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A peridynamics simulation on the orthogonal glass cutting

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Abstract

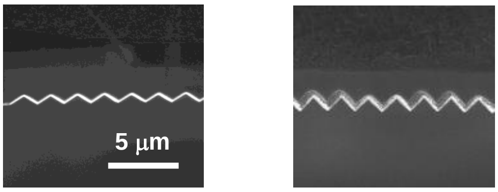
A peridynamic (PD) simulation on the orthogonal glass cutting is discussed. The PD simulation was performed to observe the effect of the critical stretch which is one of material parameter in the PD and the rake angle on the cracking characteristics. In these simulations, the fractured area in the material cut is expanded with the decreasing of the “stretch constant” which is determined of the critical stretch of the material fracture. And the fractured area is also expanded at the large negative rake angle.

Keywords: Peridynamics, Fused silica, Orthogonal cutting, Brittle fracture, Stretch constant, Rake angle.

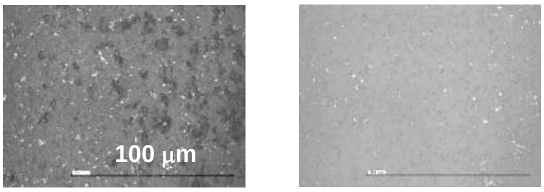
1. Background

Glass materials have been used in many products such as optical parts, heat-resistant products, chemical inspection instruments and anymore. Especially in a production of optical parts, high precision and high quality of the surface finish are required to achieve the high performance of the optical features. The cutting and abrasive machining (for example, grinding and polishing) are widely used in the curve generation and the surface finish of optical parts. In these processes, avoidance of a brittle fracture is most important requirement to guarantee the quality and function of the product. In cutting on glasses, many cracks are left on the machined surface with inappropriate conditions. A non-uniformly of the edge profile of the cutting tool (such as the edge roughness) is one of the important factors of the fracturing because it makes the un-uniform edge engaging. The ununiform engaging causes the ununiform stress distribution on cutter engaging points. Such unbalanced stress distribution may make the cracks on the machined surface. However, if the edge roughness has the uniform (or periodic) shapes, the cutter engaging is also made uniformly. Such “controlled edge roughness” (like the periodic serrations) does not only makes the uniform or periodic cutter engaging, but also may processes the” controllable” stress distribution on the material surface.

Based on this idea, the new cutting method with artificial serrated edge tool to avoid the large brittle cracking during cutting process has been proposed [1-3]. Fig. 1 shows an example of the artificially serrated cutting edge on the Single Crystal Diamond (SCD) rounded nose tool (R0.5), processed by Focused Ion Beam (FIB) machine tool. The main machining conditions are also summarized in figure. These serrations were processed by “image scanning” method with bitmap image. In this case, the serration has the periodic triangular shape, both ridge of the triangle roles the cutting edge to engage on the material cut with keeping its vertex angle. Fig. 1 shows the example of the effect of artificial serrations. The brittle cracks were suppressed at the vertex angle of serrations of 90 degrees (Fig.1(b), (d)) than that of 120 deg. ((a), (c)). By these results, it is concluded that a crack propagation is changed by changing the vertex angle of the serration. In usual, many flaws are left on the machined surface in these methods. On the other hand, it is well known that the flaw is suppressed at the small cutting depth less than 0.1 - 1.0 μm in these processes. Usually, this phenomenon is called "ductile mode cutting" by many researchers. However, the mechanics of this "ductile to brittle mode transitions" phenomenon has not been understood enough because of its physical size and complexity of the effects of material components on mechanical properties of (fractured) surface, especially the water component. Therefore, the research for this phenomenon by "traditional" experimental approaches is difficult because of its size restrictions.



(a) Vertex angle φ: 120 deg. (b) φ: 90 deg.



(c) Surface (φ: 120 deg.) (d) (φ: 90 deg.)

Fig.1 An effect of vertex angle of the edge serrations on the brittle cracking [2]

Cutting conditions: feed rate, 0.24 mm/min; rotational speed, 20000 rpm; depth of groove, 20 μm; tool inclination angle, 45 deg. with water lubrication.

