Elastic–plastic deformation of single-crystal silicon in nano-cutting by a single-tip tool

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Received May 13, 2019; revised June 15, 2019; accepted June 19, 2019; published online July 11, 2019

A material removal mechanism of a single-tip tool cutting/scratch is the foundation for the analysis and prediction of the grinding process. A novel method for conducting single-tip, relatively high speed, and force-measurable nano-cutting tests with controllable cutting length are proposed to investigate the elastic–plastic deformation. Nano-cutting tests of single-crystal silicon are implemented at the cutting speeds of 0.1 m s⁻¹ and 1 m s⁻¹ which are close to the real grinding speed and much higher than that of single-tip tool scratch tests reported. Remarkable elastic recovery rate over 50% is observed in both cutting speeds. A semi-empirical model describing the relationship between the elastic recovery rate and residual depth is proposed. The normal force is studied in the whole cutting range. The findings of the elastic–plastic deformation behavior under relatively high cutting speed are valuable for the further mechanisms and process analysis of the ultra-fine grinding of brittle materials.

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1. Introduction

Grinding is a complicated machining process that utilizes an enormous number of abrasive particles with randomly positioned cutting edges to remove workpiece surface materials. Successful implementation of the grinding process relies on the understanding of the material removal mechanism in grinding. To obtain better surface integrity, the mechanism of the ductile-regime grinding of hard-and-brittle materials should be further explored. However, few methods have been reported to predict the surface integrity in ductile-regime grinding due to the lack of comprehensive understanding of the interaction between the abrasive grains and the workpiece.

Grain depth-of-cut is a predominant parameter that affects the grinding process. Analytical grinding models have been proposed for predicting the material removal at the level of a grain depth-of-cut based on the assumption of rigid-plastic deformation. However, the predicted grain depth-of-cut in ultra-fine self-rotating grinding is about several nanometers, which is too small to make physical sense. The unreasonable grain depth-of-cut is caused by the arbitrary assumption of the grain-workpiece interaction, which has strong elastic-plastic characteristics. In recent years, analytical models for grain depth-of-cut incorporating elastic–plastic material response have been proposed for the prediction of material removal in grinding. For these models, the quantification of the elastic–plastic material removal process is an essential prerequisite for the prediction and optimization of ductile-regime grinding. However, the elastic–plastic removal characteristics of hard-and-brittle materials with nano-cutting depth have not been thoroughly studied.

In order to reveal the fundamental mechanisms of the material removal, the well-known scratch test, in which a diamond stylus moves over the surface of a sample at a constant slow speed with a defined force over a defined distance, has been widely conducted to investigate the material deformation and removal mechanisms in the grinding process experimentally and theoretically since the 1960s. Malkin et al. and Klocke et al. have reviewed and discussed the state-of-art of the research on the grinding mechanism. The material removal is considered as a combination of three fundamental phases, namely rubbing, plowing and cutting. For brittle materials, it has been demonstrated that a brittle-regime to ductile-regime transition (BDT) will take place when the depth-of-cut is below a certain critical value, regardless of the material hardness and brittleness. In ductile-regime cutting, it is generally accepted that materials are removed by plastic flow and rigid-plastic theory is employed. However, several articles have reported obvious elastic–plastic characteristics in brittle material nanoscratch tests under penetration depth of hundreds of nanometers. The elastic recovery of the workpiece could reach up to 80% ~ 90%. The remarkable difference between the rigid-plastic hypothesis and the significant elastic–plastic response indicates that the rigid-plastic hypothesis is not suitable for the analysis and modeling in ductile-regime grinding of brittle materials. Many studies have conducted nano-cutting tests to reveal the grinding mechanism of silicon. But the cutting speeds in most of these reported tests are typically in the range of 1 μm s⁻¹ to 1 mm s⁻¹ which is far smaller than the grain-cutting speed in actual grinding. The deformation mechanism of some kinds of hard brittle materials has been proved to be cutting speed related, even under slow cutting speed for single-crystal silicon. Nevertheless, there have been few reports on the single-tip nano-cutting method characterized by the cutting speed around 1 m s⁻¹.

