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# Nanotwinning in monocrystalline silicon upon nanoscratching

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Nanoscratching-induced deformation in monocrystaline silicon is found to depend on the loading conditions. Molecular dynamics simulations reveal that amorphous phase transformation and nanotwins are the two major mechanisms. At a relatively low scratching depth, amorphous transformation occurs on the surface; however, when the scratching depth is greater than 1 nm, nanotwinning also emerges in the subsurface along ⟨1 1 0⟩ direction and its formation is associated with the body-centred-tetragonal-5 Si phase transformation. The twinning deformation stops at a Shockley partial dislocation.


*Keywords:* Silicon; Nanoscratching; Nanotwinning; Phase transformation; Molecular dynamics

Monocrystalline silicon undergoes mechanical deformation during the fabrication of electronic devices. As electronic devices become increasingly miniaturized, the manufacturing methods involved have also become more and more complicated. For most applications, silicon wafers are thinned down by nanogrinding. During this process the nanoscratching of abrasives on a grinding wheel governs the material removal mechanisms [1] and the control of nanoscopic deformation in silicon plays a critical role in satisfactory fabrication.

Investigations using high-resolution scanning and transmission electron microscopy and micro-Raman spectroscopy have shown that surface morphologies created by nanoscratching are strongly influenced by the scratch velocity and load [2]. At low speeds, nanocrystals can appear within the amorphous silicon region, whereas at high speeds only amorphous silicon exists. At a high load, dislocations would be initiated. A recent transmission electron microscopy investigation [3] of nanoscratch-induced deformation of silicon also showed that the normal load and tip radius have a significant influence on the deformation. Amorphization occurred at extremely small loads, and stacking faults and twins nucleated at a load smaller than that for dislocation. Nanotwinning has also been observed in silicon nanocrystals of diameters larger than 6 nm, produced by ion implantation [4]. It is therefore important to know the mechanisms and conditions of nanoscratching under which twinning and dislocation will take place.

Silicon crystals have a face-centred-cubic (fcc) structure. On mechanical loading, three types of dislocations are common: a full dislocation with Burgers vector $b = (a/2)\langle 1\ 1\ 0\rangle$; a Shockley partial dislocation with $b = (a/6)\langle 1\ 1\ 2\rangle$; and a Frank partial dislocation with $b = (a/3)\langle 1\ 1\ 1\rangle$. So far twinning/dislocation has not been observed in molecular dynamics (MD) simulation studies of silicon although dislocations have been reported in the MD simulation of monocrystalline fcc materials such as Ag [5] and Al [6]. Twinning deformations have been predicted by Yamakov et al. [7,8] for nanocrystalline Al polycrystals. Previous MD studies on silicon scratching showed that amorphous phase transformation was the main deformation of silicon when subjected to contact sliding [1,9]. However, those studies were performed under relatively low loads with a small indenter. The present study will investigate the microstructural changes during scratching using a relatively larger probe tip.

MD was used to simulate the scratching on a Si(0 0 1) surface using a hemispherical diamond tip of radius 7.5 nm. Large silicon samples of size $57.02 \times 15.20 \times 5.97$ and $37.47 \times 15.20 \times 9.77$ nm$^3$ were used. Two layers of thermostat atoms and boundary atoms were arranged to surround the Newtonian atoms (except those on the top and front surface) of silicon to ensure reasonable outward heat conduction during scratching and to eliminate rigid body motion [1,10]. Interactions between silicon atoms were described by the Tersoff potential and those between silicon and diamond atoms

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were described by a modified Morse potential, as explained by Zhang and Tanaka [10] and Cheong and Zhang [11]. The diamond tip was placed 0.3 nm above the Si(0 0 1) surface and the scratching simulations were done at depths of 0.5, 1.0 and 1.5 nm on fresh samples by moving the tip at a speed of 40 m $s^{-1}$. Here the scratching depth is considered as the penetration of the tip measured from the surface of the workpiece assuming that the surfaces are defined by the envelopes at the theoretical radii of their surface atoms [12].