To solve this problem, the numerical approaches such as classical molecular dynamics (MD) has been discussed [4]. In many cases, the MD simulation is performed with an assumed material model. And assumed models are verified by comparing with the experimental result which conducted under the same conditions. However, although many research results have been reported so far, since MD basically deals with problems on the molecular scale, it is difficult to apply it to problems which caused in the submicron scales such as crack propagation during cutting.

To solve this technical issue, a "Peridynamics" (PD)

[5] has been attracted attention from many researchers. This method is one of numerical method of the mesh free (particle) approach to solve the fracture with large deformations in continuum mechanics. This method bases on the integral equation to avoid the divergence in the discontinuous region such as the crack. In the conventional method which is based on the partial difference equation such as finite element method requires some numerical technics for example a J-integral to avoid the divergence in the discontinuous region. However, J-integral, the scope of application based on the original definition of the is limited. And it is difficult to apply on crack growth problems including unloading process [6]. On the other hand, the PD does not require such numerical technics because it can simulate the dynamics on the discontinuous region directory with the integral based equation.

In this paper, the PD simulation on orthogonal cutting on fused silica is introduced. This simulation was performed by LAMMPS, which is one of the molecular-dynamics source code developed by Sandia National Laboratory in United State. This code has a feature for PD simulation which is called "PD-LAMMPS"[13]. This module has based on four material models [7-10]. In this paper, calculations were performed with the PMB model [7] to simplify the calculation. In this method, an interaction function between particles depends only on a bond stretch. If the bond stretch exceeds the threshold value in the interaction of the particles, the interaction is lost. In this calculation, PD simulations were performed with various critical bound stretch [5,7,13] and rake angle of the cutter on the material removing process.

2. Peridynamics simulation on the glass cutting

2.1 Peridynamics theory

The peridynamics is a formulation of continuum mechanics that is oriented toward deformations with discontinuities, especially fractures. The peridynamic theory can simulate the deformation include the singularities such as the brittle cracks because it is based on integral equations. Fig. 2 shows the schematic of deformed body in the peridynamics theory. In this figure, Ω is deformable body, ξ: = *x' – x* is the relative position between particle x and neighbourhood particle *x',* and *R* is a spherical region in the neighbourhood surround the *x* with radius δ (in usual, which is called “horizon” in this method). The equation of the motion for *x* in this method is described as following:

$$\rho(x)\cdot\ddot{u}(x,t) = \int_R \{T[x,t]\langle x'-x\rangle - T[x',t]\langle x-x'\rangle\} dV_{x'} + b(x,t) \quad \text{(Eq. 1)}$$

In Eq. 1, where ρ(x) is the mass density of the un-deformed material, *u(x,t)* is the vector of the displacement, t is the time, and b(x,t) is the external body force density, respectively. Each particle experiences two types of forces: short range forces and long-range forces i.e. bond-forces. Short range forces are repulsive in nature. The bond-force on each particle is generated from the bonds it shares with the neighbourhood particles. Here, the *T* is an infinite dimensional vector operator that maps the deformed image of the vector contained in the angle brackets <>, into the force acting on *x*. *T* = τ*M* is defined as a force vector-state. In this function, τ and *M* are the scalar force state and deformed direction vector state. The *M* described as following:

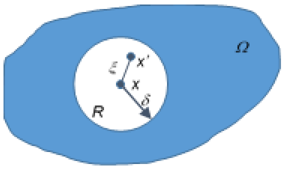


Fig. 2 Schematic of deformed body in PD

$$M\langle\xi\rangle = \begin{cases} \dfrac{\xi+\eta}{\|\xi+\eta\|} & \|\xi+\eta\| \neq 0 \\ 0 & \|\xi+\eta\| = 0 \end{cases} \quad \text{(Eq. 2)}$$