The pendulum cutting method could provide a high cutting speed by the circular movement of a cutting tool mounted to the end of a pendulum. However, considering the cutting depth at the nanometer level, the ductile-regime cutting length is too short for the force transducer to record enough force data due to its limited natural frequency. The absence of high speed, single-tip nano-cutting experiments leads to the uncertainty of the actual material removal and...
normal force for a given depth-of-cut, which further results in the material response being roughly assumed to be rigid-plastic\textsuperscript{18} and the normal force being approximately estimated by the Meyer indentation hardness equation in theoretical grinding analysis.\textsuperscript{23,24} In addition, it is still unclear whether the remarkable elastic–plastic material response found in the nanoscratch test of single-crystal silicon remains significant under the grinding speed of m/s magnitude. Therefore, it is necessary to study the elastic–plastic deformation behavior of single-tip tool cutting at a relatively high speed compared with conventional scratch tests.

To study the grinding mechanism under more realistic scenarios, a novel high-speed single-tip nano-cutting method is proposed to bridge the gap between the conventional scratch test under slow speed and the actual grinding process under relatively high cutting speed. Compared with the reported methods, this novel method could perform nano-cutting tests characterized simultaneously by relatively high speed, single-tip tool, nano-scale depth-of-cut, controllable cutting length and force monitoring. With this method, nano-cutting tests of single-crystal silicon are implemented to investigate several important characteristics of material removal such as the elastic recovery rate, the normal force, and the residual groove topography. The effect of the cutting speed on the elastic–plastic response of single-crystal silicon is also investigated and analyzed to discuss whether it should be taken into account for the actual grinding process modeling.

2. Experimental setup and procedures

2.1. Single-tip nano-cutting method

When cutting speed comes to 1 m s\(^{-1}\), the major difficulty for the cutting tests is to select a reasonable cutting length with a ramp depth-of-cut. In this research, minimum cutting length \(L_{\text{min}}\) was determined by the product of the cutting speed \(v\) and the cutting time \(t\) during which sufficient force data could be recorded with respect to changing residual depth:

\[
L_{\text{min}} = t \cdot v = \frac{\rho d}{f} \cdot v
\]

where \(d\) is the maximum residual depth, \(\rho\) is the force data points per depth and \(f\) is the natural frequency of the piezoelectric dynamometer. The maximum residual depth was given as 100 nm because the critical depth of BDT was in the range between 6.5 \(\sim\) 70 nm,\textsuperscript{4,13,18,25} as shown in Table I. A dynamometer with the high natural frequency, \(f = 50\) kHz was adopted in this method. If \(\rho\) was expected to be more than 1 point per 1 nm depth and \(v\) to be 1 m s\(^{-1}\), the cutting length \(L\) should be larger than 2 mm. In addition, the cutting length should not be too large not only for the convenience of measuring procedure but also to minimize the cutting depth sensitivity to original surface waveness. In summary, \(L\) was expected to be less than 3 mm and a ramp residual depth increasing from 0 to 100 nm along the cutting length within 2 \(\sim\) 3 mm was suitable for this study.

The novel single-tip nano-cutting method is illustrated in Fig. 1. Commercially polished doped p-type single-crystal (100) silicon wafer (\(\Phi = 200\) mm) with an ultra-flat and smooth surface for lithography was employed in the experiments in order to minimize cutting depth sensitivity to workpiece’s surface waviness. A protrusion with an arc-shaped profile on the wafer was created to ensure a ramp depth-of-cut within a selected range of cutting length, as shown in Fig. 2. It was realized by attaching a strip of thin film (dicing tape) to the backside of the silicon wafer before clamped on the vacuum chuck. All the cutting processes were performed along the \(\langle 110 \rangle\) crystalline direction in order to avoid the effect of crystal orientation on the deformation mechanism.

