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Smoothed-particle hydrodynamics investigation on brittle-ductile transition of quartz glass in single-grain grinding process

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Abstract:

The smoothed particle hydrodynamics (SPH) method was introduced to simulate the quartz glass grinding process with a single grain under micro-nano scale. To investigate the mechanism of brittle-ductile transition, such factors as machining depth, grinding force, the maximum equivalent stress, residual stress were analyzed. The simulation results indicate that cracks in quartz glass at different grinding depths (0.1 ~ 1 μm) are observed, and the critical depth of brittle-ductile transformation is 0.36 μm. At different grinding depths, the grinding force ratio is greater than 1. When the cutting depth is 0.4 μm, the crack propagation depth is about 1.2 μm, which provides a basis for the prediction of subsurface damage depth. In addition, the correctness of the simulation result was verified by carrying out scratch experiments of varying cutting depth on optical quartz glass.

Keywords : quartz glass, brittle-ductile transition, ultra-precision grinding, SPH

1. Introduction

As a kind of special glass composed of single component of silica, quartz glass is increasingly widely used in many areas such as aerospace, microelectronics, information because of its excellent characteristics of high purity, high temperature resistance, radiation resistance, optical transparency, great stability etc. [1,2]. However, it is very difficult to obtain ultra-smooth surface and low/no damage of optical glass due to its high brittleness and hardness, which badly limits the application of optical glass [3,4].

In 1991, Bifano et al. [5] first proposed the view of brittle-ductile transition and the concept of critical depth, proved brittle material can be removed in ductile region. An et al. [6] compared BK7 glass with fused silica and found the fused silica was more difficult to machine than BK7 glass. The brittleness of fused silica is larger than BK7. Jia [7] conducted an experimental study on SF6 glass with increasing cutting depth, and explained the effect of cutting fluid on the cutting performance of SF6 glass. Under the condition of dry cutting, the brittle transition depth is 0.71 μm, and when the cutting fluid was

added, the critical depth increases to 1.08 μm. Liu et al. [8] analyzed the removal mechanism of glass materials through the micro-milling experiment of soda lime glass, and obtained the critical brittle-ductility transition condition considering the size effect. At the same time, it was found that when the cutting depth is less than 30 μm, soda lime glass can be processed in the ductile domain. Zhou et al. [9] carried out the indentation experiment of glass-ceramics using a microhardness tester, analyzed and discussed the mechanism of crack generation and propagation, and studied the effect of temperature on the brittle-ductile transition of glass-ceramics. Sun et al. [10] used the CSM technology to test the performance of glass ceramic hard substrates, studied the brittle-tough transition mechanism of glass ceramic hard substrates through nano-scratch technology, and obtained the critical depth of brittle-ductile transition of ceramic hard substrate (0.335 μm). Zhao et al. [11] investigated the fused silica by micro-nano indentation and single grit experiments, and considered the depth of the cut value for ductile model grinding was around 0.5 μm. Our team [12] established cutting model of K9 glass by using the smoothed particle hydrodynamics (SPH) method and found the

critical cutting depth was about 0.2 μm .

Grinding experiment is expensive and it is very difficult to observe the material behavior at micro scale. Therefore, a mesh-free method—SPH was introduced to simulate the single grain grinding process which can reveal the fundamentals of the grinding process. A remarkable advantage introduced by SPH is the “natural” chip/workpiece separation and no fracture criterion is necessary [13]. At present, the SPH method has been applied in a large number of materials, and its effectiveness has been proved. Wang et al. [14] used the SPH method to simulate the grinding process of titanium alloy with single particle cubic boron nitride (CBN), studied the influence of cutting depth on grinding force and chips, and compared the chip formation effect of SPH and FEM, proving the applicability of the SPH method for metal cutting simulation. Amir et al. [15] studied the flank wear effect of the tool by establishing a SPH simulation model of single-point diamond tool cutting silicon and the effect of tool wear on the brittle-ductile transition of silicon during the cutting process was studied microscopically by combining with experimental phenomena. In order to study the material removal mechanism in ultrasonic machining, Wang et al. [16] simulated the process of a single silicon carbide abrasive particle hammering float glass by the SPH method, then observed and analyzed the crack generation and propagation on the workpiece, and verified the correctness of the simulation model through ultrasonic experiment. Guo et al. [17] used the SPH method to establish the indentation simulation model on the KDP crystal plane (001). The effects of four types of indenters, including Vickers indenter, Bosch indenter, conical indenter and spherical indenter, on the depth of plastic damage layer were analyzed.