Damage was examined by (i) projecting a thin layer of atoms in that region onto the set of {1 1 0} planes; (ii) through the evaluation of slip vector, $s_i$, defined by:

$$s_i = -\frac{1}{N_s}\sum_{j\neq i}^{N_{nn}}\left(r_{ij} - r_{ij}^0\right) \quad (1)$$

where $N_s$ and $N_{nn}$ are the number of slipped neighbours and the nearest neighbours of atom $i$ and $r_{ij}$, $r_{ij}^0$ are the vectors linking atom $i$ and all its nearest neighbours $j$ in the current and reference positions; and (iii) by structural analysis.

Table 1 shows the average normal and scratching forces at different nanoscratching depths. The normal and scratching forces in the steady nanoscratching states are the averages of the corresponding vertical and horizontal instantaneous forces, respectively. Under the shallow scratching depth of 0.5 nm, amorphous phase transformation is the only type of subsurface damage to emerge. However, other types of structural changes took place at depths greater than 1 nm as seen in Figure 1b and c; one of these is marked by dotted lines in Figure 1b.

**Table 1.** Effect of nanoscratching depth on forces.

| Nanoscratching depth (nm) | Normal force, $F_N$ (μN) | Scratching force, $F_S$ (μN) | $F_S/F_N$ |
|---|---|---|---|
| 0.5 | 0.35 | 0.225 | 0.64 |
| 1.0 | 0.69 | 0.45 | 0.65 |
| 1.5 | 0.95 | 0.65 | 0.68 |

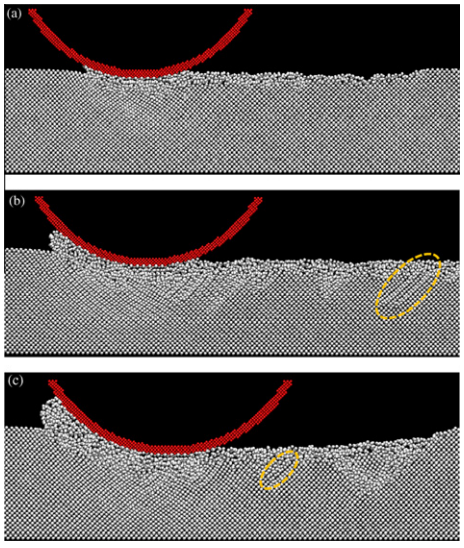


**Figure 1.** Cross-sectional view of subsurface damage—effect of nanoscratching depth: (a) 0.5 nm, (b) 1.0 nm and (c) 1.5 nm.

When scratching at a depth of 0.5 nm (Fig. 1a) the tip ploughs through the substrate with a negligible pile-up of substrate atoms in front of the probe. In all other cases, ploughed atoms accumulate in front of the probe and form chips. A deeper scratching leads to a greater chip volume, resulting in a higher resistance to scratching, and hence a larger scratching force, as demonstrated by the increase of the force ratio, $F_S/F_N$, in Table 1.

In Si(1 0 0), it is known that a crack can propagate more easily along the highest closed packing planes [13,14]. In the present study, we found that when scratching at a depth of 1 nm or greater, a series of microstructural changes occurred, as shown in Figure 1b and c. A close examination, as detailed below, shows that nanotwinning emerged during the nanoscratching, but stopped at a Shockley partial dislocation.

Twinning can be identified on {1 1 0} planes [15]. Thus by projecting the atoms of a monolayer within the region marked by the dotted line in Figure 1b onto a (1 1 0) plane, we obtain the nanotwins with the twin plane (1 1 1) as shown in Figure 2. It is clear from Figure 2 that the nanotwinning stops at the Shockley partial dislocation. Generally, frequent twins and high density of uniform dislocations occur in materials with low