2.2. System setup

Figure 3 illustrates the developed setup according to the proposed cutting method. The setup was built on a granite base. To provide a relatively high cutting speed, an air bearing rotary table was adopted, on which a vacuum chuck was fixed. The workpiece, i.e. the silicon wafer was clamped on the vacuum chuck. The spindle rotating speed was adjusted to provide the cutting speed from 0.1 m s\(^{-1}\) to 1 m s\(^{-1}\).

A two-stage feed mechanism composed of a linear stage and a piezo stage was applied in the system. The piezo stage containing the moving tip was fixed on the linear stage and allowed nano-scale depth-of-cut through the nano-positioning change of the cutting tool. It has a positioning resolution of 0.4 nm with a short travel range of 100 \(\mu\)m. The linear stage driven by a stepper motor was vertically mounted on the granite base beside the rotary table. It has a positioning resolution of 1 \(\mu\)m with a long travel range of 50 mm. If the desired displacement exceeded the travel range of the piezo stage, the linear stage would be driven to compensate for the position change.

A dynamometer (9215A, Kistler, Switzerland) with natural frequency up to 50 kHz and sensitivity up to 95 pC N\(^{-1}\) was applied to record the normal force during cutting tests. The force signal was amplified by an amplifier (9018, Kistler, Switzerland) and was recorded by a personal computer. A custom triangular-based pyramidal diamond tool was mounted on the dynamometer which was fixed on the piezo stage. The edge reversal method was adopted to measure the diamond tip geometry. First, an indium sample with excellent plasticity/ductility was prepared. Then, an indent was created on the sample by the diamond tip to transform the geometry of the diamond tip onto the surface of the indium. Finally, the atomic force microscope (AFM) (XE-200, Parker, Korea) was utilized to measure the geometry of the indent, which

\[
H_{\text{silicon}} = 13 \text{ GPa}, E_{\text{silicon}} = 168 \text{ GPa}, K_{\text{silicon}} = 0.75 \text{ MPa m}^{1/2}
\]
**Fig. 1.** (Color online) Schematic illustration of the cutting length control method in the single-tip nano-cutting test.

**Fig. 2.** (Color online) Interferometric fringe pattern (a) and the calculated surface profile (b) of the cutting region. A protrusion with an arc-shaped profile on the wafer was created to ensure a ramp depth-of-cut within a selected range of cutting length. Its cross-sectional profile was qualitatively described by the black line in (b).

**Fig. 3.** (Color online) A schematic of (a) the nano-cutting setup and (b) the photo of the setup.
2.3. Experimental procedures

Figure 5 illustrates the flow chart of the proposed experimental procedures. Tool setting was accomplished via the linear stage to make a fast approach towards the protrusion area. The nano-scale tool feed was driven by the piezo stage to execute a periodic stepwise movement including a vertical 50 nm movement along the Z-axis and a radial approximate 5 μm horizontal step movement along the Y-axis. Each tool feed was executed before the cutting tool acting with the protrusion area. The tool feed movement transverse to the cutting direction was designed to avoid a duplicate cut and thus there would be no damage from the previous tool passes in the machined workpiece, as shown in Fig. 6. It should be mentioned that the radial movement of the cutting tool was executed by tilting the piezo stage around the X-axis. The closed-loop tilt angle in ϑx was ±0.4 mrad and the rotating radius of the cutting tool was 44 mm. Consequently, the corresponding radial feed travel length equaled 35 μm and the resulted tip displacement in the Z-direction was negligible. Each travel included 7 step feed movements. Once a travel was finished, the cutting tool was lifted up to check the force signal. If no force signal was detected, the tip started to feed transversely in the opposite direction, and that cycle was repeated until the force signal was detected.

