Key Engineering Materials Vols. 389-390 (2009) pp 521-526
Online available since 2008/Sep/26 at www.scientific.net

doi:10.4028/www.scientific.net/KEM.389-390.521

Scale Effect of Nano-indentation of Silicon – A Molecular Dynamics Investigation

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Keywords: Silicon, molecular dynamics, indentation, scale effect.

Abstract. This paper investigates the scale effect of indenter tip radius on the deformation of silicon under nanoindentation using molecular dynamics simulation. It was found that with larger diamond tips a six-coordinated silicon phase different from β-silicon on loading and a diamond like crystal beneath the indenter on unloading would appear as a result of the indentation stressing. This is a new phenomenon that has not been observed previously.

Introduction

Understanding the mechanical properties of silicon mono-crystals has become increasingly important in developing high performance electronic devices for nanotechnology and biotechnology. The fabrication and application of these devices require that the mechanical behaviour of silicon mono-crystal subjected to various loading conditions need to be more deeply understood. It is well known that phase transformations in silicon occur during indentation and a vast amount of literature, both theoretical [1-4] and experimental [5-10], is available. Previous studies have identified various stable and non-stable phases during the loading-unloading cycles of indentation on silicon. Experimental studies have revealed that under indentation during loading silicon transforms from its diamond cubic structure to a metallic body-centered tetragonal structure known as β-silicon. In indentation experiments, the metallic nature of the β-silicon is inferred by the fall in resistivity [8]. Evolution of β-silicon phase was also explained by monitoring the positions of atoms during indentation using molecular dynamics (MD) simulation [2]. During unloading, the β-silicon phase was transferred to either the amorphous or the high-pressure R8/BC8 phase or a mixture of them. The high-pressure phases have been identified using high resolution transmission electron microscopy (HRTEM).

In this work we will perform MD simulations of indentation with different diamond tip radii to identify the phase transformations – especially the onset and evolution of different phases during loading and unloading and the effect of tip radius on the deformation of silicon.

Molecular Dynamics Modeling

The MD simulation of indentation is on <100> silicon sample. Hemi-spherical rigid diamond tips of radius 50, 75 and 100 Å were used as indenters. To avoid the boundary effect, silicon samples of dimensions 217.2 x 217.2 x 97.7 $Å^3$ and 244.4 x 244.4 x 119.5 $Å^3$ were used. The boundary atoms and thermostat atoms were arranged to surround the Newtonian atoms of silicon to eliminate the rigid body motion and realise a reasonable heat conduction as has been detailed elsewhere [1]. The interactions among silicon atoms were described by Tersoff potential [11,12] and those among silicon and diamond atoms were described by Morse potential with specially developed parameters, as explained by Zhang and Tanaka [1]. Initially the tip of the indenter is placed 5 Å above the surface of the silicon workpiece and moved towards the workpiece by 0.001 Å per time step of 2.5 fs.

Results and Analysis

(a) Indentation with a hemi spherical indenter of radius 50 Å. A complete load–displacement curve, consisting the loading and unloading path, is shown in Fig. 1(a). The indentation load increased with indenter tip displacement, except at the preloading path where the force is negative due to the attraction between indenter and silicon atoms when they are in distance. The behaviour is very similar to previously observed MD simulation results of Zhang and Tanaka [1] and Cheong and Zhang [2] using a much smaller spherical indenter of radius 21.4 Å. Fig. 2(b) shows the location of atoms at an indentation depth of ~40 Å. The atoms beneath the indenter tip have a six coordinated β-silicon crystalline order as have been identified by previous studies. After unloading, the surface beneath the indenter is not smooth due to the formation of amorphous silicon and has an average residual indentation depth of ~11.5 Å. It is clear that up to the indenter radius of 50 Å, there is not any scale effect in terms of deformation mechanisms in silicon.

