Deformation induced complete amorphization at nanoscale in a bulk silicon

Zhang, Zhenyu; Meng, Fanning; Cui, Junfeng; Wang, Bo; Wang, Ziguang; Lu, Yang; Hassan, Hamad ul; Guo, Dongming

Published in:
AIP Advances

Published: 01/02/2019

Document Version:
Final Published version, also known as Publisher’s PDF, Publisher’s Final version or Version of Record

License:
CC BY

Publication record in CityU Scholars:
Go to record

Published version (DOI):
10.1063/1.5079819

Publication details:
Zhang, Z., Meng, F., Cui, J., Wang, B., Wang, Z., Lu, Y., Hassan, H. U., & Guo, D. (2019). Deformation induced complete amorphization at nanoscale in a bulk silicon. AIP Advances, 9(2), [025101].
https://doi.org/10.1063/1.5079819

Citing this paper
Please note that where the full-text provided on CityU Scholars is the Post-print version (also known as Accepted Author Manuscript, Peer-reviewed or Author Final version), it may differ from the Final Published version. When citing, ensure that you check and use the publisher's definitive version for pagination and other details.

General rights
Copyright for the publications made accessible via the CityU Scholars portal is retained by the author(s) and/or other copyright owners and it is a condition of accessing these publications that users recognise and abide by the legal requirements associated with these rights. Users may not further distribute the material or use it for any profit-making activity or commercial gain.

Publisher permission
Permission for previously published items are in accordance with publisher's copyright policies sourced from the SHERPA RoMEO database. Links to full text versions (either Published or Post-print) are only available if corresponding publishers allow open access.

Take down policy
Contact lbscholars@cityu.edu.hk if you believe that this document breaches copyright and provide us with details. We will remove access to the work immediately and investigate your claim.

Download date: 11/01/2021
Deformation induced complete amorphization at nanoscale in a bulk silicon

Cite as: AIP Advances 9, 025101 (2019); https://doi.org/10.1063/1.5079819
Submitted: 03 November 2018 . Accepted: 23 January 2019 . Published Online: 01 February 2019

Zhenyu Zhang, Fanning Meng, Junfeng Cui, Bo Wang, Ziguang Wang, Yang Lu, Hamad ul Hassan, and Dongming Guo

ARTICLES YOU MAY BE INTERESTED IN

Analytical modelling for p-i-n structured semiconductor devices
AIP Advances 9, 025102 (2019); https://doi.org/10.1063/1.5045090

A study of strain-induced indirect-direct bandgap transition for silicon nanowire applications
Journal of Applied Physics 125, 082520 (2019); https://doi.org/10.1063/1.5052718

Effect of distance between the laser spot and the cavity center on spatially confined laser-induced copper plasma
AIP Advances 9, 025001 (2019); https://doi.org/10.1063/1.5080181
Deformation induced complete amorphization at nanoscale in a bulk silicon

Zhenyu Zhang,1,a) Fanning Meng,1 Junfeng Cui,1 Bo Wang,1 Ziguang Wang,1 Yang Lu,2 Hamad ul Hassan,3 and Dongming Guo1

AFFILIATIONS
1Key Laboratory for Precision and Non-Traditional Machining Technology of Ministry of Education, Dalian University of Technology, Dalian 116024, China
2Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Kowloon, Hong Kong, China
3Interdisciplinary Center for Advance Materials Center, Ruhr-University Bochum, Bochum 44801, Germany

a)Email: zzy@dlut.edu.cn (Z.Y.Z.).

ABSTRACT

Solid state amorphization is induced by shock, irradiation and deformation, while deformation induced complete amorphization remains a challenge in a bulk solid. Brittle-to-ductile transition (BDT) mechanism is elusive at loading speeds of m/s at nanoscale depth of cut. Existing formula has no effects of shape and radius of cutting edges on the critical depth of cut at BDT. In this study, a new route of deformation induced complete amorphization at nanoscale is proposed in a bulk solid confirmed by transmission electron microscopy (TEM). This is performed by a novel approach of ultraprecision grinding, conducted on a specially designed setup. The grinding is carried out by a developed single diamond grain with a cutting edge radius of 2.5 \( \mu \)m, at depth of cut of 24 nm under a loading speed of 40 m/s. BDT takes place at depth of cut of 419 and 172 nm for Si (100) respectively, ground by single diamond grains with tip radii of 5 and 2.5 \( \mu \)m correspondingly. A new model is suggested for BDT, considering the effects of radius and shape of cutting edges. The findings provide new insights for design and fabrication of high performance devices used in flexible electronics, nanodevices, microelectronics and optoelectronics.

