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A study of surface residual stress and crystal quality during ultra-precision diamond cutting of ZnSe crystals

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Abstract

In this paper, single-point diamond cutting experiments were conducted on soft-brittle ZnSe crystals, and the residual stress and crystal quality of cut surfaces are investigated. The results show that it is possible for negative compressive stress and positive tensile stress to coexist in the cut surfaces. The cut surface exhibits residual compressive stress ranging from tens to several hundreds of MPa. The residual stress and crystal damages of cut surfaces increase with increasing tool feed rate, while they almost remain unchanged with the cutting depth. The interaction effect of cutting parameters on residual stress and crystal quality is minimal. Moreover, a response surface model is developed to determine the residual stress with cutting parameters. This study will provide a reference for the defect-free ultra-precision machining of ZnSe crystals.

Ultra-precision machining, defect-free diamond cutting, ZnSe crystal, residual stress, crystal quality

1. Introduction

ZnSe crystal has stable physical and chemical properties, and it exhibits good transmission performance within a wavelength range from 0.5 μm to 22 μm, which basically cover the visible and infrared bands. It can be made into the fundamental elements for optical detection devices, nonlinear optical devices, and semiconductor lasers, etc [1, 2]. Single-point diamond turning enables efficient and mass production of precision elements, making it to be the most widely used method for processing ZnSe crystals [3, 4]. However, due to the high brittleness, low fracture toughness, and grain anisotropy of ZnSe crystals, various common damages inevitably arise, including fractures, cracks, and pits [5]. These damages greatly limit the utilization of the fabricated elements due to increased absorption or scattering. How to remove these common damages has been a hot research topic [6-8]. However, with the increasing demand for better surface quality of ZnSe crystals in the semiconductor and high-power laser fields, the research is no longer limited to the common damages. Nowadays, the research needs to encompass more subtle damages, especially residual stress and crystal disorder/damage of ZnSe crystals.

Few researchers have publicly reported on the residual stress and crystal quality of the machined ZnSe crystals. Sotillo et al. [9] investigated the residual stress distribution around Vickers indentation on the surface of ZnSe crystals. It is found that the compressive stress occurred inside the indentation, while the tensile stress appeared at the periphery of the indentation. Shojaee et al. [10] were the first to study the residual stress and crystal quality of ZnSe crystals after diamond turning. They identified the tensile stress, and demonstrated that a higher tensile stress and more severe lattice damages generally occurred with increasing feed rate. In the latest research, Huang et al. [11] believed that the stress in ZnSe crystals beneath the cutting tool could be decomposed into the hydrostatic stress caused by tool compression and the deviatoric stress applied by tool friction, with the former being dominant. Obviously, it is still unclear when tensile stress or compressive stress appears and what the magnitude of compressive stress is. The interaction effect of cutting parameters has never been reported.

In this paper, single-point diamond cutting experiments were conducted on ZnSe crystals under different cutting conditions. Raman spectroscopy is used to evaluate the residual stress and crystal quality of cut surfaces. The main and interaction effects of cutting parameters on residual stress and crystal quality are analyzed. Moreover, a response surface model is developed to determine the residual stress. This study will provide a reference for the defect-free machining of ZnSe crystals.

2. Experimental work

One ultra-precision polished ZnSe crystal (Φ25 ×1 mm) was prepared for the single-point diamond cutting experiments by Moore Nanotech 350FG, as shown in Fig. 1(a). The material properties of ZnSe crystal are shown in Table 1. As shown in Fig. 1(b), two groups of surfaces, i.e., Group A above and Group B under the horizontal line, were obtained by plunge cutting. Within each group, there are sixteen cut surfaces. Among them, one half on the left of vertical line was cut by tool 1, and the other half on the right of vertical line was cut by tool 2. The size of each cut surface was 2 mm × 2 mm, and the interval of adjacent cut surfaces was 0.5 mm. The geometrical parameters of tool 1 and tool 2 are shown in Table 2. The cutting parameters for Group A and Group B were determined using random and optimal Latin hypercube designs, respectively, as shown in Table 3. Group A and Group B were performed at different positions of ZnSe crystal. The values or ranges of cutting speed (v), feed (f), and cutting depth (a_p) were 800 mm/min, 0.5–5.0 μm/rev, and 0.5 μm –5.0 μm, respectively. A laser micro-Raman spectrometer (HR-800) was utilized to measure the residual stress and crystal quality of cut surfaces. Before the measurement, all cut surfaces were cleaned with alcohol, acetone, and deionized water for at least 5 min in an ultrasonic cleaning machine.

