CIRP Annals - Manufacturing Technology xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

CIRP Annals - Manufacturing Technology

journal homepage: http://ees.elsevier.com/cirp/default.asp

# Investigation of the cutting mechanisms and the anisotropic ductility of monocrystalline sapphire

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ARTICLE INFO

*Keywords:*
Machinability
Anisotropy
Sapphire

ABSTRACT

In this study, plunge-cut tests are conducted on single-crystal sapphire to investigate the brittle and ductile deformation mechanisms from the viewpoint of crystal anisotropy. The anisotropic deformation behaviour of the machined sapphire substrate manifests itself in the critical depth of cut and the diverse crack morphologies. Based on a resolved stress model that is adapted to the experimental procedure, weighted resolved stresses are computed, and the tendency of brittle–ductile transition depending on the peculiarities of the low-symmetry hexagonal crystal structure is discussed. Rhombohedral twinning is assumed to dominate the brittle–ductile transition.



## 1. Introduction

Aluminium oxide ($\alpha$-$Al_2O_3$), with its combined singular chemical and physical material properties, is a multifunctional, high-performance engineering material. Its extreme hardness and scratch resistance are applied in protective cover glasses (watches, mobile phones, lenses, etc.). The high optical transparency, one of the favourable optical properties that sapphire exhibits, is in the range of 200–5000 nm for optical devices such as LEDs and projectors. Furthermore, sapphire is suitable for applications in extremely harsh environments owing to its superior chemical and radiation resistance. Moreover, the biocompatibility is highly useful for bio-medical applications [1]. However, the machinability of sapphire is still an issue, owing to its hardness, brittleness, and crystal anisotropy.

For hard–brittle ceramics, the machinability depends on the cutting mode, i.e. the ductile and brittle modes [2]. Ductile regime cutting is associated with crack-free surfaces and low surface roughness, owing to plastic flow and chip formation. Plastic deformation is generated by dislocation movement initiated through a slip glide. The brittle mode is dominated by brittle fractures with crack formation and chipping caused by breakages along the cleavage planes.

The crack formation and deformation mechanisms of alumina [3] and single-crystal sapphire [4–6] were investigated in scribing processes using diamond indenter tips. It was found that the ductile cutting portion could be enhanced by using higher negative rake angle tools [4] and that increasing the scratch velocity was advantageous for the ductile plastic deformation [5]. The plunge-cut experiment with a round-nosed diamond tool is a common experimental investigation method used to study the anisotropic brittle–ductile transition (BDT) of single-crystal ceramics under orthogonal cutting conditions, e.g., in the case of $CaF_2$ [7], $MgF_2$ [8] or silicon substrates [9]. For the rhombohedral R-plane of sapphire, the anisotropic critical depth of cut (CDC) was measured using plunge-cut experiments [10]. However, the anisotropic deformation behaviour was not discussed with regards to the hexagonal crystal structure and the inherent deformation system, i.e., cleavage planes and slip systems.

Unlike high-symmetry crystal structures, such as $CaF_2$ or silicon, sapphire does not feature distinct primary and secondary slip systems and has several types of deformation systems (slip and cleavage) owing to its low-symmetry hexagonal crystal structure [11]. Twinning is also assumed to be involved in the deformation process of sapphire [12]. A resolved stress model is proposed to overcome this challenge.

In this study, plunge-cut tests were conducted to deeply analyse the brittle-ductile transition on the basal (0001) plane. The weighted resolved stresses were computed by incorporating critical resolved shear stress (CRSS) and fracture energy. The anisotropic deformation behaviour of the machined sapphire was inclusively discussed in terms of slip systems, cleavage, and twinning.