© 2019 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/). https://doi.org/10.1063/1.5079819

Amorphous materials have structural and functional applications, attracting much attention.1,2 Solid state amorphization from crystals is a pivotal method to prepare amorphous materials. However, it is difficult to realize amorphization from a brittle single crystal. For instance, dislocation-driven plasticity takes place under compression in a monocrystalline nanoparticle, rather than amorphization.3 Amorphous transition occurs at the compressed site in nanowires (NWs), whereas crack happens on the tensed side.4 At present, methods of solid state amorphization consist of mechanical scratching,2 diamond anvil cell under hydrostatic pressure,5 electron irradiation at low temperatures,6 indentation,6 impact of electrospayed nanodroplets,6 electron beam irradiation7 and extension.8

Mechanical scratching induces a small amorphous region, surrounded by damaged crystallites and cracks at a scratching speed of 10 mm/s.2 This means that the partially amorphization takes place. Amorphization is formed in a diamond anvil cell of porous free-standing films with thickness varying from 30 to 50 \( \mu \)m. It is generated by methanol/ethanol or Ar as a pressure medium at a high pressure of 10.1 GPa.3 Irradiated amorphization with a diameter of 400 nm happens under electron irradiation with a dose of 2 MeV for 15 min at 25 K.9 Indented amorphization occurs in the central area of an indent with a size of 500 nm, which is encompassed by cracks.9 This indicates the partial amorphization produced by indentation, which is in good agreement with that of mechanical scratching. Shock-induced amorphization takes place at the periphery of a crater with a diameter of 300 \( \mu \)m. It is bombarded by nanodroplets at 4620 m/s for 15 min at a high pressure of 15 GPa.8 Partial amorphization occurs at the periphery and damaged crystallites forms in other area of the crater.
Amorphization is demonstrated in a NW with a diameter of 37.8 nm, which is bombarded by electron beam in vacuum for 25 min at 3.24 A/cm².2 Axial extension induces amorphization in NWs carried out in high resolution transmission electron microscopy (HRTEM) at a strain rate of 10⁻⁵/s.⁴ There are three methods for amorphization, i.e. shock, irradiation and deformation. Shock and irradiation are performed in vacuum for 15 or 25 min, and they are time-consuming. Moreover, the sizes of amorphization induced by shock and irradiation are 400 nm, 15-70 nm and periphery of 300 µm,²⁵ which are very small. For deformation, amorphization is verified in NWs by tensile tests in TEM and porous films under hydrostatic pressure.²³ Partial amorphization takes place in a bulk solid via deformation, which is surrounded by damaged crystallites and cracks.²⁵ In bulk deformation, the loading speed is very low up to 10 mm/s.² Deformation induced complete amorphization has not been demonstrated in a bulk solid. As a result, it remains a challenge for deformation induced complete amorphization in a bulk solid.

Material removal on a brittle solid contains brittle and ductile modes. In brittle removal mode, cracks are found on the surface and/or subsurface,²⁻⁵ and damaged layer is thick. This removal mode generates rough surface, which is not qualified for high performance devices and setups, producing waste products. For ductile removal mode, cracks are absent on both surface and subsurface, and damaged layer is extremely thin. Only in this mode, ultrasmooth and ultralow damage surface can be obtained and used for high performance devices and setups. For instance, ductile removal mode is testified by ultraprecision grinding at a speed of 33 m/s,³⁻¹⁵ and fly-cutting at speeds ranging from 15 to 18 m/s.²⁻⁵ Nevertheless, an amorphous layer is at the topmost, followed by a damaged crystalline layer beneath, indicating the partial amorphization happened. Ductile removal mode is vital for solid state amorphization and applications of brittle materials in their high performance devices and setups. Fundamental mechanisms of brittle-to-ductile transition (BDT)¹⁰⁻¹⁵ are essential for the solid state amorphization and ductile removal on brittle materials.

Silicon (Si) is a representative brittle material, dominating the semiconductor and solar cells industries, and becoming the foundation of electronics industry.¹⁴ It is widely used in optoelectronics,¹⁵⁻¹⁶ flexible electronics,¹⁶⁻¹⁸ microelectronics,¹⁹⁻²⁰ nanodevices²¹⁻²² and quantum computing.²³ The band gap of amorphous Si varies from 1.5 to 1.7 eV, which is higher than 1.1 eV of crystalline Si.²⁴ Furthermore, amorphous Si has a low sensitivity to high energy radiation, which is a unique property of amorphous semiconductors.²⁴ Consequently, Si is selected as the specimen of solid state amorphization and BDT. The critical diameter of BDT for Si pillars under uniaxial compression is between 310 to 400 nm.¹³ The compression speed is 5 nm/s. However, the BDT is sensitive to the strain rate,¹⁰ and therefore the critical depth of cut (CDC) of BDT at loading speed of m/s remains elusive. The CDC at BDT, Dc, is calculated,²⁵

\[ D_c = 0.15 \left( \frac{E}{H} \right) \left( \frac{K_{IC}}{H} \right)^2 \]  

where E is the Young’s modulus, H is the hardness and \( K_{IC} \) is the fracture toughness. The hardness, Young’s modulus and fracture toughness of Si (100) are 13.2 GPa, 150.2 GPa and 0.99 MPa m⁵ respectively. The CDC at BDT calculated is 9.6 nm, which is 30 to 40 times lower than critical diameter of BDT for Si pillars under uniaxial compression. Moreover, Equation (1) does not consider the effects of radius and shape of a cutting edge on the CDC at BDT. Nevertheless, it is reported that the radius²⁷ and shape of cutting edges²⁸ affect the CDC of BDT respectively. As a result, it is necessary to propose a new model to calculate the CDC at BDT.

