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Effect of bct-5 Si on the indentation of monocrystalline silicon

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Abstract. Mono-crystalline silicon experiences various phase transformations under different loading conditions. This paper reveals, with the aid of molecular dynamics simulations, that scratching the silicon {001} surface along the [110] direction under a load of 0.8 μN or more would produce stable 5 coordinated body centered tetragonal (bct-5) silicon in the subsurface. By examining the effect of this bct-5 silicon on indentation, it was found that the resistant to deformation of bct-5 silicon is higher than a-Si but lower than diamond Si.

Introduction

Monocrystalline silicon is a key material for a wide range of applications. Most micro-electro-mechanical systems (MEMS) and integrated circuit (IC) technologies use silicon as the substrate material. Extensive research has been carried out to produce MEMS and ICs. An important step is to obtain integrated and miniaturized systems of high surface integrity. Hence, to control the subsurface quality, an in-depth understanding of the microstructural changes with stresses and other external factors is of increasing importance.

Silicon experiences various phase transformations under different loading conditions [1]. So far thirteen different stable and meta-stable silicon phases have been identified either experimentally [2,3] or theoretically [4]. For example, with increasing the hydrostatic pressure in a diamond anvil cell, silicon undergoes various phase transformations. In loading at a pressure of 10 GPa to 12 GPa the original diamond structure of silicon (Si-I) transforms into a denser β-Sn phase (Si II). When the pressure reaches the range of 13 GPa to 16 GPa, Imma silicon (Si-XI) occurs. More phase changes take place upon further increment of the pressure: primitive hexagonal (Si-V) at 14 GPa to 16 GPa, Cmca (Si-VI) at above 38 GPa, hexagonal close-packed structure (Si-VII) at 40 GPa to 49 GPa, and the face centered cubic silicon (Si-X) at around 79 GPa. The phase transformation routes can become different under different loading and unloading conditions. For instance, Si-II forms under indentation loading and then Si-III, Si-XII or a-Si can appear during unloading, depending on the maximum indentation load and unloading rate [3,4,5,6]. A new six-coordinated meta-stable silicon phase Si-XIII, can also appear on loading [4]. On exploring the strain space of silicon using plane-wave pseudopotential method, Boyer et al. [7] uncovered an interesting transformation that takes the diamond structure into a body-centered-tetragonal structure with fivefold-coordinated atoms. They reported that non-hydrostatic pressure could transform diamond cubic silicon to bct-5 silicon and once transformed it could well be stable at ambient pressure.

This paper investigates the possibility of the emergence and growth of the bct-5 silicon in the sub surface by scratching the silicon {001} surface along the [110] direction. Molecular dynamics simulation will be used.

Computational Methodology

A hemi-spherical diamond tip of radius 7.5 nm and a large silicon sample size of 50.0 × 38.4 × 6.0 nm^3 were used to simulate the nano-scratching process of mono-crystalline silicon {001} surface. Two layers of thermostat atoms and boundary atoms were arranged to surround the Newtonian atoms

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(except the front and top surfaces) of silicon to ensure reasonable outward heat conduction during sliding and to eliminate the rigid body motion [8]. Interactions among silicon atoms were described by Tersoff potential [9,10] and those among silicon and diamond atoms were described by a modified Morse potential, as explained elsewhere [11]. The surface was scratched along the [110] direction under a load of about 1 μN by moving the tip with a speed of 40 m/s.

Portions of the scratched Si with and without the a-Si were taken for indentation studies. Except the top surface of the sample, two layers of the surface atoms of each of the other sample surfaces were taken as boundary atoms and the next two layers of the atoms were taken as thermostat atoms to eliminate the rigid body motion and to ensure reasonable outward heat conduction during indentation. The contact area, A, was calculated using an atomistic approach by counting the number of silicon atoms that were in contact with the diamond indenter and multiplying it by the projected area of an atom, πr^2 [11].

Results and Discussion

Scratching the {001} silicon surface along [110] direction under a depth-of-cut of 1.5 nm resulted in a-Si to a depth of ~1 nm on the surface and a crystalline phase to a depth of ~1 nm in the subsurface beneath the a-Si as shown in Fig. 1(a).