In this paper, a single grain grinding model for quartz glass is established and emphasis is put on brittle-ductile transition of quartz glass and the critical cutting depth needed for the ductile mode. The reliability of simulation results is also verified by scratch experiment.

2. Establishment of Single-grain Grinding Model

2.1 Theoretical Basis of SPH

Lucy et al. [18] proposed the SPH method in 1977. It has been verified by plenty of experiments that the problems of solid dynamic response and high velocity impact can be solved by the SPH method due to its self-adaptability.

The analysis model of SPH is shown in the Fig. 1, where i is the evaluation point particle, j is the other particle, the distance between particle i and j is $x-x'$, h is the smooth length of particles, and the value is 1.2 μm . When $x-x' < h$, particle j will participate in the calculation. The theoretical basis of the SPH algorithm is interpolation theory. Arbitrary macrovariable such as density, temperature, pressure can be represented as the form of integral interpolation by virtue of a group of unordered point. Using core estimated value of scalar field at one point provided by interpolating function can represent particle movement information. The approximate kernel function of a particle is:

$$\Pi^h f(x) = \int f(x') W(x-x', h) dy, \text{Error! Reference source not}$$

found. (1)

where W is a smooth function (or kernel function). If the smooth kernel function is the cubic B-spline function, it is defined as follows:

$$W(x-x', h) = a_d \begin{cases} 2/3 - R^2 + 0.5R^3, 0 \leq R < 1 \\ 1/6(2-R)^3, 1 \leq R < 2 \\ 0, R \leq 2 \end{cases} \quad (2)$$

In the formula, $R = |x-x'|/h$, a_d is a constant coefficient related to the smooth length h : $a_d = 1/h$, $a_d = 15/7\pi h^2$ and $a_d = 3/2\pi h^3$ Error! Reference source not found. are respectively in the 1D, 2D and 3D spaces.

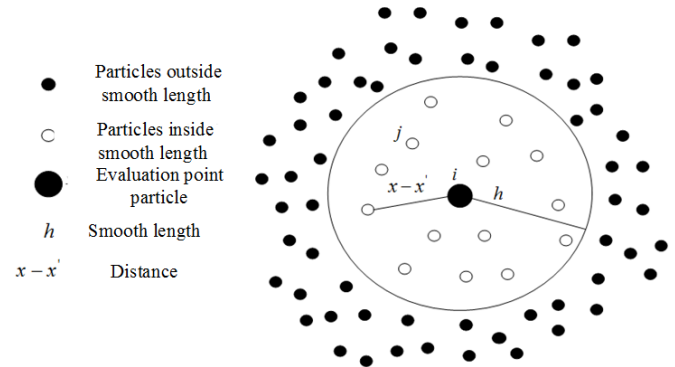


Fig. 1 SPH analysis model

2.2 Modeling of Single-grain Grinding Quartz Glass by the SPH Method

The material of grain is diamond in model. The density is 3.51 $\text{g}\cdot\text{cm}^{-3}$ and elastic modulus is 1141 GPa. The Poisson's ratio is 0.07. The single-particle diamond is simplified to the ideal spherical rigid body, as shown in Fig. 2.