In Eq. 2, η := *u(x0; t) - u(x; t)* is the displacement vectors of two bonded points x’ and x, respectively. In usual, the scaler force state τ is described in following 4 models, the prototype micro-elastic brittle (PMB)[7], the linearly elastic solid (LPS)[8], the elastic-plastic solid (EPS)[9] and viscoelastic solid (VES)[10] models. In this paper, the scaler force state τ is determined by the PMB model to observe the crack propagation with the low computational cost. In this model, τ described only on the scalar quantity called bond stretch *s*. If the *s* exceeds the threshold value s_0 in the region *R*, the interaction among molecules is eliminated and the fracture occurs. In this model, the τ is described as following:

$$\tau(t,\eta,\xi) = \frac{18K}{\pi\delta^4} s(t,\eta,\xi)\cdot\mu(t,\eta,\xi) \quad \text{(Eq. 3)}$$

In Eq. 3, *K* is the bulk module. An interaction between *x* and *x’* is called a "bond". The bond state is evaluated by its stretch length *s*. The bond stretch *s* is described as follows:

$$s(t,\eta,\xi) = \frac{\|\eta+\xi\| - \|\xi\|}{\|\xi\|} \quad \text{(Eq. 4)}$$

Bonds are made to break when they are stretched beyond a given limit. Once a bond fails, it is failed forever [11]. Further, new bonds are never created during the simulation. We discuss only one criterion for bond breaking, called the critical stretch criterion. Define μ to be the history-dependent scalar function as follow:

$$\mu(t,\eta,\xi) = \begin{cases} 1 & s(t,\eta,\xi) < \min\left(s(t',\eta,\xi), s(t',\eta',\xi') : 0 \le t' \le t\right) \\ 0 & \textit{otherwise} \end{cases} \quad \text{(Eq. 5)}$$

The history function μ breaks bonds when the bond stretch *s* exceeds the critical stretch s_0. Although $s_0(t, \eta, \xi)$ is expressed as a property of a particle, bond breaking must be a symmetric operation for all particle pairs sharing a bond. That is, particles *x* and *x’* must utilize the same test when deciding to break their common bond. This can be done by any method that treats the particles symmetrically. In the definition of φ above, we have chosen to take the minimum of the two s_0 values for particles *x* and *x’* when determining if the *x-x’* bond should be broken.

2.2. Effect of the stretch constant s_{00}

In the PD simulation, the critical bond stretch s_0 is one it is concerned with the fracture toughness of the of the

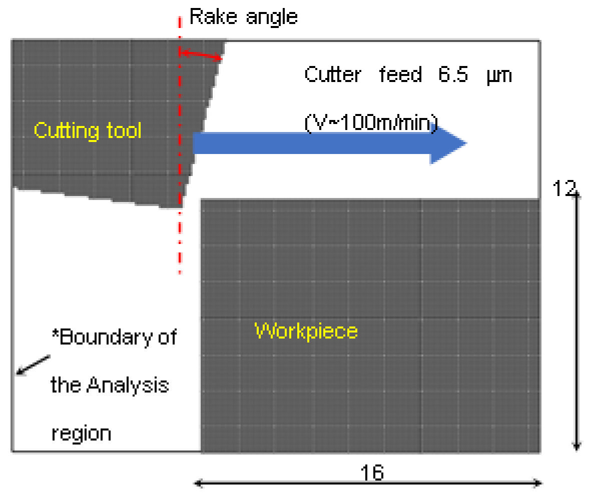
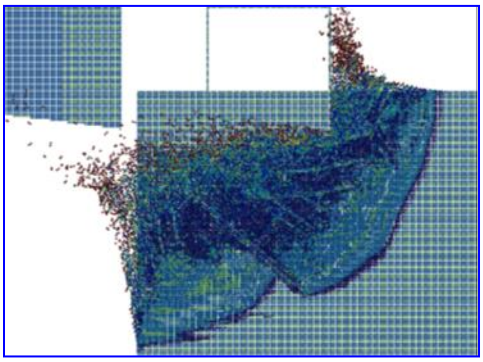
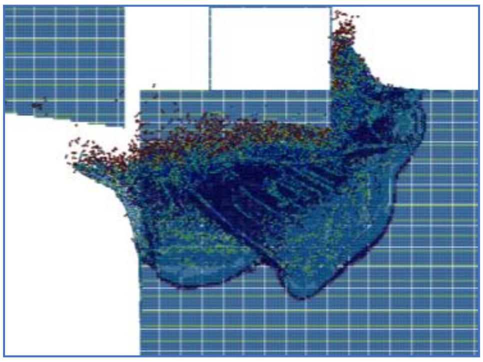