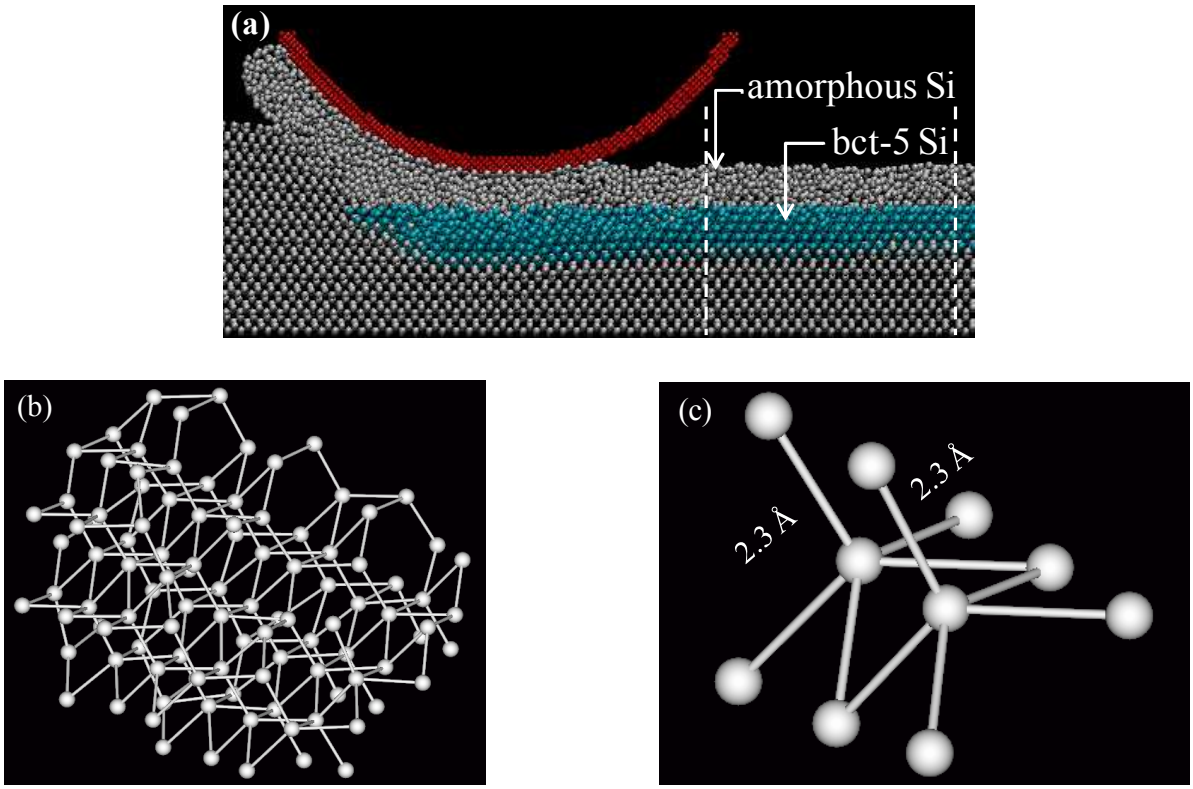

Figure 1: (a) Cross-sectional view of a portion of the scratched surface when scratched along [110] direction, (b) a portion of the bct-5 silicon formed in the sub surface, and (c) structure of the five coordinated atom.

On examining the coordination number of this different crystalline phase showed that the atoms are five coordinated with one short and four slightly long bonds having a structure similar to the bct-5 Si. A portion of this five coordinated silicon is shown in Fig. 1(b) and two of these atoms are shown in Fig. 1(c). Even after completing the scratching, this five-coordinated phase remains in the subsurface along the path traversed by the tip. The bct-5 silicon phase was also observed in our recent nano-indentation studies under loading but it disappeared on unloading [4].

A portion of the scratched material was used in the indentation study. Fig. 2(a) shows the cross-sectional view of the initial setup for indenting the scratched surface consisting of a-Si, bct-5 Si and diamond cubic silicon. During the loading process, the diamond tip would first indent on the a-Si to a depth of ~1 nm, then on the bct-5 silicon to a depth of further ~1nm and then finally it would reach the diamond cubic silicon. Fig. 2(b) shows the deformation pattern at an indentation depth of 2.6 nm. It is evident that on loading, the six coordinated β-tin Si formed at a greater distance below the indenter tip, similar to the indentation on fresh surface. This β-tin Si is surrounded by five coordinated bct-5 silicon. In addition, similar to the diamond-like crystalline patches observed when indenting the fresh surface, here the bct-5 Si patches were observed in between the indenter tip and the β-tin Si. However, upon unloading, unlike the fresh surface where the diamond-like crystalline patches grow to a bigger crystalline, here the bct-5 Si patch disappeared and the deformed zone contained mainly amorphous silicon.