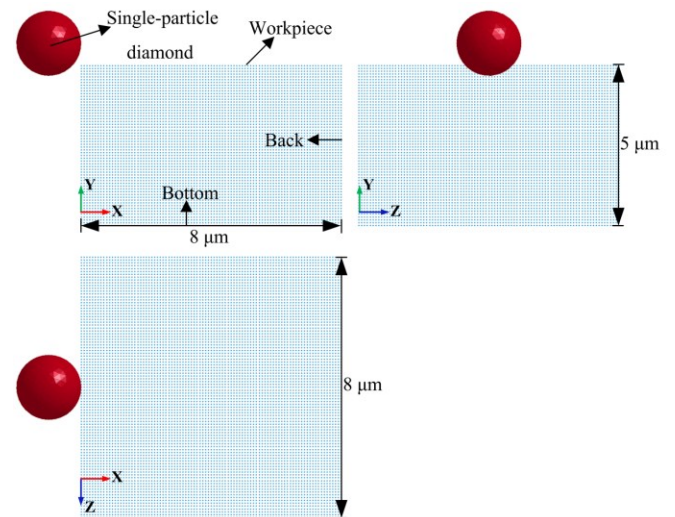


Fig. 2 SPH model of single grain grinding

To take into account both high efficiency and precision, the workpiece of quartz glass is designed as a cube of 8 μm ×5 μm ×8 μm . The number of particles in SPH is nearly 500,000, which is achieved by LS-PrePost. The key step in the SPH algorithm is neighborhood search. In this process, SPH's unique "ghost particle method" plays an important role [19, 20]. The bottom and back of the workpiece are constrained by using the virtual particle method. As shown in Fig. 3,

the SPH particles located at the boundary of the model automatically create virtual particles with the same mass, pressure and absolute velocity within the range of 2h in the vicinity of the self-mapping. In this way, the real particles can search the neighborhood normally, and constrain the particles at the boundary at the same time.

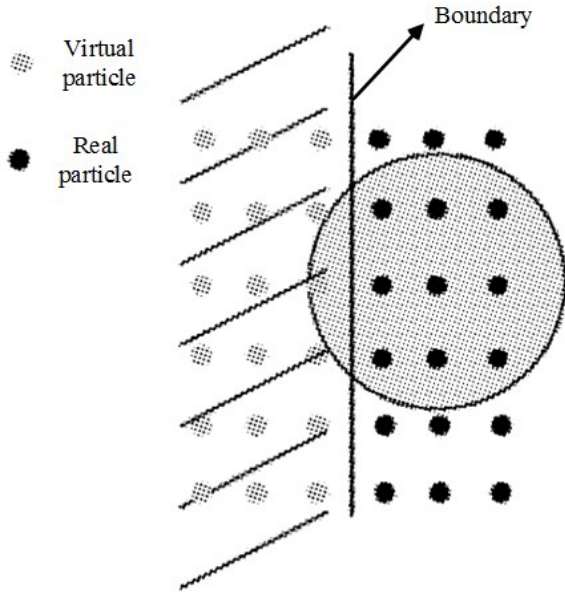


Fig. 3 The schematic of “ghost particle method”

Considering the damage during machining processes and the accumulation of compression failure, Johnson Holmquist Ceramics (JH-2) material model is chosen [21]. This model is rational to describe the constitutive relation of hard-brittle material. It is appropriate to large-strain and large-strain rate of material. Part parameters of the mode are shown in Tab.1 [22, 23]. The model of non-dimensional strength can be expressed as:

$$\sigma^* = \sigma_i^* - D(\sigma_i^* - \sigma_f^*) \tag{3}$$

In the formula, **Error! Reference source not found.** σ_i^* , **Error! Reference source not found.** σ_f^* are the complete strength and breaking strength of the material respectively (parameter variables with * indicate that they have been standardized). D is the damage variable ($0 \leq D \leq 1$), and its expression is:

$$D = \sum \Delta \varepsilon^p / \varepsilon_f^p \tag{4}$$

where **Error! Reference source not found.** $\Delta \varepsilon^p$ is the plastic strain during a cycle of integration and ε_f^p is the plastic strain to fracture under a constant pressure.

