislocations with 1/2<110> Burgers vectors and Shockley partial dislocations with 1/6 <112> Burgers vectors are significantly increased under stress-assisted machining. As mentioned above, these two dislocations can slip, which can facilitate plasticity of 3C-SiC. MD simulation results further show that stress-assisted machining can effectively activate dislocation activities, resulting in the improvement of ductile machining.

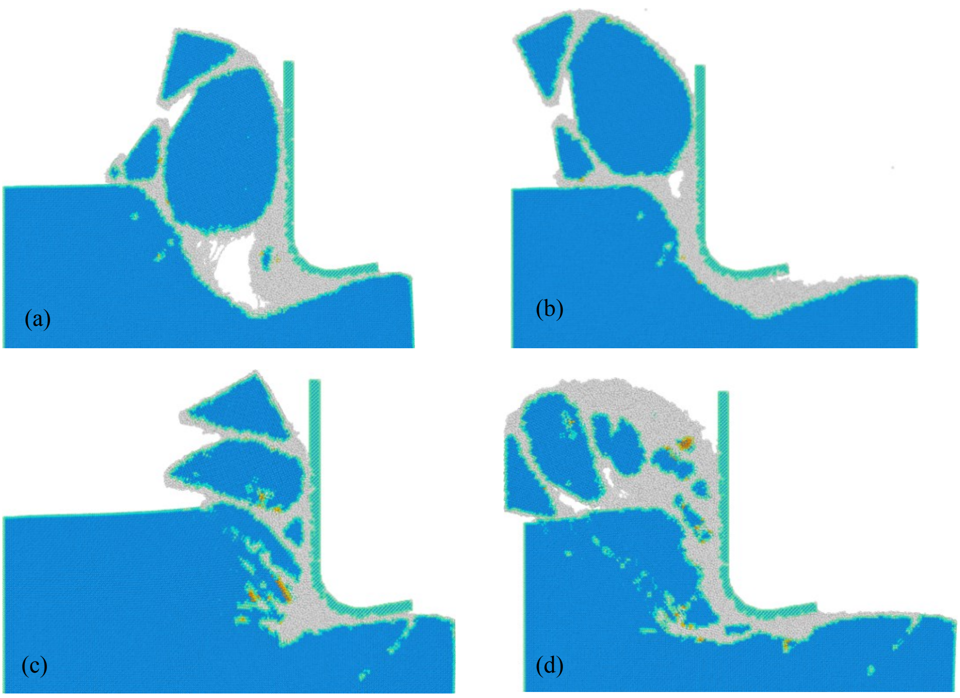

Figure 6. Snapshots from the different nanometric cutting simulation with 10 nm depth of cut. (a) Normal nanometric cutting at 300 ps. (b) Normal nanometric cutting at 500 ps. (c) Stress-assisted nanometric cutting with a stress of 7 GPa at 300 ps. (d) Stress-assisted nanometric cutting with a stress of 7 GPa at 500 ps.

4. Conclusions

The molecular dynamics simulation is performed to investigate the nanometric cutting mechanism of 3C-SiC in the ductile-brittle cutting mode transition. The stress-assisted machining method is studied to improve 3C-SiC ductile machining ability. The following conclusions can be drawn from the simulation results:

(1) The deformation mechanism of 3C-SiC is the combination of plastic deformation dominated by dislocation activities and localization of shear deformation in the ductile-brittle transition stage.

(2) Stress-assisted nanometric cutting can obtain better quality of the finished surface indicated by the subsurface damage depth and lower cutting resistance. But the results also indicate that there will be a threshold for the pre-stress setup.

(3) Furthermore, the stress-assisted nanometric cutting can further enhance its plastic deformation ability through the active dislocations' movements, including perfect dislocations with 1/2<110> Burgers vectors and Shockley partial dislocations with 1/6 <112> Burgers vectors.

References

Chang, K. J., and Cohen, M. L. (1987), "Erratum: ab initio pseudopotential study of structural and high-pressure properties of sic", *Physical Review B Condensed Matter*, Vol. 35 NO. 15, p. 8196.