The CDC at nanoscale is crucial to perform solid state amorphization and explore the fundamental mechanisms of BDT. Nonetheless, there are no commercial instruments and methods to conduct BDT at nanoscale at loading speeds of m/s used for machining and manufacturing. At present, there are four methods to simulate the machining and manufacturing at nanoscale. The first is performed by atomic force microscopy (AFM) at loading speeds of 5,²⁷ 15,²⁵ and 100 µm/s. The second is conducted by the Tribolindenter at scratching speeds of 0.33²⁵ and 133 µm/s. The third is carried out by scratch testers at a scratching speed of 8.3 µm/s.²⁴ The fourth is executed by a 3D mobile platform at a scratching speed of 16.7 µm/s.²⁷ All the four methods are performed by commercial instruments at loading speeds varying from 0.33 to 100 µm/s, which is 4 to 7 orders magnitude lower than m/s used in machining and manufacturing. Moreover, it is extremely difficult to prepare TEM specimens at BDT, and there is no TEM characterization in the literatures for the four methods²⁷⁻²⁹⁻³⁴ The scratched surfaces are characterized by scanning electron microscopy (SEM) and AFM. As a consequence, the CDC of BDT at loading speeds of m/s is unclear. It is a challenge to develop a novel approach to explore the CDC at BDT at loading speeds of m/s at nanoscale depth of cut. Even at nanoscale depth of cut, an amorphous layer is at the topmost, and a damaged crystalline layer beneath. It is performed at a cutting speed of 8.3 mm/s at depth of cut of 30, 50, 60 and 120 nm.³⁵ This is in good agreement with those induced by ultraprecision grinding and fly-cutting,¹¹⁻¹² indicating partial amorphization occurred in a bulk solid.

In this study, a novel approach of ultraprecision grinding is developed on a specially designed setup, which is performed by developed single diamond grains at a loading speed of 40 m/s at nanoscale depth of cut. With this method, a new route is proposed for deformation induced complete amorphization in a bulk solid. A new model is proposed to calculate the CDC at BDT, considering the effects of radius and shape of a cutting edge.

Table I lists the matching terminologies between grinding and nanoscale scratching. Three diamond grains were fabricated from natural diamonds with sizes ranging from 1 to 1.5 mm, which were imported from South Africa. A diamond was brazed on a stainless steel rod by high-frequency welding. After brazing, the diamond was ground by resin bond diamond wheels with mesh sizes at a sequence of 600, 2000 and 3000 to form a conical tip. Then, the conical tip was further ground by a vitrified diamond wheel with a mesh size of 5000. Finally,
the diamond grain was finished by a cast iron plate. During finishing, the reaction between diamond and cast iron plate was activated by the polishing-heat. After finishing, the surface of diamond cutting edge was smooth. Three diamond cutting tools developed were designated as C30, C5 and C2.5 respectively, as listed in Table II. C30, C5 and C2.5 had conical shape, and their cutting edge radii were 30, 5 and 2.5 \( \mu \text{m} \), respectively.

A diamond cutting tool was fixed in a hole with a diameter of 320 mm of an aluminum (Al) alloy plate with a diameter of 336 mm. The Al alloy plate developed was mounted on an ultraprecision grinder (Okamoto VG401 MKII, Japan), forming a specially designed setup to perform grinding induced by a single diamond grain at nanoscale depth of cut, as illustrated in Fig. 1(a).

Commercially available Si (100) wafers (Grinm Advanced Materials Co., Ltd.) of 150 mm in diameter were used as specimens for grinding. The Si wafers had a flatness of about 100 nm after chemical mechanical polishing (CMP). Prior to grinding, a Si wafer was fixed on the ultraprecision grinder by a vacuum chuck. The diamond cutting tool was fed manually. A subtle ground track was generated when touching the Si wafer, and then the readout was taken. The diamond cutting tool was lifted for 30 \( \mu \text{m} \). Grinding was set up automatically, and then it was started until to the readout. During grinding, wheel and table speeds and feed rate were 40 m/s, 140 rpm and 10 \( \mu \text{m/min} \), respectively. Coolant was not supplied in grinding. When reaching the readout, the diamond cutting tool was uplifted immediately. After grinding, ground tracks were formed on a Si wafer, as depicted in Fig. 1(b). Nanoscale depth of cut during grinding was guaranteed by a combination of 150 nm, in which the face runout of air spindle was 50 nm in the ultraprecision grinder and the flatness was 100 nm on a Si wafer. Si wafers were cleaned and dried by deionized water and compressed air respectively prior to characterization.

Diamond cutting tools after grinding and ground surfaces on Si wafers were characterized by a field emission SEM (Lyra3 Tescan, Czech Republic) equipped with focused ion beam (FIB) technique. Widths at onset of grinding and BDT were measured by SEM, and their depths were measured by in situ SEM after FIB cutting. TEM samples at onset of grinding and BDT were prepared by FIB (Auriga, Carl Zeiss, Germany). TEM examinations were performed by an FEI Tecnai F20 microscope operated at an accelerated voltage of 200 kV.

Figure 2 shows the top and side views of SEM images on the cutting tool of diamond C30 grain after grinding. The C30 diamond grain has a conical shape (Figs. 2(a), 2(b) and 2(c)) with a cutting edge radius of 30 \( \mu \text{m} \) (Fig. 2(d)) and an included angle of 143.5\(^{\circ}\) (Fig. 2(d)).