2.4. Experimental measurement

Residual cutting grooves were observed by a laser scanning confocal microscope (VK-X250, Keyence, Japan). Figure 7 shows an overview micrograph of the residual groove at the cutting speed of 0.1 m s⁻¹ and five magnified inset micrographs. Parallel residual cutting grooves were created due to the radial displacement of the cutting tool. The whole surface topography of the groove with the maximum depth-of-cut was further examined by an AFM (XE-200, Parker, Korea) with tapping mode in detail.

3. Results and discussion

3.1. Cutting grooves profile analysis

The cross-sectional profile in Fig. 8 shows the residual depth and residual width of grooves which are obtained from AFM images. A1A2 is the residual cutting width and B1B2 is the residual cutting depth. These variables were measured on the cross-sectional profile at positions with 10 μm intervals along the axial direction of the groove at cutting velocities of 0.1 m s⁻¹ and 1 m s⁻¹. This profile data has been plotted as
scatter lines in Fig. 9(a) as a function of the cutting length. Above the graph, the normal force has been plotted in Fig. 9(b) as a solid black line with respect to time. The background is an optical micrograph showing the panorama of the residual grooves. Both the force curve and the background graph were scaled to the cutting length axis and visually aligned with it, as shown in Fig. 9(b).

An interesting phenomenon is found in Figs. 9(a) and 9(b), in that the variation trend of normal force versus cutting length is closer to the change of residual depth in the whole cutting range, even if brittle crack occurred as observed in Fig. 9(c). And the linear relationship coefficient between the normal force and the residual depth is about 0.169 for \( v = 1 \text{ m s}^{-1} \) and 0.202 for \( v = 0.1 \text{ m s}^{-1} \). An important phenomenon found is that the residual width increases with increasing normal force until the residual width reaches approximately 1200 nm, at which point the residual depth begins to fluctuate obviously. The critical point of residual width may be the result of the change of the material deformation mechanism.

Four AFM images with residual depths of 10 nm, 30 nm, 50 nm, and 80 nm have been shown in Fig. 9(c). No obvious features representing the onset of cutting (chip formation) are observable in the force and profile measurements. Initially, at the residual depth of 10 nm, pile-ups on both sides of the residual groove and irregular protuberance at the bottom of the residual groove can be directly observed which indicates severe plastic deformation. Following the initial transformed area, periodic protrusions are found at the residual depth of 30 nm. As the residual depth increases, protrusions gradually extend laterally away from the edge of the cutting groove and finally evolve into brittle cracks at the residual depth of 50 nm. Previous studies have reported that obvious fluctuations of force signals indicate brittle fracture occurrence.\(^{28}\) However, force signals in this study keep changing smoothly over the whole cutting process. This is a reasonable phenomenon because crack intervals range from several to tens of micrometers. Considering the cutting speed, the crack generation frequency approximately equals 1000 kHz, which
far exceeds the natural frequency of the piezoelectric
dynamometer.

Relationships between residual depth and width below the
critical point where the residual depth begins to
fluctuate have been plotted in Fig. 10(a). It is commonly assumed that the contact width of the tool tip is the same as the residual width of
the groove$^{17,23,29}$ as shown in Fig. 10(b). Thus, contact depth could be determined from the diamond tip profile and it is also plotted as a solid line in (a) with respect to the residual width $w$. The vertical error bars in (a) represent one standard deviation based on a dataset with 5 ~ 10 data at each data point.

$\text{ERR} = \frac{h - h_f}{h}$  \hspace{1cm} (2)

where $h_f$ is the residual depth and $h$ is the corresponding penetration depth. Residual depth could be determined from AFM images as mentioned before. Penetration depth was evaluated according to the previous work reported by Oliver et al.$^{29}$ where $h_s$ and $h_c$ are given by:

$h_s = \frac{\pi - 2}{\pi} (h - h_f)$ \hspace{1cm} (3)

$h_c = h - h_s$ \hspace{1cm} (4)

Fig. 10. (Color online) Residual depth $h_f$ as a function of residual width $w$ at cutting speeds of 1 m s$^{-1}$ and 0.1 m s$^{-1}$ (a), and a schematic illustration of a cross-sectional profile showing penetration depth $h$, contact depth $h_c$, residual depth $h_f$, and residual width $w$ in the analysis (b). The contact width is assumed to be equal to the residual depth.$^{17,23,29}$ Thus, the contact depth $h_c$ could be determined from the diamond tip profile and it is plotted as a solid line in (a) with respect to the residual width $w$. The vertical error bars in (a) represent one standard deviation based on a dataset with 5 ~ 10 data at each data point.