## 2. Resolved stress model

The tendency for plastic deformation associated with slip deformation can be geometrically expressed by the resolved shear stress on a specific slip system that consists of the slip plane and slip direction (Fig. 1(a)). Schmid's law describes this relation [13] by:

$$\tau = \sigma_a m \quad (1)$$

$$m = \cos\theta \cos\lambda \quad (2)$$

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http://dx.doi.org/10.1016/j.cirp.2017.04.018

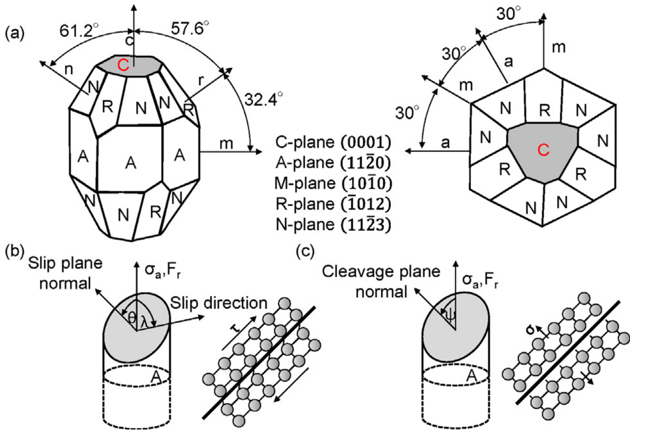


**Fig. 1.** (a) Crystallographic diagram of sapphire with commonly used crystal facets (tracht) [1], (b) slip deformation and (c) cleavage fracture.

where $\tau$ is the resolved shear stress, $\sigma_a$ is the applied stress, $m$ is the Schmid-factor, $\theta$ is the angle between the applied stress and slip plane normal vector, and $\lambda$ is the angle between the applied stress and slip direction (Fig. 1(b)). If the shear stress component surpasses a critical value, the CRSS, the slip dislocation for the applied stress can glide along the slip plane. The Schmid-factor $m$ quantifies how easily the slip system is activated in terms of the geometrical relationship between the force direction and slip system. Shibata discussed the influence of slip systems on the brittle-ductile transition of single-crystal silicon in a turning process based on the calculation of the Schmid-factor [14].

For low-symmetry hexagonal crystal structures such as sapphire, the resolved shear stress is not sufficient to fully describe the plastic deformation tendency; the plain geometrical calculation of the Schmid-factor only describes the relative magnitude of the resolved shear stress values. Hence, in order to include the tendency for activation under shear stress, the deformation systems were ranked by incorporating the CRSS for each specific slip system (as shown in Table 1), which is analogous to the approach of Nowak in the nano-indentation of sapphire [15]. The plastic deformation parameter $P_i$ describes the weighted Schmid-factor for the $i$th slip system or twinning:

$$P_i = \frac{m_i}{\left(\tau_i^{crit}/\min_i \tau_i^{crit}\right)} \tag{3}$$

As shown in Fig. 1(c), in a similar manner, the resolved tensile stress on a cleavage plane is given as:

$$\sigma = \sigma_a c \tag{4}$$

$$c = \cos\psi^2 \tag{5}$$

where $\sigma$ is the resolved tensile stress, $\sigma_a$ is the applied stress, $c$ is the cleavage factor and $\psi$ is the angle between the applied stress and cleavage plane normal vector. The cleavage planes are quantified by the fracture energy, which is necessary for the separation of the atomic bonds. Assuming that different cleavage planes have similar values for the resolved tensile stress, the cleavage plane that occupies the lowest fracture energy is more likely to be separated. Therefore, a cleavage fracture parameter $F_j$ is introduced by:

$$F_j = \frac{C_j}{\left(E_j^{frac}/\min_j E_j^{frac}\right)} \tag{6}$$

At the beginning of the computation, the slip and twinning systems given by the Miller-Bravais indices were transformed into the Cartesian coordinate system. The vector of the resultant force with an inclination angle $\beta$ on the main orientation plane is computed by utilising the Rodrigues-rotation calculation specification. The Rodrigues calculation formula describes a three-dimensional rotation for a given axis and rotation angle. The force inclination angle $\beta$ is calculated to be 40° on the basis of the resulting vector of the measured force component of the thrust force and cutting force. For each slip system $i$, with cutting direction angle $\delta$ on the main crystal plane and constant force inclination angle $\beta$, the Schmid-factor $m$ can be calculated by computing the angle $\theta$ between the resultant force vector and the slip plane normal vector, as well as the angle $\lambda$ between the force vector and slip direction. For each cleavage plane $j$, the angle between the applied force and cleavage plane normal is also calculated accordingly.