Figure 3 illustrates the SEM and TEM images on the surface and cross-sections at onset of grinding induced by the C30 diamond grain. Width and depth at the onset of grinding are 455 (Fig. 3(a)) and 26 nm (Fig. 3(b)) respectively. An amorphous layer is at the topmost, followed by a damaged crystalline layer beneath, as shown in Fig. 3(c). Partial amor phization is formed at the topmost. The damaged crystalline layer is confirmed by the selected area electron diffraction (SAED) pattern in the inset of Fig. 3(c). Cracks are found in Fig. 3(c). Diamond cubic Si-I phase is observed in Fig. 3(d), which is in good agreement with SAED pattern in the inset of Fig. 3(c). Edge dislocations form a grain boundary (Fig. 3(d)).

Figure 4 depicts the SEM and TEM images on the surface and cross-sections at BDT generated by the C30 diamond grain. Cracked surface is observed on the ground track in Fig. 4(a), and there are no chips left aside the ground track.

### Table II. Specifications of the grinding conditions and measured width and depth at onset of grinding and BDT.

| Diamond grain | Included angle (\(^{\circ}\)) | Cutting edge radius (\( \mu \text{m} \)) | Mesh size | Width (nm) | Depth (nm) | Onset of grinding | BDT Width (nm) | BDT Depth (nm) | Wheel speed (m/s) | Table speed (rpm) | Feed rate (\( \mu \text{m/min} \)) |
|---------------|-----------------------------|------------------------------------------|-----------|------------|-----------|-----------------|----------------|---------------|-----------------|----------------|----------------|
| C30           | 143.5                       | 30                                       | 250       | 455        | 26        |                 | 2660           | 265           | 40              | 140            | 10             |
| C5            | 90                          | 5                                        | 1500      | 394        | 20        |                 | 1360           | 419           |                 |                |                |
| C2.5          | 93                          | 2.5                                      | 3000      | 174        | 24        |                 | 2560           | 172           |                 |                |                |

© Author(s) 2019

AIP Advances 9, 025101 (2019); doi: 10.1063/1.5079819
Width and depth at onset of grinding are 394 (Fig. 6(a)) and 20 nm (Fig. 6(b)) respectively. An amorphous layer is at...
FIG. 6. SEM (a), (b) and TEM (c), (d) images on the surface (a) and cross-sections (b), (c), (d) at onset of grinding produced by the C5 diamond grain at low (c) and high magnifications. (b) is taken from the area marked by a black rectangle in (a). Inset in (c) shows the corresponding SAED pattern marked by a pink circle. (d) is taken from the area marked by a pink square in (c).

FIG. 7. SEM (a), (b) and TEM (c), (d) images on the surface (a) and cross-sections (b), (c), (d) at BDT induced by the C5 diamond grain at low (c) and high (d) magnifications. (b) is taken from the area marked by a black rectangle in (a). Inset in (c) shows the corresponding SAED pattern marked by a pink circle. (d) is taken from the area marked by a pink square in (c).

At BDT induced by the C2.5 diamond grain, the width is 2.56 µm (Fig. 10(a)) and depth is 172 nm (Fig. 10(b)). The topmost is an amorphous layer, and the bottom is a damaged crystalline layer confirmed by the SAED pattern in the inset of Fig. 10(c). A crack takes place in the damaged layer. A twin boundary is shown in Fig. 10(d).

FIG. 8. Top (a), (b) and side (c), (d) views of SEM images at low (a), (c) and high (b), (d) magnifications on the cutting edge of C2.5 diamond grain after grinding.

Chips are present aside the ground track, and they have the ductile characteristics, as shown in Fig. 7(a). Ductile ground track is found in Fig. 7(a), which is distinct from the cracked one in Fig. 4(a). Width and depth at BDT are 1.36 µm (Fig. 7(a)) and 419 nm (Fig. 7(b)), respectively. There is an amorphous layer at the topmost and a damaged crystalline layer beneath (Fig. 7(c)). The damaged crystalline layer is verified by SAED pattern in the inset of Fig. 7(c).

Cracks occur in the cross-sectional microstructure in Fig. 7(c). A grain boundary is found in Fig. 7(d).

The C2.5 diamond grain has a conical shape, as illustrated in Figs. 8(a) and 8(b). A ribbon-like chip is observed in Figs. 8(b), 8(c) and 8(d), exhibiting obvious ductile characteristics. C2.5 diamond grain has a cutting edge radius of 2.5 µm and an included angle of 93°, as depicted in the inset of Fig. 8(d).