Table 1 Partial material parameters of optical quartz glass

Tensile strength	0.05 GPa
Bulk modulus	30 GPa
Hug elastic limit	9 GPa
Maximum normalized fractured strength	0.5
Fractured strength parameter (M)	0.29
Intact strength parameter (N)	0.75

3. Results and Analysis

3.1 The Brittle-ductile Transition of Quartz Glass

By the dichotomy, lots of simulation experiments are carried out to explore critical depth of brittle-ductile transition of single-grain grinding with the grinding depth ranging from 0.1 to 1 μm . Three sets of data chosen from simulation results are shown in Fig. 4a - Fig. 4c, in which the grinding depths are 0.1 μm , 0.36 μm , 0.6 μm respectively. Diameter of grain is 2 μm . When the cutting depth is 0.1 μm (Fig. 4a), quartz glass has no crack or fracture. It can be deemed that quartz glass achieved removal in plastic region under such conditions. As shown in Fig. 4b, when the cutting depth is 0.36 μm , crack is generated and extended to the edge of the workpiece at the initial moment, causing the brittle fracture of material. In the stable processing stage, from the plastic strain map (Fig. 4d), it can be seen that there is a plastic strain band extending obliquely from below the grains, indicating that cracks will occur here. When cutting depth is 0.6 μm (Fig. 4c), quartz glass generates the transverse crack obviously. Hence the critical depth of brittle-ductile transition is 0.36 μm by single-grain grinding in above conditions. Yao et al. [24] by using diamond grinding wheel to grind quartz glass in linear velocity of 31.5 $\text{m}\cdot\text{s}^{-1}$, measured the critical depth of brittle-ductile transition is 0.329 μm . The critical depth of brittle-ductile transition obtained by simulation is 0.36 μm , which is approximately close to the experimental result of Yao et al. Therefore, the validity of the SPH method is verified to some extent.

Using the SPH method to simulate the cutting process of quartz glass under the condition of 0° tool rake angle and 10 $\text{m}\cdot\text{s}^{-1}$ cutting speed, the critical depth of brittle-ductile transition is 0.18 μm [22]. The difference lies in that grain grinding is similar to cutting process in negative rake angle which can restrain the generation of cracks and the grinding process is more stable than cutting process.

Parameters	value
Density	2.2 $\text{g}\cdot\text{cm}^{-3}$
Young modulus	70 GPa
Poisson ratio	0.17
Shear modulus	31 GPa

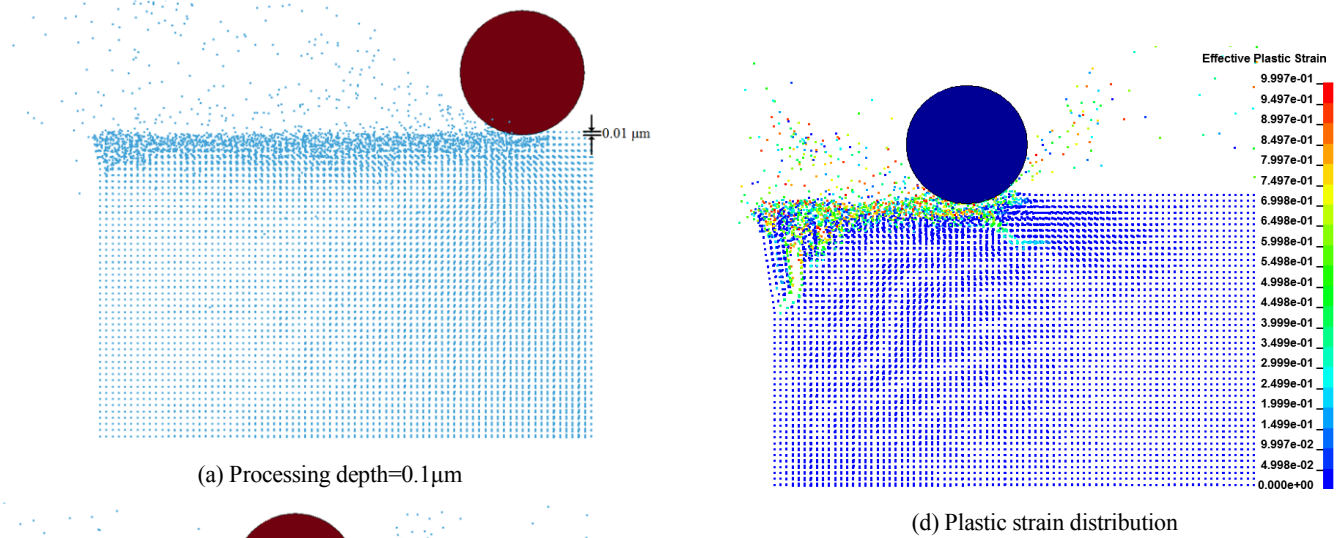
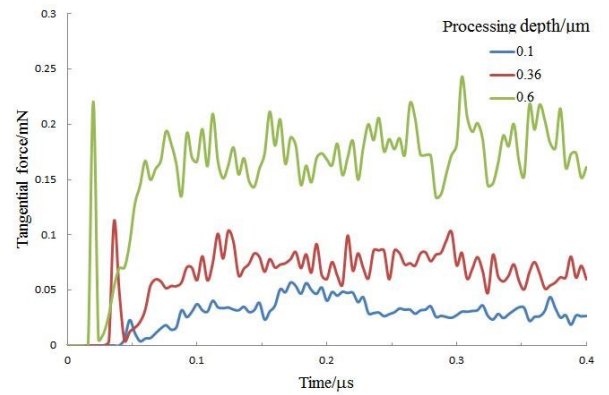