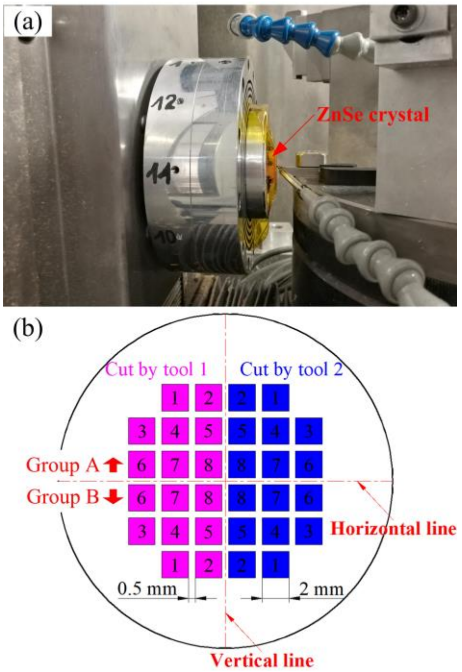

Figure 1. (a) Experimental setup for single-point diamond cutting experiments; (b) two groups of cut surfaces by tools 1 and 2, i.e., group A above and group B under the horizontal line.

Table 1 Material properties of ZnSe crystal

Young's modulus (GPa)	Density ($g \cdot cm^{-3}$)	Poisson ratio	Vickers hardness (GPa)	Fracture toughness ($Mpa \cdot m^{1/2}$)
70.3	5.3	0.3	1.5	0.9

Table 2 Geometry parameters of tool 1 and tool 2

Tool No.	Nose radius (mm)	Nominal rake angle (°)	Clearance angle (°)	Cutting edge radius (nm)
1	1.004	0	12	≈ 25
2	0.201	−25	12	≈ 20

Table 3 Groups A and B of cutting parameters

No. of cut surfaces	Group A		Group B	
	Tool Feed rate f (μm/rev)	Cutting depth a_p (μm)	Tool Feed rate f (μm/rev)	Cutting depth a_p (μm)
1	1.1	0.5	3.1	2.4
2	2.4	1.1	1.1	1.8
3	5.0	1.8	2.4	0.5
4	1.8	2.4	0.5	3.7
5	0.5	3.1	4.4	1.1
6	4.4	3.7	1.8	5.0
7	3.7	4.4	3.7	4.4
8	3.1	5.0	5.0	3.1

3. Results and discussions

Fig. 2 shows a typical Raman spectrum of an uncut surface. The transverse-optical (TO) and longitudinal-optical (LO) modes are centered at 205.6 cm^{-1} and 252.4 cm^{-1}, respectively. The third peak located at 140.3 cm^{-1} corresponds to the second order transversal acoustic (2TA) phonon mode. The Raman spectrum is sensitive to strain, and consequently, the residual stress can be measured by the shift of Raman peaks. A shift of Raman peaks towards a lower wavenumber indicates residual tensile stress, whereas the opposite shift indicates residual compressive stress. Fig. 2 also displays a Raman spectrum of a cut surface. A slight shift of Raman peaks towards a higher wavenumber reveals residual compressive stress in the cut surface. Shojaee et al. [10] reported that the residual stress in the diamond-turned ZnSe surface was tensile. Whether it is compressive or tensile stress depends on various factors, especially tool rake angle [12].

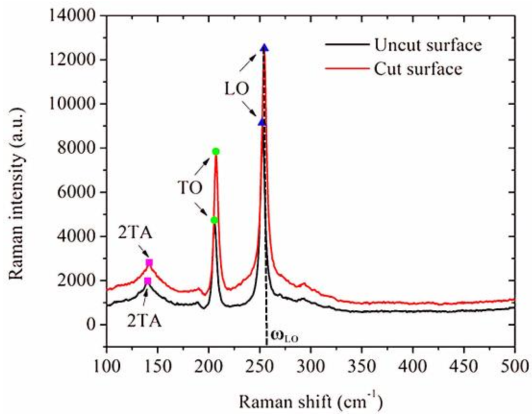

Figure 2. Raman spectrum of an uncut surface and a randomly selected cut surface.