At BDT induced by the C2.5 diamond grain, the width is 174 nm (Fig. 9(a)) and a depth is 24 nm (Fig. 9(b)). An amorphous layer is at the topmost, followed by a crystalline layer beneath demonstrated by the SAED pattern in the inset of Fig. 9(c). Thickness of the amorphous layer varies from 36 to 50 nm. There are no cracks in the TEM image of Fig. 9(c). Deformation induced complete amorphization is confirmed by HRTEM in Fig. 9(d), and Si-I pristine crystalline lattice is below the amorphous layer. There is no damaged crystalline layer at onset of grinding, which is different from those ground by the C30 and C5, in which there is a damaged crystalline layer below an amorphous layer (Figs. 3(c) and 6(c)).
The CDC at BDT measured is 265, 419 and 172 nm induced by the C30, C5 and C2.5 diamond grains respectively, as listed in Table II, and the former is 9/1000, 8/100 and 7/100 that of cutting edge radii of the latter correspondingly. The cutting edges of three diamond grains are hemispheric. In such small depth of cut compared to the cutting edge radii of diamond grains, effect of included angle of diamond grains can be neglected. Hence, radius plays the most important role on the surface and cross-sectional microstructure induced by the three diamond grains. An amorphous layer is at the topmost and a damaged crystalline layer beneath, as illustrated in Figs. 3(c), 4(c), 7(c) and 10(c), which is consistent with previous reports.\textsuperscript{11,12} Mesh size of a diamond wheel, \( M \) is presented,\textsuperscript{36}

\[
M = \frac{15.2}{d_g(\text{mm})} \quad (2)
\]

where \( d_g \) is an equivalent diameter of a grain. The C30, C5 and C2.5 diamond grains have the cutting edge radii of 30, 5 and 2.5 \( \mu \text{m} \) respectively, corresponding to mesh sizes in diamond wheels of 250, 1500 and 3000. At onset of grinding in Fig. 3(c), cracks take place, indicating brittle removal mode. This means that a diamond wheel with a mesh size of 250 is disabled to perform ductile removal, and it can only perform brittle removal. Ductile removal demands that there are no cracks on the surface and cross-section produced by a diamond wheel. The C5 and C2.5 diamond grains can perform ductile removal. This is attributed to the absence of cracks on the surface and cross-section at onset of grinding, as depicted in Figs. 6(c) and 9(c) respectively. Deformation induced complete amorphization is demonstrated (Fig. 9(c)) induced by the C2.5 diamond grain, which is distinct from previous partial amorphization,\textsuperscript{11,12} in which there is an amorphous layer at the topmost and a crystalline damaged layer beneath. Thickness of the solely amorphous layer varies from 36 to 50 nm, which is one order magnitude lower than 170 nm\textsuperscript{37} induced by a diamond wheel with a mesh size of 3000. This predicts that a solely amorphous layer with thickness ranging from 36 to 50 nm could be formed, by a new diamond wheel with a mesh size of 3000. It is extremely significant for industries of semiconductor, optoelectronics and microelectronics. The damaged layer induced by grinding is required to be removed by subsequent CMP. However, CMP is the most expensive in machining processes of semiconductor manufacturing. The thinner thickness left by grinding, the less cost and time needed for subsequent CMP processes.

The CDC at BDT is 9.6 nm calculated according to Eq. (1), which is two orders magnitude lower than those measured values experimentally ranging from 172 to 419 nm, as listed in Table II. In consequence, Eq. (1) is not appropriate to calculate the CDC at BDT. It is a challenge to propose a new model to calculate the CDC at BDT, containing the effects of radius and shape of a cutting edge. To solve this difficulty, Hertz contact and plastic deformation theories are employed to calculate the CDC at BDT.

Thrust force, \( F_t \) is proposed,\textsuperscript{38}

\[
F_t = \frac{2\pi a H a^2}{\lambda^2} \quad (3)
\]

where \( a \) is a half of width and \( \lambda \) is a dimensionless parameter. For an axisymmetric cutting edge, \( \lambda \) is 1. Size of plastic deformation, \( S_p \) generated by a grain is introduced,\textsuperscript{38}

\[
S_p = 2\alpha \left[ \frac{3(1-2\nu)}{5-4\nu} + \frac{2\sqrt{3}}{\pi(5-4\nu)} \frac{E}{\sigma_y \cot \alpha} \right]^{0.5} \quad (4)
\]

where \( \nu \) is the Poisson’s ratio, \( \sigma_y \) is the yield strength and \( \alpha \) is the half included angle. The Poisson’s ratio of Si (100) is 0.3.\textsuperscript{26}
Grinding force $F_g$ is suggested,

$$F_g = \mu F_t$$  \hspace{1cm} (6)

where $\mu$ is the friction coefficient, which is 0.08 between a diamond grain and a Si (100) wafer.\textsuperscript{39} The CDC at BDT, $D_c$ is given,\textsuperscript{40}

$$D_c = \left[ \frac{3F_t}{4E'\sqrt{R}} \right]^{2/3}$$  \hspace{1cm} (7)

where $E'$ is the effective indentation modulus, and $R$ is the cutting edge radius of a diamond grain. $E'$ is obtained,\textsuperscript{40}

$$\frac{1}{E'} = \frac{1}{E_c^*} + \frac{1}{E_c}$$  \hspace{1cm} (8)

where $E$ is the Young's moduli and $\nu$ is the Poisson's ratios of a Si (100) wafer ($s$) and a diamond grain ($c$). The Young's modulus and Poisson's ratio of diamond are 1141 GPa and 0.07,\textsuperscript{40} respectively. Calculated force, stress, depth of cut and plastic size are listed in Table III at onset of grinding and BDT. Depth of cut at onset of grinding, $D_{\text{on}}$ calculated is 16 nm, and $D_c$ is 259 nm (Table III), which is in good agreement with experimentally measured values of 26 and 265 nm (Table II), respectively.