Elastic recovery rate has been plotted with respect to the residual depth at cutting speeds of 1 m s$^{-1}$ and 0.1 m s$^{-1}$ in Fig. 11. Both sets of data show that the elastic recovery rate approaches 100% initially and decreases gradually as the residual depth increases, which indicates a decline in the portion of elastic deformation. The recovery rates still exceed 50%, even if the residual depth increases to 100 nm. The increasing offset between both sets of data demonstrates evidence of the cutting speed dependence. In this case, the elastic recovery rate decreases with the cutting speed for a given residual depth. Figure 11 also compares the data obtained with reported experimental results from Gassilloud$^{14}$ and Youn,$^{15}$ who performed single point scratch tests with a similarly shaped diamond tip on the Si(100) surface along the $\langle 110 \rangle$ direction except for the lower cutting speed on the scale of 1 $\mu$m s$^{-1}$. Results show that the variation trend of elastic recovery versus residual depth and cutting speed agrees well with previous experimental results.

A semi-empirical relationship between elastic recovery and residual depth is further deduced. According to Fig. 9, there is a linear correlation between normal force and residual depth.
depth. Normal force $P$ could be expressed as:

$$P = kh_f$$  \hspace{1cm} (6)$$

where $k$ is a constant related to cutting speed. For spherical tip geometry, the normal force could be conveniently obtained by:20)

$$P = \alpha (h - h_f)^{3/2}$$  \hspace{1cm} (7)$$

where $\alpha$ is a constant. By substituting Eq. (6) and Eq. (7) into Eq. (2), elastic recovery rate could be derived by:

$$ERR = \frac{1}{1 + C \cdot h_f^{1/3}}$$  \hspace{1cm} (8)$$

$$C = \left(\frac{\alpha}{k}\right)^{2/3}$$  \hspace{1cm} (9)$$

where coefficient $C$ is a constant depending on the mechanical properties of the workpiece, the geometric feature of the tool tip and the cutting speed. The value of $C$ is determined by a fitting procedure in the range before crack initiation. Fitted curves shown in Fig. 11 suggest that the model describes the experimental results well.

Previous literature on BDT has suggested that grain depth-of-cut plays a crucial role in deformation mechanism transformation from the plastic-regime to brittle-regime. According to the experimental results in this paper, the influence of elastic recovery should be considered when analyzing critical cutting depth based on the residual profile. With the elastic recovery rate calculated by the derived semi-empirical equation, the penetration depth and normal force could be further estimated, which is valuable for the research on the critical depth-of-cut of BDT and the ductile-regime grinding mechanism.

### 3.2. The normal force during nano-cutting tests

Figure 12 plots the variations of the normal force versus residual width with cutting speeds of 0.1 m s$^{-1}$ and 1 m s$^{-1}$. Similar to the variation trend of the elastic recovery rate, the difference between both sets of data is also negligible initially and becomes pronounced as the residual width increases. The normal force is positively related to the cutting speed for a given residual width. Based on the preceding hypothesis that contact width is equal to residual width, it becomes evident that the normal force in the cutting process is positively affected by the cutting speed under the same contact depth condition.