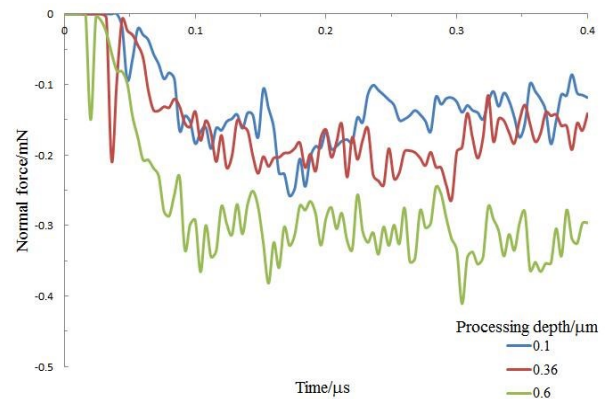
Fig. 4 Simulation results of grinding under different processing depth

3.2 Grinding Force

In general, the grinding force is divided into tangential grinding force F_t and normal grinding force F_n . Compared with tangential force and normal force, the axial grinding force is so small that it can be neglected. Tangential force and normal force are shown as Fig. 5 in different grinding depth.



(a) Tangential force



(b) Normal force

Fig. 5 Tangential and normal forces under different processing depth

With the increasing of cutting depth, material is removed more rapidly by grain and the resistance force acted on material is larger in speed direction. As a result, tangential force is increasing (Fig. 5a). The material removal undergoes a transition from plastic separation to brittle fracture in this process. When entering the brittle domain, the material removal is discontinuous, which causes serious fluctuation of tangential force. The tangential force forms a sharp increasing peak at the initial processing position in different grinding depth as a result of the collision between grain and workpiece.

As seen from the Fig. 5, the tangential force is more sensitive with the increase of the grinding depth. The stable grinding force is very important to improve the surface quality of the machined surface, and the smaller grinding force is helpful to avoid brittle collapse and achieve plastic removal. Generally, a crack-free surface obtained by ductile removal can be regarded as ideal. Therefore, it can be shown that controlling the grinding depth makes the removal of brittle materials in the plastic domain, which is more favorable to obtain the ideal surface quality.

Through the previous simulation analysis, it is found that when the cutting depth of the optical quartz glass is 0.36 μm, cracks occur in the quartz glass for the first time. To some extent the normal force load at this time can be regarded as the critical pressure load for cracking.

When the applied pressure just exceeds the critical value, the median crack begins to appear, and the load at this time is the critical pressure, and its calculation formula [25] is:

$$P_C = \lambda_0 K_{IC}^2 / H_V^3, \tag{5}$$

where, P_C is the pressure load on the test piece, K_{IC} is the fracture toughness of quartz glass [26], λ_0 is the proportional constant ($1.0 \sim 1.6 \times 10^4$), H_V is the Vickers hardness.