Thrust force at onset of grinding under the C30 grain calculated is 2145 $\mu$N, which is the maximum force among the three diamond grains, leading to cracks happened in Fig. 3(c). The calculated depth of cut at onset of grinding for three diamond grains vary from 10 to 24 nm (Table III), which agrees well with measured values changing from 20 to 26 nm (Table II). $D_c$ calculated for three diamond grains changes from 126 to 368 nm, which is consistent with measured results varying from 172 to 419 nm. This confirms that the new model is valid considering effects of radius and shape of a cutting edge. Depth of cut at onset of grinding and BDT calculated is in good agreement with experimental measured results.

Under nanocompression, the compressive stress of 18 GPa. However, all the CATs taken place in Figs. 3(c), 4(c), 6(c), 7(c) and 9(c) are under stress varying from 0.44 to 2.79 GPa (Table III), which is far lower than the predicted critical value of 9.7 GPa for CAT.\textsuperscript{48} Under nanocompression on a Si pillar, amorphization happens from a single crystal via an intermediate diamond-hexagonal under the compressive stress of 18 GPa. However, all the CATs taken place in Figs. 3(c), 4(c), 6(c), 7(c) and 9(c) are under stress varying from 0.44 to 2.79 GPa (Table III), which is far lower than the predicted critical value of 9.7 GPa. As a result, grinding speed at nanoscale depth of cut has a significant effect on CAT. Nevertheless, the stress calculated in Table III is the average stress under the grain cutting edge of C2.5 at BDT is 26.04 GPa, which is 57.8 GPa for Si (100). $b_p$ is proposed,\textsuperscript{43}

$$b_p = \frac{L_p}{\sqrt{6}}$$  \hspace{1cm} (11)

where $L_p$ is the lattice parameter of Si. $L_p$ is 0.5431 nm,\textsuperscript{44} and $b_p$ is 0.2217 nm. Average thickness of $\lambda$ is 3.67 nm, as measured in Fig. 10(d), $\gamma$ is 69 mJ/m$^2$.\textsuperscript{45} The critical twinning stress of Si (100) calculated is 3.8 GPa.

An amorphous layer is at the topmost and a damaged crystalline layer beneath, as shown in Figs. 3(c), 4(c), 6(c), 8(c) and 10(c), which is consistent with previous findings of partial amorphization.\textsuperscript{11,12} Nanoscale amorphous layer is formed at the topmost in Figs. 3(c) and 6(c). Deformation induced complete amorphization takes place in Fig. 9(c) with thickness varying from 36 to 50 nm, which is different from previous literatures.\textsuperscript{11,12} In this study, deformation induced complete amorphization is ground by a single diamond grain with a cutting edge radius of 2.5 $\mu$m at depth of cut of 24 nm, as listed in Table II. The grinding speed is 40 m/s, which is 4 to 8 orders magnitude higher than previous loading speeds from 0.33 $\mu$m/s to 8.3 mm/s.\textsuperscript{27,29-35} Grinding speed plays an important role in deformation induced complete amorphization. Complete amorphization is formed in Fig. 9(c), which is different from partial amorphization induced by nanoscratching at a speed of 400 nm/s,\textsuperscript{46} in which an amorphous layer with thickness of about 10 nm at the top, followed by a damaged crystalline layer beneath with a thickness of approximately 6 nm. The normal stress under the grain cutting edge is 0.84 GPa for the complete amorphization in Fig. 9(c), as listed in Table III. This is basically consistent with the hydrostatic pressure of 1.5 GPa for dislocation-controlled plastic deformation of nanoparticles,\textsuperscript{9} while it is distinct from those in nanoscale compression.\textsuperscript{47,48} In a core/shell configuration, the crystalline-to-amorphous transition (CAT) is induced by nanocompression under 8.5 GPa, which is close to the predicted critical value of 9.7 GPa for CAT.\textsuperscript{48} Under nanocompression on a Si pillar, amorphization happens from a single crystal via an intermediate diamond-hexagonal under the compressive stress of 18 GPa. However, all the CATs taken place in Figs. 3(c), 4(c), 6(c), 7(c) and 9(c) are under stress varying from 0.44 to 2.79 GPa (Table III), which is far lower than the predicted critical value of 9.7 GPa. As a result, grinding speed at nanoscale depth of cut has a significant effect on CAT. Nevertheless, the stress calculated in Table III is the average stress under the cutting edges of diamond grains, and the local stress might reach the critical value of CAT. The stress under the grain cutting edge of C2.5 at BDT is 26.04 GPa, which is

| Diamond grain | $F_t$ ($\mu$N) | $F_g$ ($\mu$N) | $S_p$ (nm) | $D_{\text{on}}$ (nm) | Normal stress (GPa) | $F_t$ ($\mu$N) | $F_g$ ($\mu$N) | $S_p$ (nm) | $D_c$ (nm) | Normal stress (GPa) |
|---------------|---------------|---------------|------------|---------------------|---------------------|---------------|---------------|------------|--------------|---------------------|
| C30           | 2145          | 172           | 836        | 16                  | 0.44                | 138805        | 1104         | 6721       | 259          | 2.79                |
| C5            | 1609          | 129           | 1219       | 24                  | 2.57                | 19166         | 1533         | 4208       | 126          | 1.52                |
| C2.5          | 314           | 25            | 525        | 10                  | 0.84                | 67908         | 5433         | 7723       | 368          | 26.04               |