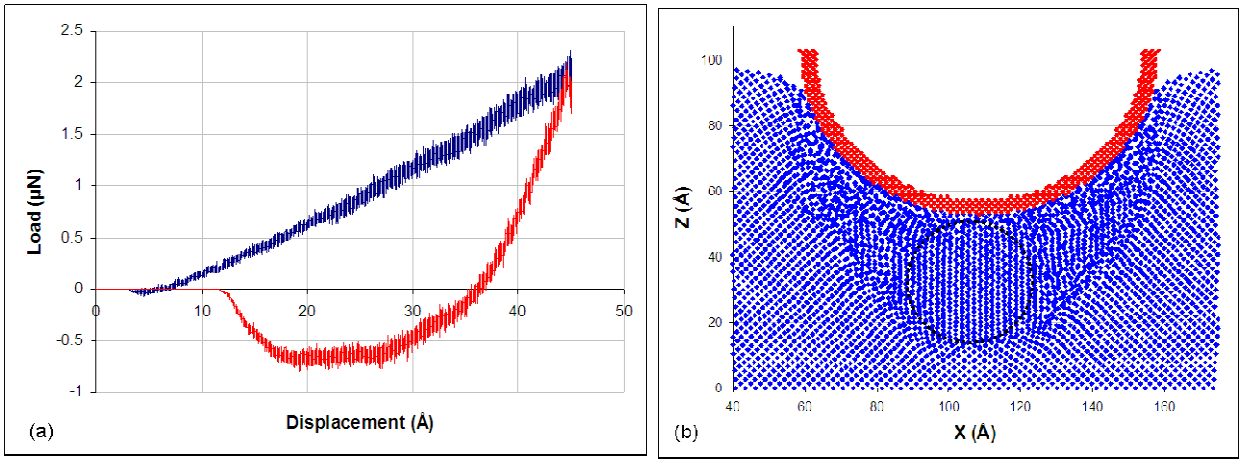

Figure 1. Nano-indentation of silicon using a diamond tip of radius 50 Å: (a) the load–displacement curve, and (b) the snapshot of a portion of the atoms under the maximum indentation depth of 40 Å. The region of six coordinated atoms is shown by a dotted circle.

(b) Indentation with a hemi spherical indenter of radius 75 Å The load–displacement curve of indentation loading and unloading is shown in Fig. 2(a) and the snapshot of the location of atoms at the maximum indentation depth of 40 Å is shown in Fig. 2 (b). In this case, two different orientations of long-range crystalline order are observed, which has never been observed before, reflecting clearly the scale effect of the indenter size on the deformation in silicon. It is evident from Fig. 2(b) that the orientation of atoms in region A is different from that of the atoms in region B. In addition, a region of disordered atoms with small patches of unaltered diamond like cubic crystalline phase is found in between the indenter and region A.

A detailed examination of the coordination number of the atoms with a bond length criterion of 2.585 Å reveals that the atoms in regions A and B are six coordinated. The number of six coordinated atoms increased rapidly around a tool displacement of ~25.5 Å. It is known that both β-silicon and Imma phases of silicon are six coordinated and forms under ~12 and 16 GPa.

A further investigation into the transformed regions A and B shows that in region A, the silicon atoms are six coordinated and have four bonds with an average bond length of ~2.43 Å and two bonds with an average bond length of ~2.58 Å. They are structurally very similar to the β-silicon phase identified in previous studies [2] with small indenters. However, unlike the indentation results described in the previous section, in the present simulation this β-silicon phase is observed at ~12 Å below the maximum indentation depth – not immediately beneath the indenter, and covers a depth of ~25 Å. In region B, although the atoms are six coordinated, their structure is different from β-silicon. A portion of these atoms is shown in Fig. 3. These atoms still maintain a crystalline order.

By monitoring the spatial coordinates of some of these atoms during indentation, we found that they were formed directly from the diamond cubic silicon atoms, rather than from the β-silicon phase, though this region started to appear after the formation of the β-silicon phase in region A.