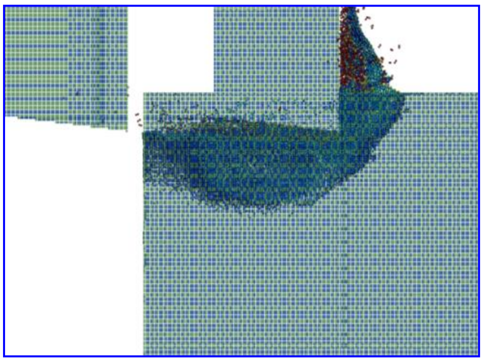
Fig. 3 Schematic of the simulation model



(a) s_{00} : 0.0125



(b) s_{00} : 0.05



(c) s_{00} : 0.2

Fig. 4 Effects of the stretch constant s_{00} on the fracture

parameters which effects on the result, because material. To observe its affect, the PD was performed with various s_0. The critical bond stretch is expressed as following function.

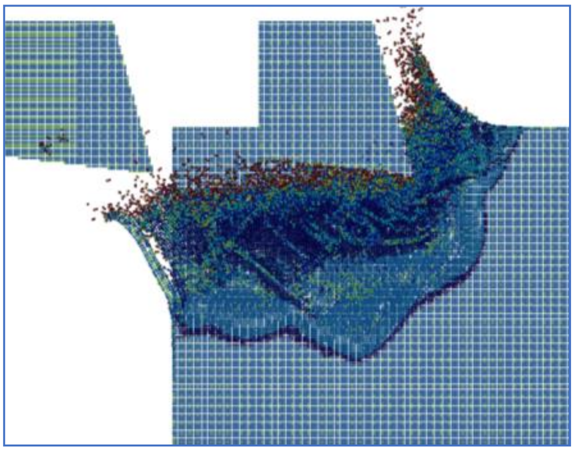
$$s_0 = s_{00} - \alpha \cdot s_{\min}(t, \eta, \xi) \qquad \text{(Eq. 6)}$$

In Eq. 6, coefficient α and stretch constant s_{00} are depends on the material properties, and $s_{min}(t, \eta, \xi)$ is the minimum bond stretch at the time t. In usual, the s_0 (also, s_{00}, α, δ, $c = 18K/\pi\delta^4$, etc) has to be determined by experimental or numerical considerations, for example, nano-indentation [16], molecular dynamics [14]. These material parameters must be determined by nano-indentation and molecular dynamics. Especially, the stretch constant s_{00} is the important parameter that is determined the s_0. However, these inspections have some restrictions (such as the difficulty of the instrumentation, or numerical assumptions). In this paper, instead of these inspections, the simulation is performed with in change the s_{00}, and observe the effect of this constant on the simulation results. Fig. 3 shows the orthogonal cutting model in PD simulations. The sharpened rigid tool which has the rake angle of 0 degrees, relief angle of 7 degrees and width of 4 μm engages on a fused silica material (W16 x H12 x D3 μm) at the cutting depth of 0.5 μm. The tool moves to x direction with the cutting velocity of 1.68 m/sec (~100m/min), from -0.5 μm to 6.0 μm (originated the side surface of the material). The PD simulation is performed with PMB model. Other parameters of PMB model expect the s_{00} {c, δ, α} are set of {1.69e5, 0.15, 0.25} chosen from the reference [12]. Also, the simulation was performed with the constant number of the particle, volume and energy (nve). The boundary condition set only the X direction as the periodic, in other directions YZ, set the expand boundaries.