The fracture toughness K_{IC} and other parameters are measured in quasi-static condition in Eq.5, which are not fit to research the generation and propagation law of dynamic cracks. In grinding, the great impact effect occurred at the moment of grain contacting with workpiece. Therefore, the actual critical pressure load should be calculated in dynamic condition:

$$P_D = \lambda_0 K_{IC}^2 / H_V^3. \tag{6}$$

In the formula, K_{IC} is the dynamic fracture toughness, which is about 30% of the static fracture toughness [27,28].

By calculation, the critical pressure load of quartz glass P_D is obtained: 0.1284 mN ~ 0.2054 mN. The average value of normal cutting force in the stable cutting stage (after 0.15 s) is 0.1866 mN. Obviously, the simulation results are within the range of theoretical calculation results, which verifies the correctness of the simulation model to a certain extent.

3.3 Subsurface damage

During the grinding process, the variation of stress also reflects the grinding characteristics of quartz glass to a certain extent. Take the two columns of SPH particles markers in the Y-axis direction (Fig. 6) and output the time history information of the effective stress and displacement of the marked particles. The grinding depth is 0.4 μm, and brittle removal starts.

The maximum effective stress of the first column particles is shown in Fig. 7a. Due to the main deformation region of workpiece nearby the grinding depth, large stress concentration lead to the material separation phenomena of plastic deformation, brittle fracture for quartz glass. In the position of shallower than grinding depth, stress state is more complex, which contain the tensile and shear stress leading to the separation of material. From grinding depth to negative direction of Y axis, the maximum effective stress has downward trend and tends to slow. However, near the depth of 0.8 μm, it is occurred slight fluctuation, which provides impetus of crack propagation.

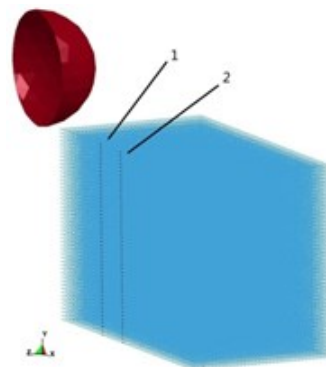
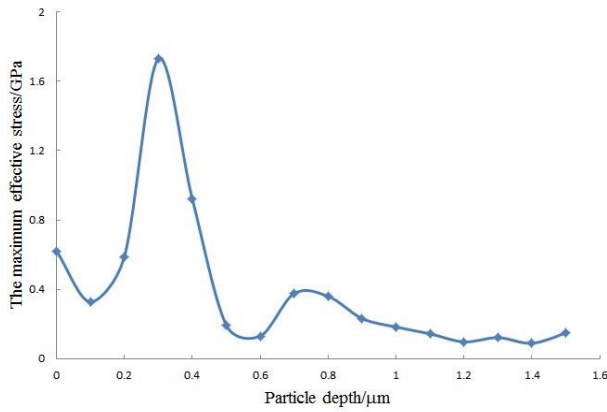
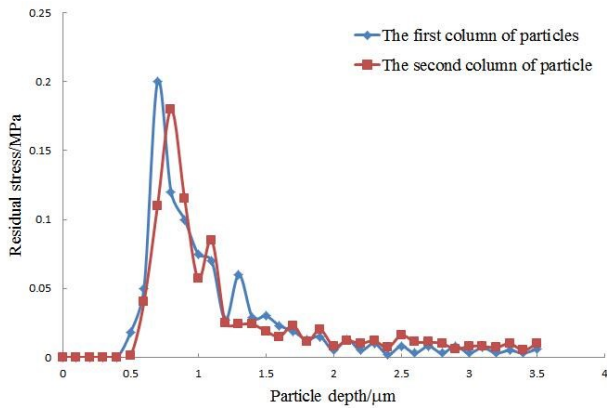