$\sigma_y$ is addressed,\textsuperscript{29}

$$\sigma_y = \frac{H}{2.8}$$  \hspace{1cm} (5)

where $\mu$ is the friction coefficient, which is 0.08 between a diamond grain and a Si (100) wafer.\textsuperscript{39} The CDC at BDT, $D_c$ is given,\textsuperscript{40}

$$D_c = \left[ \frac{3F_t}{4E'\sqrt{R}} \right]^{2/3}$$  \hspace{1cm} (7)

where $E'$ is the effective indentation modulus, and $R$ is the cutting edge radius of a diamond grain. $E'$ is obtained,\textsuperscript{40}

$$\frac{1}{E'} = \frac{1}{E_c^*} + \frac{1}{E_c}$$  \hspace{1cm} (8)

where $E$ is the Young's moduli and $\nu$ is the Poisson's ratios of a Si (100) wafer ($s$) and a diamond grain ($c$). The Young's modulus and Poisson's ratio of diamond are 1141 GPa and 0.07,\textsuperscript{40} respectively. Calculated force, stress, depth of cut and plastic size are listed in Table III at onset of grinding and BDT. Depth of cut at onset of grinding, $D_{\text{on}}$ calculated is 16 nm, and $D_c$ is 259 nm (Table III), which is in good agreement with experimentally measured values of 26 and 265 nm (Table II), respectively. Thrust force at onset of grinding under the C30 grain calculated is 2145 $\mu$N, which is the maximum force among the three diamond grains, leading to cracks happened in Fig. 3(c). The calculated depth of cut at onset of grinding for three diamond grains vary from 10 to 24 nm (Table III), which agrees well with measured values changing from 20 to 26 nm (Table II). $D_c$ calculated for three diamond grains changes from 126 to 368 nm, which is consistent with measured results varying from 172 to 419 nm. This confirms that the new model is valid considering effects of radius and shape of a cutting edge. Depth of cut at onset of grinding and BDT calculated is in good agreement with experimental measured results.

The critical twinning stress of Si (100) is calculated,\textsuperscript{41}

$$\tau_c = \frac{2aGb_p}{A} + \frac{\gamma}{b_p}$$  \hspace{1cm} (9)

where $a$ is a constant, $G$ is the shear modulus, $b_p$ is the magnitude of the Burgers vector of the Shockley partial dislocation, $\lambda$ is the thickness between two adjacent twin boundaries, and $\gamma$ is the stacking fault energy. $\alpha$ is 0.5 for edge dislocations,\textsuperscript{41} $G$ is obtained,\textsuperscript{42}

$$G = \frac{E}{2(1+\nu)}.$$  \hspace{1cm} (10)
higher than the critical twinning stress of 3.8 GPa for Si (100), resulting in the formation of a nanotwin in Fig. 10(d).

In summary, complete morphization is realized in a bulk solid, which is ground by a developed single diamond grain on a specially designed setup. The diamond grain has a cutting edge radius of 2.5 µm. The complete amorphization is ground at 40 m/s at depth of cut of 24 nm. A nanotwin is found by HRTEM at BDT induced by the diamond grain at depth of cut of 172 nm. The critical twinning stress calculated is 3.8 GPa for Si (100). It is demonstrated that radius and shape of cutting edges affect the CDC at BDT. A new model is proposed to calculate the force, stress, plastic size and CDC at BDT, under the cutting edges of single diamond grains, and the effects of radius and shape of cutting edges are taken into account. The calculated results of CDC at BDT are consistent with those experimentally. The outcomes in this study provide new viewpoints for manufacturing high performance devices employed in nanodevices, flexible electronics, semiconductor, microelectronics and optoelectronics.

The authors acknowledge the financial supports from the Excellent Young Scientists Fund of NSFC (51422502), Science Fund for Creative Research Groups of NSFC (51621064), Changjiang Scholar Program of Chinese Ministry of Education, Program for Creative Talents in University of Liaoning Province (LR2016006), Distinguished Young Scholars for Science and Technology of Dalian City (2016R05), the Xinghai Province (LR2016006), and the Collaborative Innovation Center of Major Machine Manufacturing in Liaoning.

