Modelling for Material Removal Modes of Monocrystalline Sapphire by Single-grit Scratch

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Abstract. Due to the randomness of the shape and distribution of abrasive grains, the number of cutting edge (NoCE) on the abrasive grains is varying during grinding process, which imparts a significant effect on material removal. In this paper, the effect of NoCE on material removal mechanism of sapphire, e.g. critical cutting depth and fracture behaviour, is studied through numerical simulation and experimental study. Single grits with conical and triangular pyramid shapes, corresponding to 0, 2 and 3 cutting edges in the scratching tests, are considered in the study. The stress distribution under various scratching conditions was simulated using a coupled smoothed particle hydrodynamics and finite element method (SPH-FEM) model. To validate the developed theoretical models, the critical cutting depth and groove topography were measured by an atomic force microscope (AFM) and a scanning electron microscope (SEM), respectively. It is concluded that the increase of NoCE of the grits results in the decrease of the critical cutting depth due to the unfavourable stress concentration in the cutting region. In the brittle regime cutting, brittle fracture is most severe when the NoCE is 3, whilst the slightest fracture corresponds to the conical-shaped grits with a zero number of cutting edge. The research results suggest that a reduced NoCE of abrasive grains favours better machining accuracy and even mirror finishing in precision grinding of monocrystalline sapphire.

Introduction

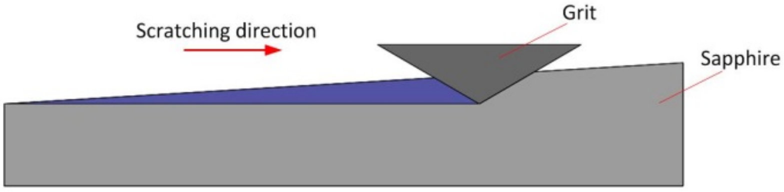
Sapphire, a single crystalline form of aluminum oxide (Al_2O_3), has been widely used in various high-tech fields, such as thin-film substrates, infrared windows, high-speed integrated-circuit chips, etc. due to its excellent optical and mechanical properties [1,2]. Sapphire is also a typical difficult-to-machine material given its extremely high hardness and brittleness. Generally, ultra-precision grinding is deemed a most suitable machining process to achieve the required surface quality on sapphire [3,4]. However, due to the random shape and distribution of abrasive grains on a grinding wheel, the number of cutting edges (NoCE) is varying during the grinding process, which influences the material removal mechanism [5–7]. Axinte *et al.* [5] have carried out a very meaningful study in this respect where single grits of controlled geometries were employed to conduct the scratch tests on sapphire sample. It was found that major plastic deformations were obtained when a circular base frustum with zero cutting edge was used, while fracturing phenomena were predominant for the square/triangular shaped grits corresponding to 2 and 3 cutting edges, respectively. In addition, the increase of NoCE contributed to significant reduction of specific cutting force. Following the footsteps of the above study, this paper further investigates the influence of NoCE on material removal mechanism of sapphire taking account of critical cutting depth and fracture behaviour though the single-grit scratch tests.

Generally, the numerical simulation of stress distribution in scratching of brittle materials was widely adopted to reveal material removal mechanism. In addition, a coupled model combining two different simulation methods—smoothed particle hydrodynamics (SPH) and finite element method (FEM)—were extensively used in recent researches [7–9]. For example, the stress distribution was analysed using SPH and FEM coupled 3D simulation of monocrystalline silicon carbide (SiC) scratching by single diamond grit [8].