Experimental results show that normal force in nano-cutting is greatly affected by the cutting speed. Although there is a rich body of literature on nanometric cutting MD simulations of single-crystal silicon, the cutting speed effect on the deformation mechanism of silicon in nanometric cutting is relatively unexplored. It is well known that the deformation of ductile metals is subjected to the Johnson–Cook model. The flow strength, which is a function of strain, strain rate, and temperature, is positively correlated to the strain rate for the given strain and temperature.30) Therefore, the flow strength could be used to explain that an increase in the cutting speed results in an evident increase in the normal force. On the other hand, the elastic–plastic response of silicon has been attributed to high-pressure phase transformations (HPPT), which is verified to be a result of the shear strain.31) However, a previous MD simulation and experimental validation by Goel et al.32) indicates that the silicon phase transformation under mechanical loading is not sensitive to the strain rate. Apart from HPPT, dislocations also play a crucial role in governing the plastic response of silicon. Therefore, it is inferred that the influence of cutting speed on the normal force in this article might be caused by the speed effect on the formation and propagation of dislocations. The exact mechanism of how the cutting speed affects the deformation mechanism of silicon in nanometric cutting still needs further investigation.

Figure 12 also compares experimental results with calculated normal forces. In the reported literature concerning single grain scratch analysis or grinding force modeling, the normal force is usually estimated by hardness formula.18,23) According to Meyer,35) the normal force $P$ could be given by:

$$P = HA_h$$  \hspace{1cm} (10)$$

where $H$ is commonly known as Meyer hardness and $A_h$ is the horizontal load support area. Typically, the load support area is assumed to be the front half of the indenter due to rigid-plastic material response assumption. In diamond tip nano-cutting
tests, however, the load support area of the cutting tool adopted is determined from the whole diamond tool tip profile projection area as a function of contact depth. Results demonstrate that the pure elastic material response assumption seems to be more appropriate due to remarkable elastic recovery estimated in Sect. 3.1. Results show that with increasing residual width, the calculated normal force at 1 m s⁻¹ is initially similar to but gradually deviates from that at 0.1 m s⁻¹. These experimental force values might be used in single-tip cutting models and grinding models where the hardness equation is used in the estimation of the normal force.

4. Conclusions

A single-tip cutting experiment with a cutting tool shaped like an abrasive grain is a direct approach for gathering evidence to identify the mechanisms of grinding. This paper proposes a novel method and setup for conducting single-tip, relatively high speed, and force-measured nano-cutting tests with a controllable cutting length. Based on experimental results and theoretical modeling, conclusions are drawn as follows.

1) The proposed method proved to be able to measure the normal force at relatively high speed in ductile-regime nano-cutting with ramp depth-of-cut.
2) The elastic recovery rate was estimated to quantify the speed dependence on the basis of precisely measured diamond tip profile. In both cutting speeds, remarkable elastic recovery rate over 50% was observed, and even residual depth reached 100 nm and the elastic recovery rate was inversely related to the cutting speed. A semi-empirical model was proposed and verified to evaluate the elastic recovery rate based on residual depth. It is significant for the understanding of the ultra-fine grinding mechanism and could be further adopted to approximate the grain penetration depth and normal force in ductile-regime grinding.
3) This paper thoroughly discussed the relationship between the resultant normal force and the groove morphology, including residual depth h_f and residual width w. It was concluded that the resultant normal force was positively related to the cutting speed based on the commonly accepted assumption that the contact width of the tool tip is the same as the residual width of the groove. The normal force was more related to the residual depth than the residual width in the whole cutting range even if brittle cracks occurred. The linear relationship coefficient between the normal force and the residual depth was further calculated to be 0.169 for v = 1 m s⁻¹ and 0.202 for v = 0.1 m s⁻¹. Additionally, it was found that the Meyer indentation hardness formula could predict the variation trend of the normal force in the cutting process. The effect of the cutting speed on the deformation mechanism of silicon under nanometer cutting still needs further investigation.

Acknowledgments

The authors appreciate the financial support from the National Natural Science Foundation of China (51875078, 51605079), National key Research and Development Program of China (Grant No. 2016YFB1102205) and the Science Fund for Creative Research Groups of NSFC of China (51621064).

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