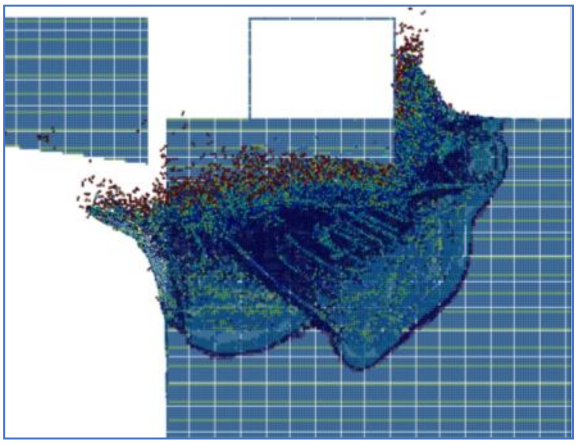
Fig. 4 shows results of PD simulations at each critical bond stretches. In this simulation, the critical bond stretch is changed by changing the s_{00} of 0.0125 (x1), 0.05 (x4) and 0.2 (x16), respectively. These images show the fractured (deleted the interaction) particle only. And particle color indicates the mieses stress distribution. In addition, the other tool model is also shown at the left side of figures. This is caused by periodic boundary condition in X direction. However, it was not deleted in the simulation because it is not affected on the simulation. As shown in these results, the fractured area is decreased with increasing the s_{00}. It is known that the fracture toughness is affected by temperature and atmosphere (Ex. water) [14,15]. However, they were not considered in this simulation. To determine a dynamic changing of fracture toughness by these parameters, now I'm trying the fracture simulation by molecular dynamics with LAMMPS with experimental validation for example the nano indentation.

2.3 Effect of the rake angle

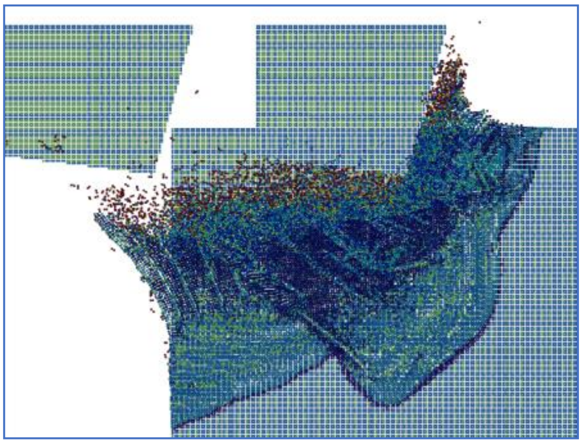
To observe the affection on the PD simulation by the tool rake angle, the simulation was performed by changing the rake angles. Fig. 5 shows results of simulations at the rake angle of -15, 0 and 15 degrees. Each simulation was performed with same condition of Fig. 3 except the s_{00} is determined as 0.05. As shown



(a) rake angle ϕ: 15 deg.



(b) ϕ: 0 deg.



(c) ϕ: -15 deg

Fig. 5 Effects of the rake angle of the cutter ϕ on the fracture

in Fig. 4, characteristics of the fracture are changed by changing the rake angle. In each figure, the crack propagation goes to similar direction. However, fracture length (or fractured area) is increased with the decreasing of rake angle. Especially, at the rake angle of -15 degrees, although the large downward material flow is caused, and the fractured area is increases than that of 0 degrees. It is considered that many laminar cracks left on front of the rake face by large share pressure with the chip deformation. The width of the land on the relief face makes the large compressive stress under the cutting point in the orthogonal cutting process. This stress may change (or suppress) the crack propagation. However, it has some issues, for examples, the expression of a friction coefficient between tool land face and fractured material (or particles) in the machining process. Now, I'm trying the PD simulation which is implemented the friction coefficient to evaluate the stress distribution under the landed material surface.

3. Conclusions

The peridynamic simulation on the orthogonal glass cutting is discussed. The PD simulation was performed to observe the effect of the critical stretch which is one of material parameter in the PD and rake angle on the cracking characteristics. In these simulations, the fractured area in the material cut is expanded with the decreasing of the critical stretch. And the fractured area is also expanded at the large negative rake angle. In this paper, the Numerical analysis showed only changes in the damage morphology. However, the validity of the analysis results could not be verified because the cutting test was stopped due to various reasons. Recently, the cutting experiment on a fused silica with similar cutting conditions of the simulation. These experimental results will be announced in near future.

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