Assuming that the cutting tool can be considered as a conical indenter, the indenter's half-apex angle is related with the tool rake angle and undeformed chip thickness. An analytical model of elastic stress field has been established for the scratching of brittle materials [13, 14]. The maximum principal stress around a scratch groove can be determined with the model. Fig. 3(a) and Fig. 3(b) show the normalized maximum principal stress around a scratch groove on ZnSe surface when the indenters with half-apex angles of 30° and 60° are used. It can be observed that the stress changes from negative to positive as the indenter is approached gradually, indicating the coexistence of compressive and tensile stresses in ZnSe cut surfaces. It provides a reasonable explanation for the possibility of detecting either compressive or tensile stresses when different process parameters are used.

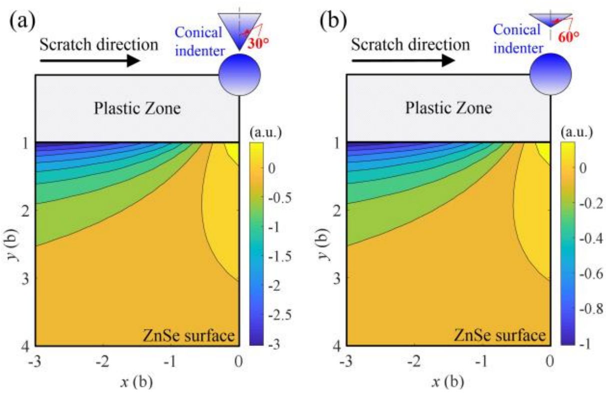

Figure 3. Normalized maximum principal stress around a scratch groove on ZnSe surface with indenter's half-apex angles of (a) 30° and (b) 60°.

LO mode is used to evaluate the residual stress and crystal quality (crystal disorder/damage) of cut surfaces. The residual stress (p) can be expressed as [15]:

$$p = \frac{\omega_{\mathrm{LO}} - 252.6}{3.14} \quad (1)$$

where ω_{LO} indicates the peak position of LO mode. The crystal quality is evaluated based on the peak width of LO mode, which can be determined by fitting the peaks to a Gauss-Lorentz type curve. An increasing peak width indicates a decrease in crystal quality. Five measuring points are selected randomly from each cut surface, and their corresponding residual stress and peak width are measured by laser micro-Raman spectrometer. Fig. 4(a) and Fig. 4(b) show the residual stress and peak width for each cut surface, respectively. It can be observed that the residual stresses range from 0 MPa to 510 MPa, and the peak widths range from 7.4 cm^{-1}to 8.6 cm^{-1}. The residual stress and peak width for cut surfaces by Tool 2 are generally larger than those by Tool 1. Tool 2 has a negative rake angle compared to Tool 1. Zhang et al. [12] found that a higher hydrostatic compressive stress was generated with a larger negative rake angle, and the stress value reduced as the negative rake angle decreased. This is consistent with the experimental results.

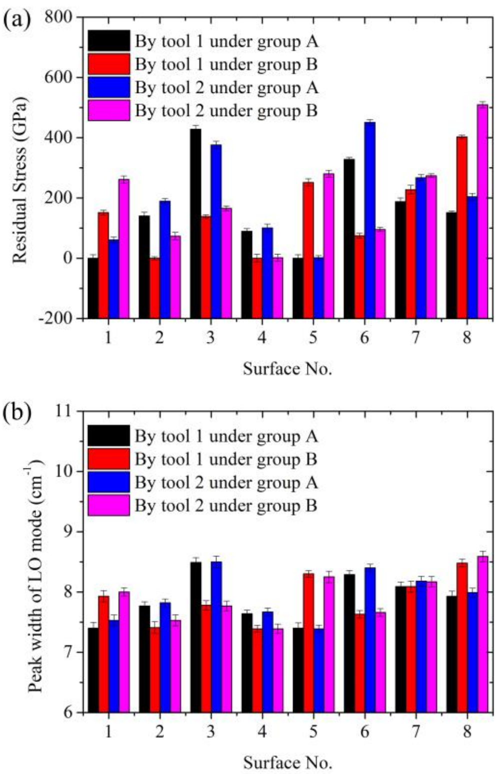

Figure 4. (a) Residual stress and (b) peak width of LO mode for cut surfaces.