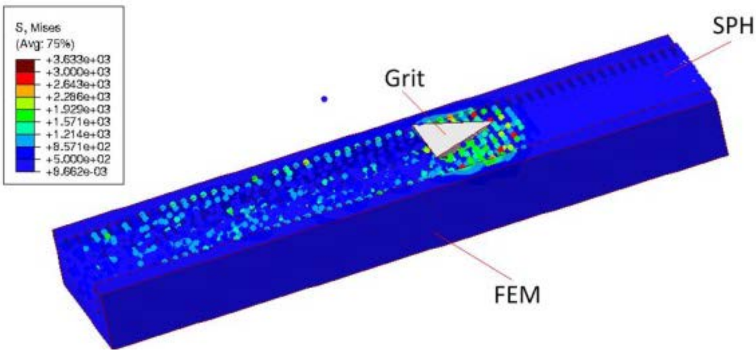
In this paper, experimental and simulation study on the effect of NoCE on material removal mechanism of sapphire will be carried out. The scratch tests will be conducted using conical and triangular pyramid shaped grits corresponding to 0, 2, and 3 cutting edges on C-plane sapphire. The stress distribution under the scratched grooves is simulated using a coupled SPH-FEM model. In order to characterise deformation features, the critical cutting depth and groove topography are measured by an atomic force microscope (AFM) and a scanning electron microscope (SEM), respectively.

SPH-FEM Coupled Simulation

Finite element method (FEM) has been extensively applied to simulate the material removal process of ductile materials in view of its suitability for the analysis of cutting mechanics. However, as for brittle material, it is less effective due to the element failure in the discontinuous problem. Besides, it is less efficient to analyse large-deformation problems due to severe mesh distortion. Compared to FEM, smoothed particle hydrodynamics (SPH) method is a mesh-free method where a set of particles is used to represent a continuum. Because of this advantage, SPH can be used to solve the problems of large deformation and material failure in the removal process. However, one should note that the computational accuracy of SPH is relatively low compared to that of FEM. Thus, the coupled SPH-FEM simulation model was proposed, where the SPH method was used to simulate the tool-work engagement region and the FEM is used for the bulk material of the small deformation region, as shown in Fig. 1. This method can not only ensure simulation accuracy but also improve simulation efficiency.



(a) Diagram of single grit scratch



(b) SPH-FEM coupled simulation model

Fig. 1 Diagram of single grit scratch and the corresponding simulation model

In this study, the SPH-FEM simulation model was developed to analyse the stress distribution under scratch groove for each scratch process. Thus, the simulation parameters such as grit geometry, scratch depth, velocity, etc. were determined according to the scratch experiments. The constitutive model and mechanical properties for sapphire in the simulation are listed in Tables 1 and 2, respectively.

Table 1 Constitutive model of sapphire used in this study [11]

ρ (kg/m^3)	G (GPa)	T (GPa)	K1	K2	K3
3,700	193	0.2	130.95	0	0
A	B	C	M	N	
0.93	0.31	0	0.6	0.6	

Table 2 Mechanical properties of sapphire [12]

Property	Unit	Value
Vikers hardness	GPa	18.5
Fracture toughness	$MPa \cdot m^{1/2}$	6.043
Young's modulus	GPa	456.5

Experiments

The (0 0 0 1) C-plane sapphire workpiece with a dimension of $10mm \times 10mm \times 10mm$ was used to investigate the effect of NoCE on removal mechanism under single grit scratch. All of the workpieces were polished to remove the original surface defects before the scratch tests. The surface roughness of them after being polished was less than 5 nm as measured by an atomic force microscope (AFM). Two types of diamond grits, i.e. conical and triangular pyramid shaped grits, with the same apex angle 120° was employed as scratch tools as shown in Fig. 2. Similar to the definition by Axinte *et al.* [5], the conical grit has 0 cutting edge, while for triangular pyramid shaped grit, the cutting edges are 2 and 3 corresponding to 'Face forward' and 'Edge forward' scratch direction, respectively, as shown in Fig. 2 (b-c). Scratch tests were conducted on a self-made scratching machine. The ramping scratch depth increased linearly from 0 to 3 µm along the scratch length of 30 mm and the scratch velocity was 10 mm/s. The topography of the scratched grooves was observed by an atomic force microscope (AFM) and a scanning electron microscope (SEM).

Results and Discussion

The characteristics of deformation and fracture under single grit scratch are shown in Figs. 3–5. It can be seen that as the scratch depth increases the material experienced three engagement phases successively, i.e. ductile-cutting phase, ductile–brittle transition phase, and brittle fracture phase in despite of different NoCEs. From the SEM images, the topography of groove scratched under the grit with zero cutting edge exhibits a greater range of ductile deformation and a smaller extent of brittle fracture. In contrast, the scratching grooves obtained under grits with 2 and 3 cutting edges experienced less ductile deformation. These features correspond to the respective critical cutting depth, d_c, of ductile–brittle transition (DBT), as shown in Figs. 3(c)–5(c). It shows that with the increase of NoCE the critical cutting depth decreases.