Fig 6 Selection of observation points

The information of residual stress from marked SPH particles is shown in Fig. 7b. Obviously, the changing trend of two polygonal lines is close to identical. The residual stress of particles is about to 0 with the depth less than 0.5 μm, which reason is this partial material has been removed in particulate abrasive dust form so the stress is released sufficiently. With the increasing of depth, the residual stress is rapidly increased and at about 0.75 μm obtains the maximum value 0.2 MPa, later decreasing slowly. Residual stress has no direct influence on the generation of crack, but will influence the propagation of crack which has been generated. When the depths of two column particles are 1.1 μm and 1.3 μm, residual stress respectively has slight fluctuation which reason is residual stress can be released by microcrack in some extend. According to the theory of fracture mechanics, the crack tip will exist plastic deformation region and stress has singularity, so the stress value in this point is larger than around. Therefore, it can be inferred that propagation stop on the depth of 1.2 μm, which provides the foundation for forecasting the subsurface damage depth.



(a) The maximum effective stress versus particle depth



(b) Residual stress versus particle depth

Fig. 7 The maximum effective stress and residual stress at different depth

4. Experiment

4.1 Experimental Device and Scheme

In order to verify the correctness of the SPH Simulation model, the varying cutting depth nano scratch experiment of optical quartz glass was carried out on the TriboIndenter nano indentation instrument. The workpiece used in the experiment is an optical quartz glass sample of 25 mm × 25 mm × 5 mm and its material properties are shown in Table 1. In the experiment, the tool adopted is a diamond Berkovich indenter. The specific experimental model is shown in Fig. 8.

The schematic diagram of the scratching process is shown in Fig. 9. The diamond indenter feeds in the X-axis direction at a constant speed. At the same time, a varying pressure is loaded on indenter in the Z-axis direction. Then the scratch with varying cutting depth is obtained. The experimental parameters are shown in Table 2 [23].

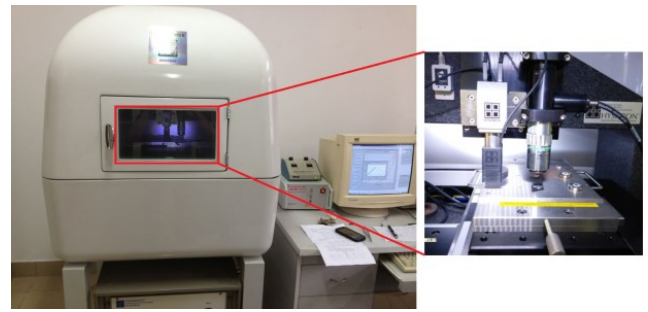


Fig. 8 Nanoindenter

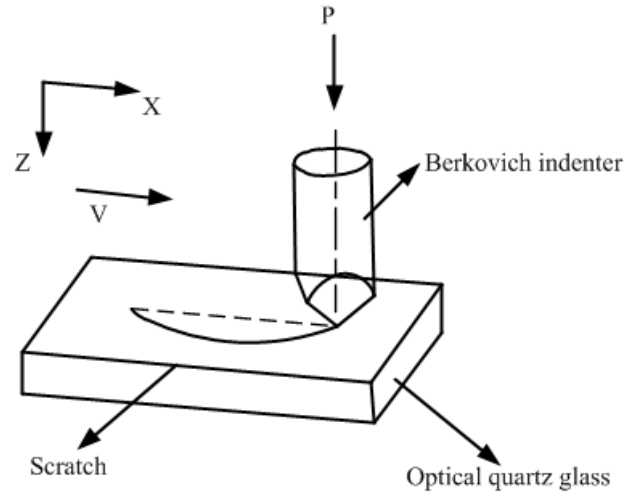


Fig. 9 Schematic diagram of scratch with variable cutting depth

Table 2 Nano scratch parameters

Parameters	value
Initial load/mN	0
Maximum load/mN	12
Velocity/(μm /s)	5

4.2 Experimental Result

To obtain the critical depth of the brittle-ductile transition of quartz glass, the scratch morphology was observed by a laser confocal microscope, as shown in Fig. 10.