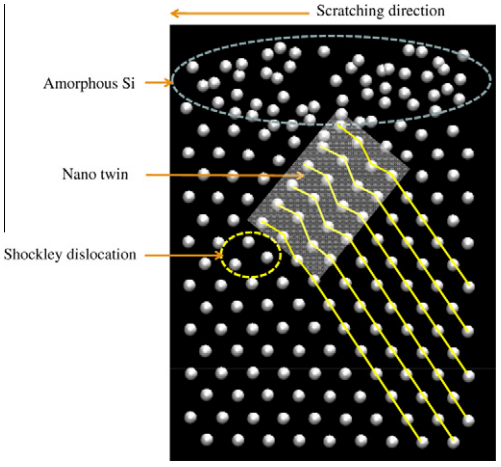


**Figure 2.** Projected atoms in the Si(1 1 0) plane showing the nanotwin and Shockley partial dislocation.

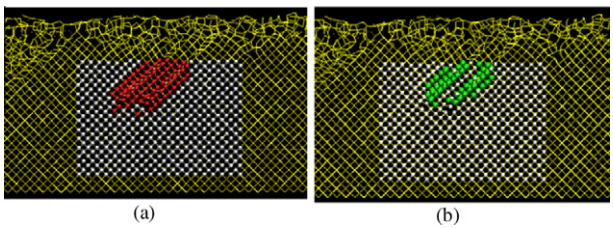


**Figure 3.** Deformation induced by nanoscratching at a depth of 1 nm: (a) atoms with non-zero slip vector (red spheres) in the region examined (white spheres); (b) atoms that have a slip vector modulus in the range 1.817–2.617 Å (green spheres). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

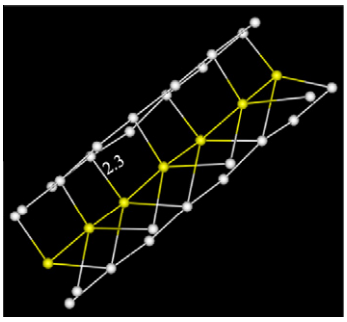


**Figure 4.** Atoms along a nanotwin with 5-coordination.

stacking fault energy (SFE), such as silicon whose SFE is about 50 mJ $m^{-2}$ [16]. In their nanoscratch TEM studies of single-crystal silicon, Wu et al. [3] reported that twins and stacking faults were nucleated, and that the nucleation load of the twins was smaller if a smaller tip radius was used.

By analyzing the marked region in Figure 1b, using Eq. (1), we found that the atoms along the ⟨1 1 0⟩ direction had slipped. Figure 3a shows the portion of the atoms selected for analysis (white spheres) and the atoms that have a non-zero slip vector (red spheres). Atoms with slip vector moduli $|S_i|$ of $(a_0/6)$ ⟨1 1 2⟩ where $a_0 = 5.43$ Å (i.e. $|S_i| = 2.217$ Å) represent the Shockley partial dislocation. Among the slipped atoms, the atoms shown in Figure 3b by green spheres have a slip vector modulus in the range of 1.817–2.617 Å. This shows that silicon undergoes Shockley partial dislocation on scratching under a load above ~0.7 μN.

An investigation into the coordination number of the atoms in the marked region of Figure 1b shows that the atoms in this region are 5-coordinated with one short (2.3 Å) and four long bonds as demonstrated in Figure 4. This is similar to the body-centred-tetragonal (bct)-5 Si structure found in nanoindentation during loading [17]. However, under indentation the bct-5 Si phase is metastable and changes to amorphous phase upon unloading. Unlike the situation in indentation, under the present nanoscratching the bct-5 Si persists after unloading (i.e. after scratching).

Gassilloud et al. [2] explained the shape of the transformed zone observed in their nanoscratching experiment, and confirmed that similar to the findings from MD simulations [1], and to the conclusions based on microscratching [18], amorphous phase transformation takes place prior to dislocation nucleation during loading. However, our present result shows that along the nanotwins, the original diamond cubic silicon (4-coordinated silicon) had transformed to 5-coordinated bct-5 silicon. This means that the emergence of the nanotwinning during nanoscratching is associated with the phase transformation to bct-5 Si.

In summary, this study has discovered the following deformation mechanisms in monocrystalline silicon under nanoscratching:

(i) When the scratching depth reaches a critical value (1 nm in the case of the probe radius of 7.5 nm used in this study), nanotwins will emerge in the subsurface in addition to amorphous phase transformation.
(ii) The nanotwins stop at Shockley partial dislocations.
(iii) The nanotwinning is associated with the phase transformation to bct-5.

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