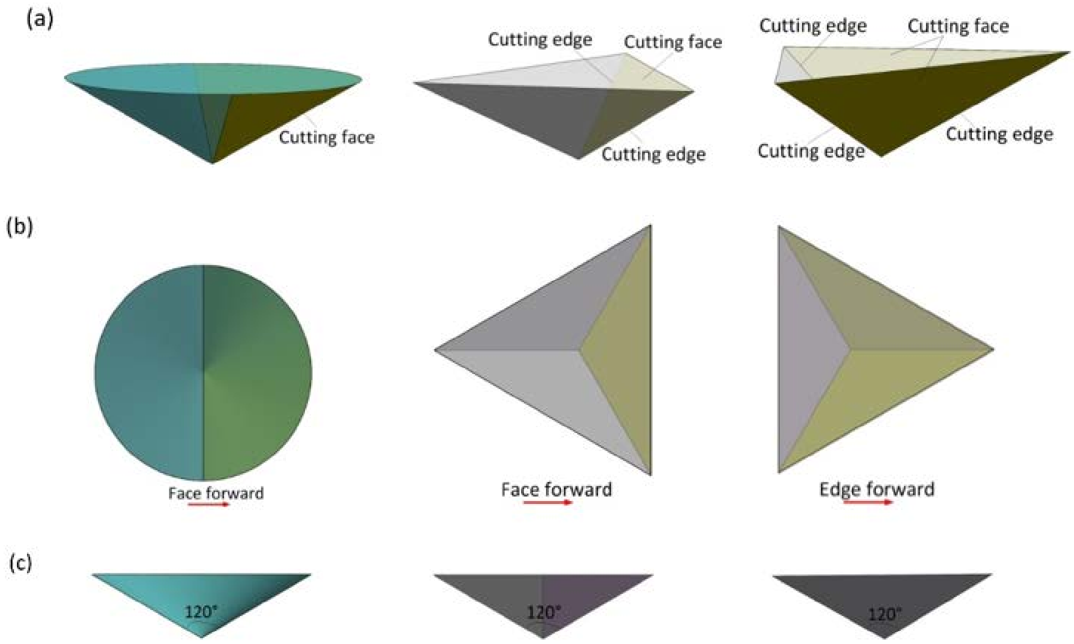


Fig. 2 (a) Three-dimension, (b) overhead view and (c) left view of grit models.

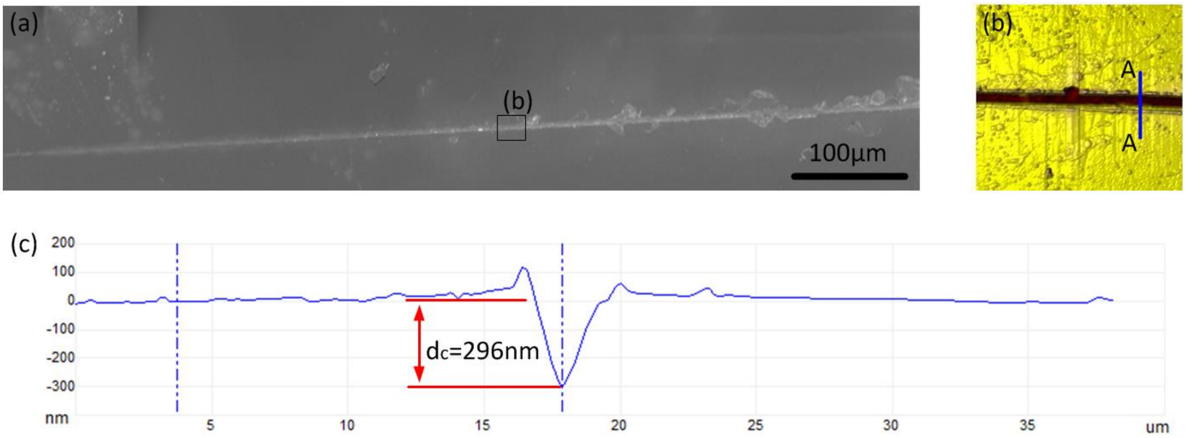


Fig. 3 SEM and AFM images of groove scratched by grit with zero cutting edge. (a) Groove surface obtained by SEM, (b) groove surface, and (c) section profile in DBT region obtained by AFM