As shown in Fig. 5 and Fig. 6, the effects of cutting parameters on residual stress and crystal quality of cut surfaces are investigated. The "Levels of factors" in Fig. 5(a) means that the cutting parameters are normalized to the range of [1.0, 2.0]. It can be found from Fig. 5(a) and Fig. 6(a) that the residual stress and peak width increase as the tool feed rate f transitions from low to high level, while they almost remain unchanged with the cutting depth a_p. This indicates higher residual stress and more severe crystal damages at higher too feed rate. The cutting depth has little effect on the crystal quality. Fig. 5(b) and Fig. 6(b) indicate a small interaction effect of cutting parameters on residual stress and crystal quality. Furthermore, the residual stress of cut surfaces is modelled with cutting parameters. The response surface model, known as the fitted second order polynomial regression model [16], is built as follows:

$$p = e_0 + e_1 f + e_2 a_p + e_{11} f^2 + e_{22} a_p^2 + e_{12} f a_p \quad (2)$$

where all coefficients e_0, e_1, …, e_{12} are obtained in Table 4 according to the values of residual stress. The coefficients of determination (R-square) are larger than 0.95, revealing that the fitting can describe the deviation in residual stress up to an extent of 95.0%.

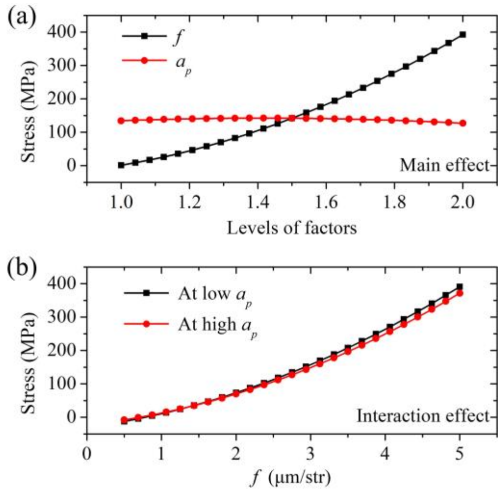

Figure 5. (a) Main and (b) interaction effects of cutting parameters (f: feed; a_p: cutting depth) on the residual stress of cut surfaces.

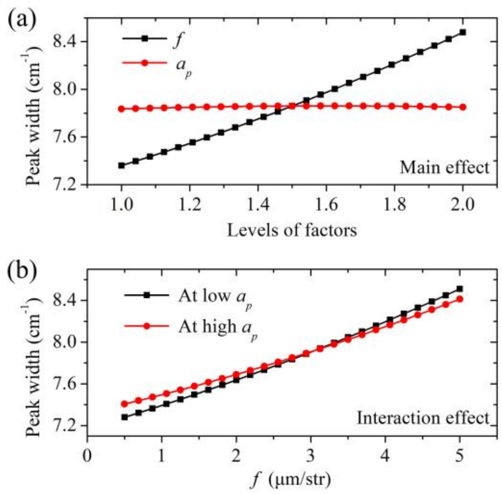

Figure 6. (a) Main and (b) interaction effects of cutting parameters (f: feed; a_p: cutting depth) on the peak width of LO mode for cut surfaces.

Table 4 Coefficients for the response surface model.

	e_0	e_1	e_2	e_{11}	e_{22}	e_{12}
Tool 1	−35.8	30.1	13.2	11.0	−2.1	−1.2
Tool 2	28.6	24.8	11.6	5.2	−9.1	15.1

4. Conclusions

This paper presents an experimental investigation of the residual stress and crystal quality of diamond cut ZnSe surfaces. The conclusions are summarized as follows:

(i) The cut surface exhibits residual compressive stress ranging from tens to several hundreds of MPa;

(ii) The residual stress and crystal damages of cut surfaces increase the with increasing tool feed rate, while they almost remain unchanged with the cutting depth. The interaction effect of cutting parameters on residual stress and crystal quality is minimal;
(iii) A response surface model is developed to determine the residual stress of cut surfaces with cutting parameters, with an R-square value greater than 0.95.

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