REFERENCES

1. M. J. Treacy and K. B. Borisenko, Science 335, 950 (2012).
2. K. Minowa and K. Sumino, Phys. Rev. Lett. 69, 520 (1992).
3. S. K. Deb, M. Wilding, M. Somayazulu, and P. F. McMillan, Nature 414, 528 (2001).
4. S. Takeda and J. Yamasaki, Phys. Rev. Lett. 83, 320 (1999).
5. D. R. Clarke, C. M. Krofi, P. D. Kirchner, R. F. Cook, and B. J. Hacker, Phys. Rev. Lett. 60, 2156 (1988).
6. M. G. Castano, A. Torrents, L. Valdevit, and J. G. Zheng, Phys. Rev. Lett. 105, 145701 (2010).
7. S. Dai, J. Zhao, L. Xie, Y. Cai, N. Wang, and J. Zhu, Nano Lett 12, 2379 (2012).
8. X. D. Han, K. Zheng, Y. F. Zhang, X. N. Zhang, Z. Zhang, and Z. L. Wang, Adv. Mater. 19, 2112 (2007).
9. D. Chrobak, N. Tymiak, A. Beaber, O. Ugurlu, W. W. Gerberich, and R. Nowak, Nanotechnology 6, 480 (2011).
10. D. Wang, C. L. Ren, M. S. Wang, X. L. Wei, N. Kawamoto, C. Liu, Y. Bando, M. Mitome, N. Fukata, and D. Golberg, Nano Lett. 12, 1898 (2012).
11. Z. Y. Zhang, F. W. Huo, X. Z. Zhang, and D. M. Guo, Scripta Mater 67, 657 (2012).
12. W. Yan, H. Takahashi, J. Tamaki, X. Gai, and T. Kuriyagawa, Appl. Phys. Lett. 87, 21901 (2005).
13. F. Ostlund, K. R. Malykse, K. Leifer, L. M. Hale, Y. Y. Tang, R. Ballarini, W. W. Gerberich, and J. Michler, Adv. Funct. Mater. 19, 2439 (2009).
14. R. S. Jacobsen, K. N. Andersen, P. J. Borel, J. Fage-Pedersen, L. H. Frandsen, O. Hansen, M. Kristensen, A. V. Lavrinenko, G. Moulin, H. Ou, C. Peucheret, B. Zsirgi, and A. Bjarklev, Nature 441, 199 (2006).
15. F. Bai, Nature 433, 691 (2005).
16. A. Martinson, J. Ballato, and T. Hawkins, APL Mater. 2, 16108 (2014).
17. J. R. Petta, Nature 455, 599 (2018).
18. J. I. B. Wilson and D. W. Weaire, Nature 275, 93 (1978).
19. D. Marinescu, CRC Press, 2010.
20. F. Ebrahimi and L. Kalwani, Mater. Sci. Eng. A 268, 116 (1999).
21. H. Wu and S. N. Melkote, J. Eng. Mater. Technol. Trans. ASME 134, 041012 (2012).
22. D. Axinte, P. Butler-Smith, C. Akgun, and K. Kolluru, Int. J. Mach. Tools Manuf. 74, 12 (2013).
23. S. H. Lee, Int. J. Mach. Tools Manuf. 61, 71 (2012).
24. L. Jiang, X. Wang, and L. F. Chi, Small 7, 1309 (2011).
25. I. L. A. Moses, J. H. Waite, and F. W. Zok, Proc. Natl. Acad. Sci. USA 104, 13559 (2007).
26. N. A. LaFranzo and J. A. Maurer, Adv. Funct. Mater. 23, 2415 (2013).
27. P. Pohl, A. Mohr, and W. Theisen, Wear 376, 947 (2017).
28. Y. W. Tan, Y. Asami, H. Harada, and T. Kuriyagawa, Precis. Eng. 33, 378 (2009).
29. S. Malkin and C. Guo, Industrial Press Inc., New York, 2008.
30. S. Gao, Z. G. Dong, R. K. Kang, and D. M. Guo, Proc. Inst. Mech. Eng. Part B J. Eng. Manuf. 227, 578 (2013).
31. X. N. Jing, S. Maiti, and G. Subhash, J. Am. Ceram. Soc. 90, 885 (2007).
32. H. H. Gatzen and M. Beck, Wear 254, 1122 (2003).
33. S. Shih, H. Wei, E. P. George, and G. M. Pharr, Scripta Mater. 59, 1095 (2008).
34. M. W. Chen, E. Ma, K. J. Hemker, H. W. Sheng, Y. M. Wang, and X. M. Cheng, Science 300, 1275 (2003).
35. M. Domingo-Espin, J. Mu. Puigoriol-Forcada, A. A. Garcia-Granada, J. Lluma, S. Borros, and G. Reyes, Mater. Des. 38, 670 (2015).
36. C. Villeges and L. L. Shaw, Acta Mater. 57, 5782 (2009).
37. L. X. Xu, X. M. Liu, Y. S. Luo, L. M. Zhou, and J. K. Kim, Prog. Mater. Sci. 90, 1 (2017).
38. H. Foll and C. B. Carter, Philos. Mag. A 40, 497 (1979).
39. Y. Q. Wu, H. Huang, J. Zou, L. C. Zhang, and J. M. Dell, “Nanoscratch-induced phase transformation of monocrystalline Si,” Scripta Mater. 63, 847 (2010).
40. Y. He, L. Zhong, F. F. Fan, C. M. Wang, T. Zhu, and S. X. Mao, Nanotechnol. 11, 866 (2016).
41. Y. C. Wang, W. Zhang, L. Y. Wang, Z. Zhuang, E. Ma, J. Li, and Z. W. Shan, NPG Asia Mater. 3, e291 (2016).