It can be seen that when the depth of the scratch is small, no cracks are generated near the scratch, indicating that the material removal form at this time is plastic. As the depth of the scratch increases, when the depth of the scratch at the cross-section C-C is exceeded, the form of removal is changed to brittle fracture, and clear cracks are generated. Obviously, a brittle-ductile transition occurred at C-C.

As shown in Fig. 11, the critical depth of brittle-ductile transition obtained in the experiment is about 0.15 μm ~ 0.31 μm. The critical depth of brittle-ductile transition obtained by simulation is 0.36 μm, which is basically consistent with the experimental results, thus verifying the correctness of SPH model. At the same time, the error between the simulated and tested results can be explained that the critical depth of brittle-ductile transition in the actual processing process is affected by temperature, fluid and other factors, while the idealized simulation process does not consider.

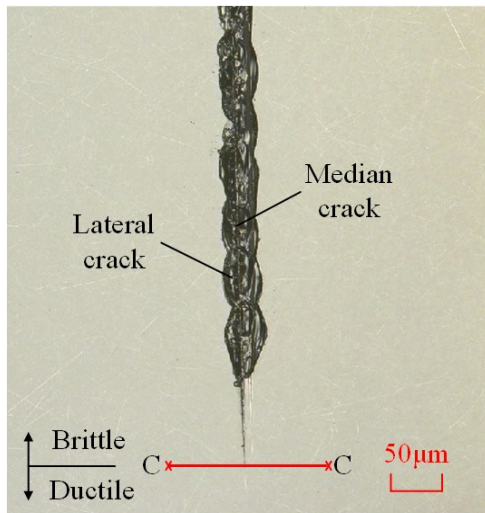


Fig. 10 Brittle-ductile transition

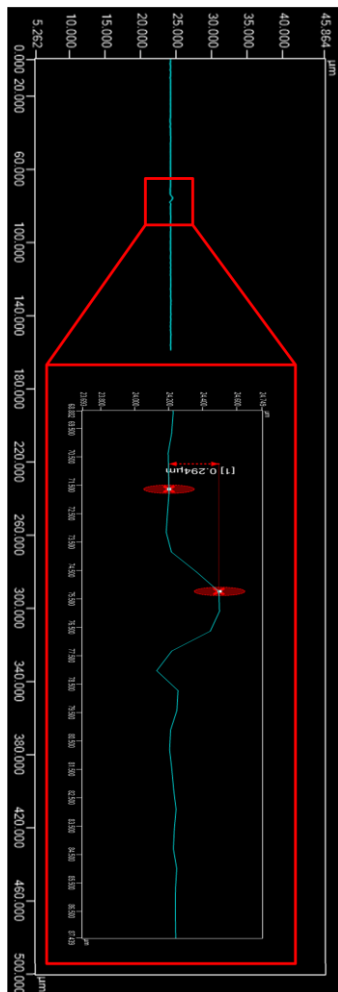


Fig. 11 Profile at section C-C

5. Conclusion

Based on the SPH method, the critical depth of the brittle-ductile transition, the change of the grinding force and the damage of the subsurface during the grinding process of the single grain of quartz glass

are studied, and the correctness of the simulation is verified. The concrete conclusions are as follows:

(1) By analyzing a large number of simulation results at different machining depths, the critical depth of brittle-ductile transition of quartz glass is $0.36 \mu\text{m}$, and the simulation results are compared with those of the cutting processes.

(2) By researching the grinding force, controlling the depth of grinding makes the removal of brittle materials in the plastic domain, which is more favorable to obtain the ideal surface quality. The maximum effective stress is concentrated in the depth of processing and above a small part of the region. The maximum residual stress is 0.2 MPa and the cracks stop at the depth of $1.2 \mu\text{m}$ under the simulated conditions, which provides the basis for the prediction of the depth of subsurface damage.

(3) The critical depth of brittle-ductile transition of quartz glass was obtained by the nano scratch experiment with variable cutting depth, which was in good agreement with the simulation result and verified the accuracy of the simulation model.

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