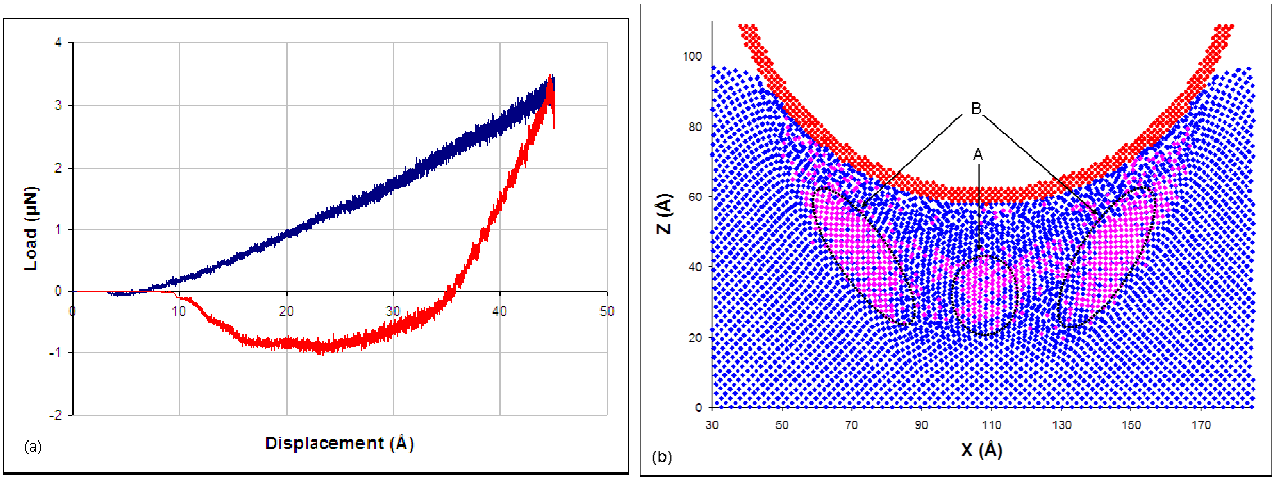

Figure 2. Nano-indentation of silicon with a diamond tip of radius 75 Å: (a) the load–displacement curve, and (b) the snapshot of a portion of the atoms under the maximum indentation depth of 40 Å.

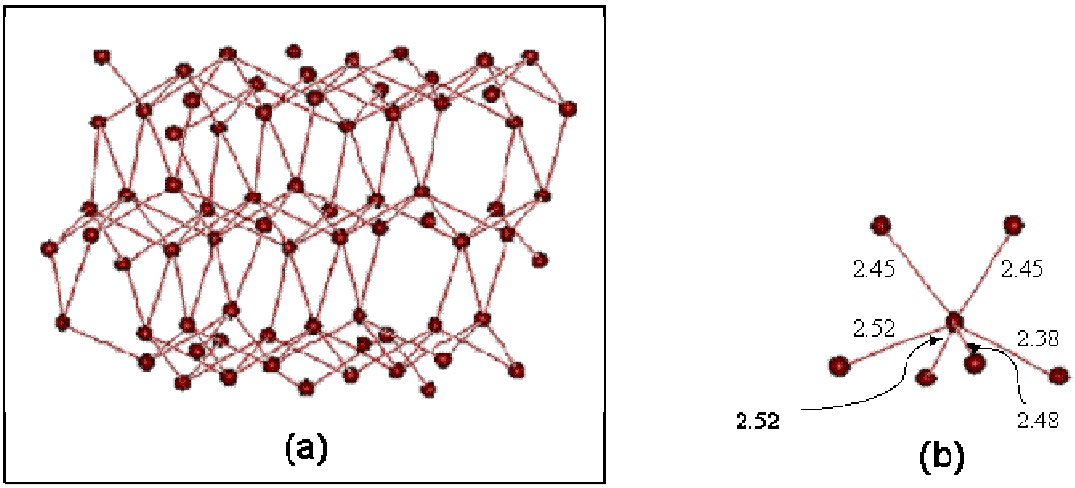

Figure 3. (a) A portion of the atoms in region B, showing the crystalline order and (b) structure of one of the atoms in region B.