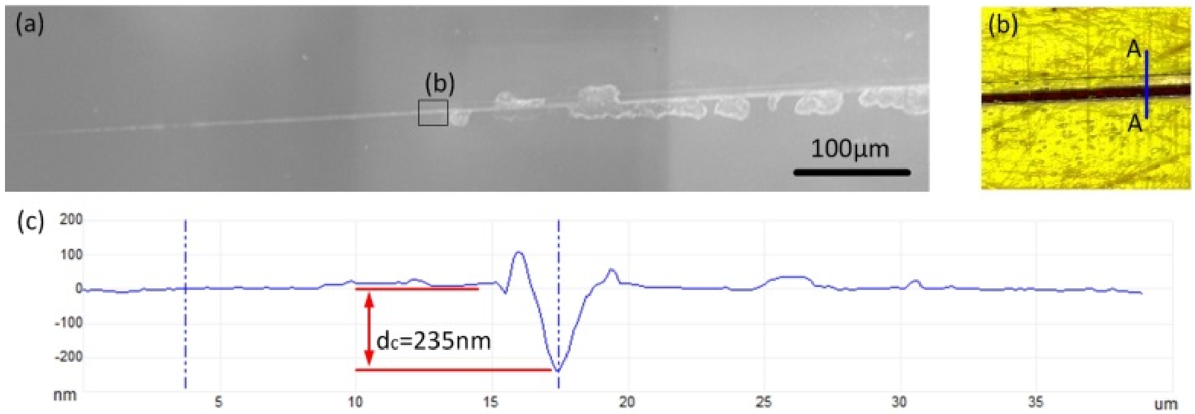


Fig. 4 SEM and AFM images of groove scratched by grit with 2 cutting edges. (a) Groove surface obtained by SEM, (b) groove surface and (c) section profile in DBT region obtained by AFM

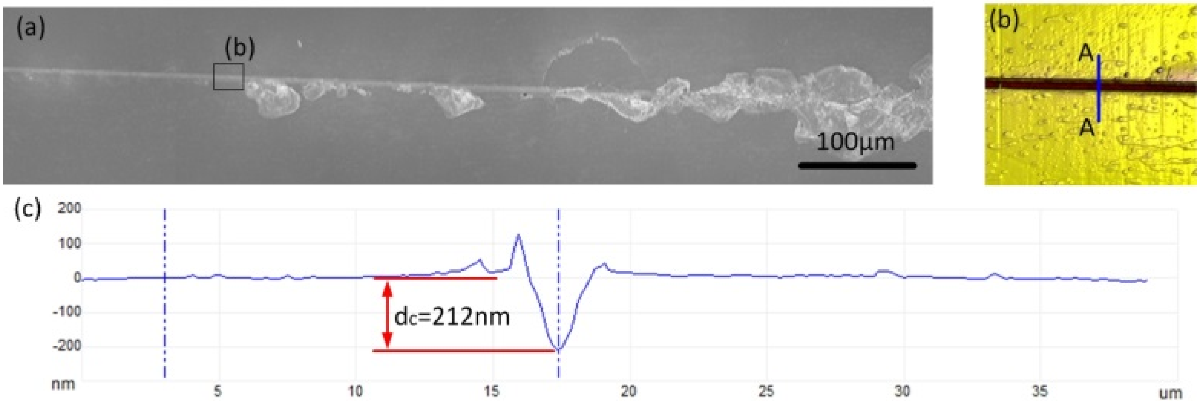


Fig. 5 SEM and AFM images of groove scratched by grit with 3 cutting edges. (a) Groove surface obtained by SEM, (b) groove surface and (c) section profile in DBT region obtained by AFM