The twinning process is unidirectional and possible under a compressive load in respect to $c$-axis, whereas the slip systems are bidirectional (except for the pyramidal slip, which is activated only in the tensile loading case). The CRSS values are temperature dependent and were taken for a temperature of 200 °C to comprise the elevated temperature in the main deformation zone near the cutting edge. The main slip systems and cleavage fracture planes are given in Tables 1 and 2.

**Table 1**
Slip/twinning systems of sapphire for the structural unit cell [11].

| Slip (twinning) system | Miller-Bravais indices | Critical resolved shear stress $\tau_{crit}$ [MPa] |
|---|---|---|
| Rhombohedral twinning (RT) | $\{1\bar{1}02\}\langle 1\bar{1}0\bar{1}\rangle$ | 0.4066 |
| Basal twinning (BT) | $(0001)\langle \bar{1}010\rangle$ | 2.2255 |
| Basal slip (BS) | $(0001)\langle 11\bar{2}0\rangle$ | 2.2255 |
| Prismatic slip (PRS) | $\{11\bar{2}0\}\langle 10\bar{1}0\rangle$ | 1.6487 |
| Pyramidal slip (PYS) | $\{0\bar{1}11\}\langle 10\bar{1}1\rangle$ | 4.4817 |

**Table 2**
Cleavage planes of sapphire for the structural unit cell [1,11,16].

| Cleavage plane | Miller-Bravais indices | Fracture energy [J/m$^2$] |
|---|---|---|
| Basal cleavage (BC) | (0001) | >40 |
| Prismatic cleavage (PC) | $\{\bar{1}010\}$ | 7.3 |
| Rhombohedral cleavage (RC) | $\{\bar{1}012\}$ | 6 |

## 3. Experimental setup and procedure

The conventional plunge-cut experimental procedure is assimilated in order to avoid sudden stress release and impact on the cutting tool at the scratch end. Similar to fly-cutting, the tool exits the specimen with the same cutting slope in a continuous motion (Fig. 2(a)). The experiments were carried out on a four-axis ultra-precision vertical machine tool (UVM-450c, TOSHIBA MACHINE Ltd.). A damage-free and pre-polished single-crystal C-plane sapphire substrate (36 × 13 × 1 mm) was fixed on a vacuum chuck. The process forces were measured by a dynamometer (9256A1, KISTLER). The brittle–ductile transition point was measured using a white light interferometer (New View TM6200, ZYGO) and the machined surface was observed with an optical microscope (VH-Z450, KEYENCE). More detailed observations were performed using a field emission scanning electron microscope (FE-SEM Merlin Compact, CARL ZEISS).

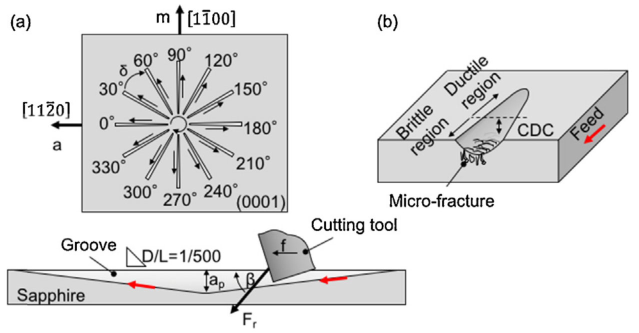


**Fig. 2.** (a) Schematic experimental procedure of in-and-out plunge-cut. (b) Brittle-ductile transition along the plunge-cut with definition of CDC.

Please cite this article in press as: Mizumoto Y, et al. Investigation of the cutting mechanisms and the anisotropic ductility of monocrystalline sapphire. CIRP Annals - Manufacturing Technology (2017), http://dx.doi.org/10.1016/j.cirp.2017.04.018