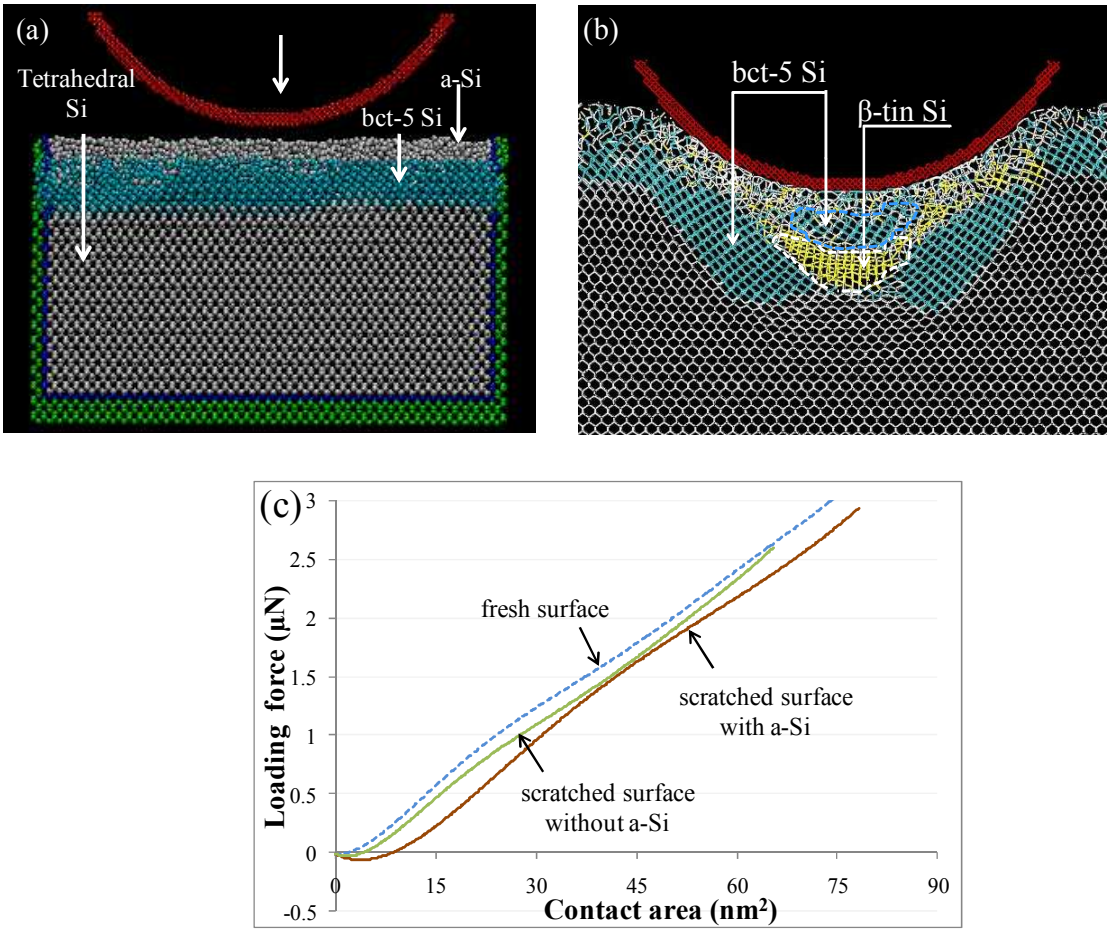

Figure 2: (a) A cross-sectional view of an initial set up for the indentation of silicon with bct-5 silicon in the subsurface, (b) a portion of the scratched surface during indentation, and (c) force-contact area curves of scratched surfaces with and without a-Si (continuous lines) and fresh (broken line) surface on loading.

In the above indentation process, the effect due to the presence of bct-5 Si alone cannot be identified because of the existense of a-Si on its top. To clarify this, we removed the top a-Si layer and indented directly on the bct-5 Si to a depth of ~1nm. It was shown in Fig.2(c) that the force varies in a similar way to the indentation with the a-Si layer. However, in the present case the force is always between the other two curves, i.e., those on the fresh Si surface and on the scratched surface with the a-Si layer. This shows that the resistant to deformation of bct-5 silicon is higher than a-Si but lower than diamond Si.

In addition the four coordinated diamond cubic silicon is semi metal whereas the bct-5 silicon could be metallic due to the decrease in the gap between the valence band and the conductance band that facilitates the formation of five coordinated silicon. Thus the presence of bct-5 silicon could have an influence on the electronic properties of the substrate.

Summary

The molecular dynamics simulations of scratching monocrystalline silicon in this study revealed that

- A stable bct-5 silicon phase could be produced in the subsurface by nano-scratching Si {001} surface along [110] direction under a load of 0.8 μN or higher.
- The resistant to deformation of bct-5 silicon is higher than a-Si but lower than diamond Si.

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