Chavoshi, S. Z., and Luo, X. (2016), "Molecular dynamics simulation study of deformation mechanisms in 3c–sic during nanometric cutting at elevated temperatures", *Materials Science and Engineering: A*, Vol. 654, pp. 400-417.

Erhart P., Albe K. . (2005), "Analytical potential for atomistic simulations of silicon, carbon, and silicon carbide", *Physical Review B*, Vol. 71, p. 035211.

Goel, S., Luo, X., Reuben, R. L., and Rashid, W. (2011), "Atomistic aspects of ductile responses of cubic silicon carbide during nanometric cutting", *Nanoscale Research Letters*, Vol. 6 NO. 1, p. 589.

Goel, S. , Stukowski, A. , Luo, X. , Agrawal, A. , and Reuben, R. L. . (2013), "Anisotropy of single-crystal 3c–sic during nanometric cutting", *Modelling and Simulation in Materials Science and Engineering*, Vol. 21 NO. 6, p. 065004.

Hoover W G. "Canonical dynamics: Equilibrium phase-space distributions", *Phys Rev A Gen Phys*, Vol. 31 NO. 3, pp. 1695-1697.

Jiang, S. Q. , Tan, Y. Q. . (2010), "Discrete Element Method (DEM) Simulation and Investigation of SiC on Pre-stressed Machining", *Journal of Inorganic Materials*, Vol. 25 NO 12, pp. 1286-1290.

Luo, X. , Goel, S. , and Reuben, R. L. . (2012), "A quantitative assessment of nanometric machinability of major polytypes of single crystal silicon carbide", *Journal of the European Ceramic Society*, Vol. 32 NO. 12.

Lai, M. , Zhang, X. , Fang, F. , Wang, Y. , Feng, M. , and Tian, W. . (2013), "Study on nanometric cutting of germanium by molecular dynamics simulation", *Nanoscale Research Letters*, Vol. 8 NO. 1, p. 13.

Madar, R. (2004), "Materials science: Silicon carbide in contention", *Nature*, Vol. 430 NO. 7003, pp. 974–975.

Nose, S. . (1984), "A unified formulation of the constant temperature molecular dynamics methods", *Journal of Chemical Physics*, Vol. 81 NO. 1, pp. 511-519.

Plimpton, S. (1995), "Fast parallel algorithms for short-range molecular dynamics", *Journal of Computational Physics*, Vol. 117 NO. 1, pp. 1-19.

Patten, J., Gao, W., and Yasuto, K. (2005), "Ductile Regime Nanomachining of Single-Crystal Silicon Carbide", *Journal of Manufacturing Science and Engineering*, Vol. 127 NO. 3, pp. 522-532.

Stukowski, A. (2009), "Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool", *Modelling and Simulation in Materials Science and Engineering*, Vol. 18 NO. 1, p. 015012.

Shimizu, F. , Ogata, S. , and Li, J. . (2007), "Theory of shear banding in metallic glasses and molecular dynamics calculations", *MATERIALS TRANSACTIONS*, Vol. 48 NO. 11, pp. 2923-2927.

Tang, M. (1995), "Elastic instabilities and structural responses of beta-silicon carbide under stress", *Nuclear Engineering*, (Cambridge, MA: Massachusetts Institute of Technology).

Wu, Z., Liu, W., and Zhang, L. (2017), "Revealing the deformation mechanisms of 6H-silicon carbide under nano-cutting", *Computational Materials Science*, Vol. 137, pp. 282–288.

Xiao, G. , To, S. , and Zhang, G. . (2015), "Molecular dynamics modelling of brittle–ductile cutting mode transition: case study on silicon carbide", *International Journal of Machine Tools and Manufacture*, Vol. 88, pp. 214-222.

Xiao, G., Ren, M., and To, S. (2018), "A Study of Mechanics in Brittle–Ductile Cutting Mode Transition", *Micromachines*, Vol. 9 NO. 2, p. 49.

Yoshino, M. , Ogawa, Y. , and Aravindan, S. . (2005), "Machining of hard-brittle materials by a single point tool under external hydrostatic pressure", *Journal of Manufacturing Science and Engineering*, Vol. 127 NO. 4, pp. 837-845.