The SPH-FEM simulation results reveal the same phenomena with experiments which can be explained from the stress distribution reasonably. As shown in Fig. 6, the high stress concentration, marked by red, orange and yellow spots, is larger when NoCE increases and concentrates in the vicinity of cutting edge at both plastic deformation and ductile removal stage, which tends to cause brittle fracture. Thus, stress concentration becomes more and more significant as the NoCE increases from 0 to 3. It is the stress concentration caused by the cutting edge that determines critical cutting depth in relation to deformation modes and brittle features. Moreover, the influence of residual stress in the model with zero cutting edge is larger than that of the model with 2 cutting edges. However, the depth of the stress concentration is on the contrary. The three-cutting-edge-grit can introduce larger residual stress and stress concentration in a wider range. Therefore, it is suggested that a reduced NoCE of abrasive grains should favour better machining accuracy and even potential mirror finishing in precision grinding of monocrystalline sapphire.

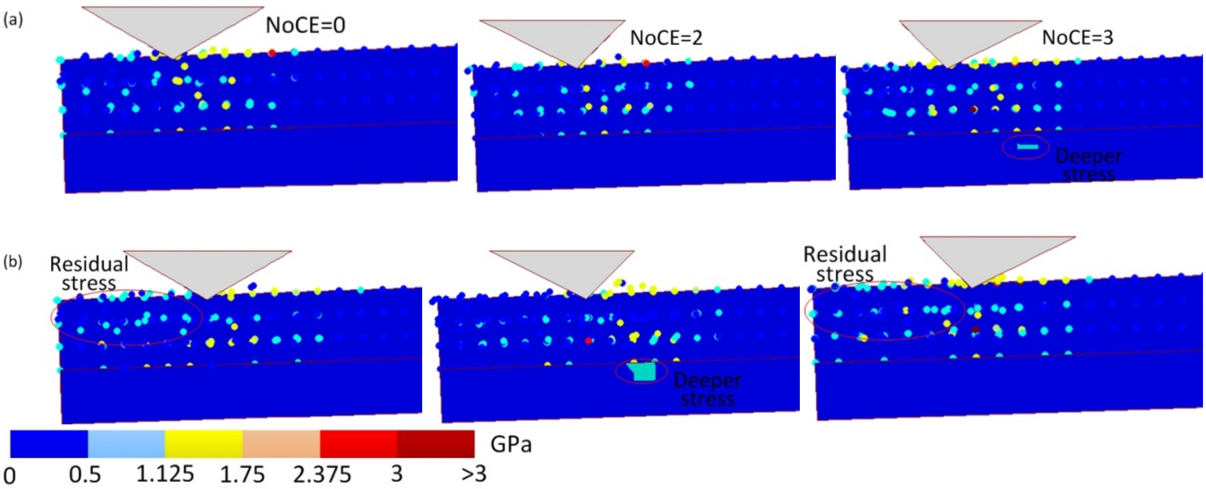


Fig. 6 Stress distribution on mid-surface of various simulation models at different scratching stage: (a) plastic deformation stage, (b) ductile removal stage

Summary

In this study, single-grit scratch experiments and the corresponding SPH-FEM simulation have been conducted to reveal the effect of NoCE on the material removal modes in monocrystalline sapphire. The conclusions can be summarised as follows:

(1) The material removal modes of sapphire correlate with the NoCE of grits. The brittle fracture is the most severe when the NoCE is 3 in the experiments, whilst the slightest fracture corresponds to the conical-shaped grits with a zero number of cutting edge. The critical cutting depth of ductile–brittle transition decreases when the NoCE increases.
(2) Stress level and distribution under the machined grooves is the dominant factor affecting the removal modes of sapphire. The stress concentration around cutting edge determines the critical cutting depth and material removal features which becomes more significant with the increase of NoCE.
(3) During scratching sapphire with single grit, zero-cutting-edge-grit may introduce larger residual stress, two-cutting-edge-grit may cause deeper stress distribution and lower level of residual stress, and three-cutting-edge-grit can potentially introduce larger residual stress and deeper stress distribution.
(4) SPH-FEM coupled model has been developed to simulate the scratching process successfully, which is proven to be an effective method to analyse the material removal mechanism for ultraprecision grinding.

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