On unloading, the small patches of the diamond-like cubic crystalline phase observed in between the indenter and region A grow into a bigger crystalline region C, as shown in Fig. 4, *i.e.* on unloading, the disordered atoms in this region formed a diamond-like crystalline lattice structure due to the nucleation of these crystalline patches. To the authors' knowledge, this have not been observed in previous small scale MD indentation studies, though crystalline patches/particles of silicon were discovered in experimental indentation studies with higher loads and micro-scale indenters [8], identified as the R8/BC8 phases [10]. Moreover, during unloading, the β-silicon phase in region A also lost its crystalline order and changed to amorphous silicon. However, during this change, the six coordination of the material in region B almost maintained, but the material's crystalline order experienced certain variations. A label identification of those six coordinated atoms in region B showed that on unloading, a portion of them changed into amorphous phase and a portion had gone back to initial diamond cubic crystalline state. Fig. 4 shows the amorphous phase and the diamond-like crystalline phase (region C) formed on complete unloading. Evidently, the

indentation with a 75 Å radius tip shows noticeable differences compared to the indentation with a tip of radii 50 Å or less.

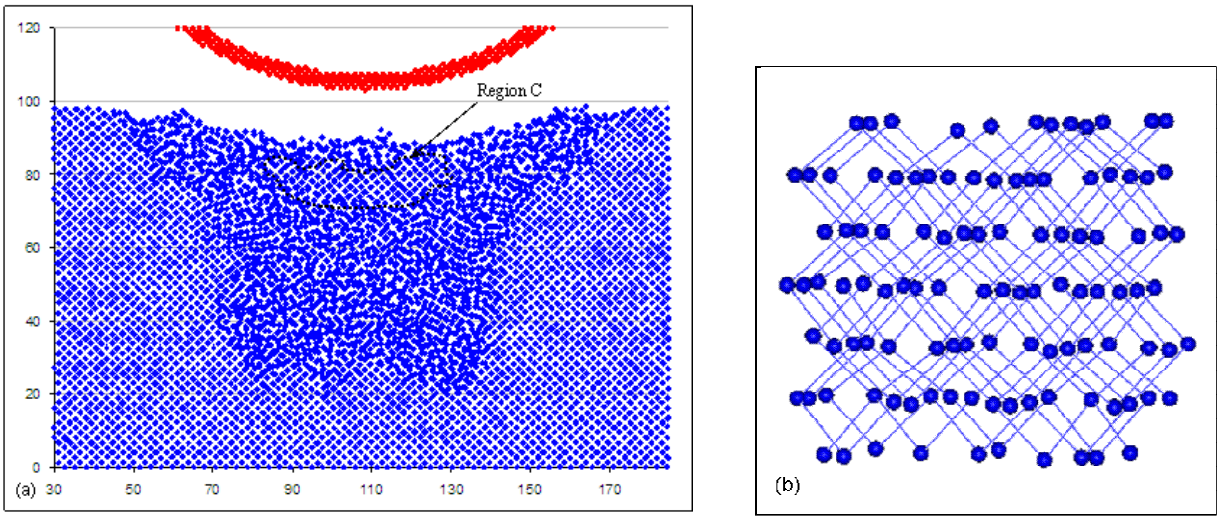

Figure 4. (a) Cross sectional view of a portion of the atomic positions on complete unloading (b) portion of the atomic arrangement in region C.

(c) Indentation with a hemi-spherical indenter of radius 100 Å. In this simulation a bigger silicon sample is indented and a snapshot of a portion of the atomic positions at an indentation depth of 40 Å is shown in Fig. 5(a). Similar to Case (b) discussed in the last section, two different orientations of long-range crystalline order are observed and the β-silicon phase is found at a depth away from the indentation surface. On unloading, a much larger diamond-like cubic crystalline region is observed beneath the indenter tip. Thus the new observations made on increasing the indenter tip radii clearly demonstrate the scale effect.

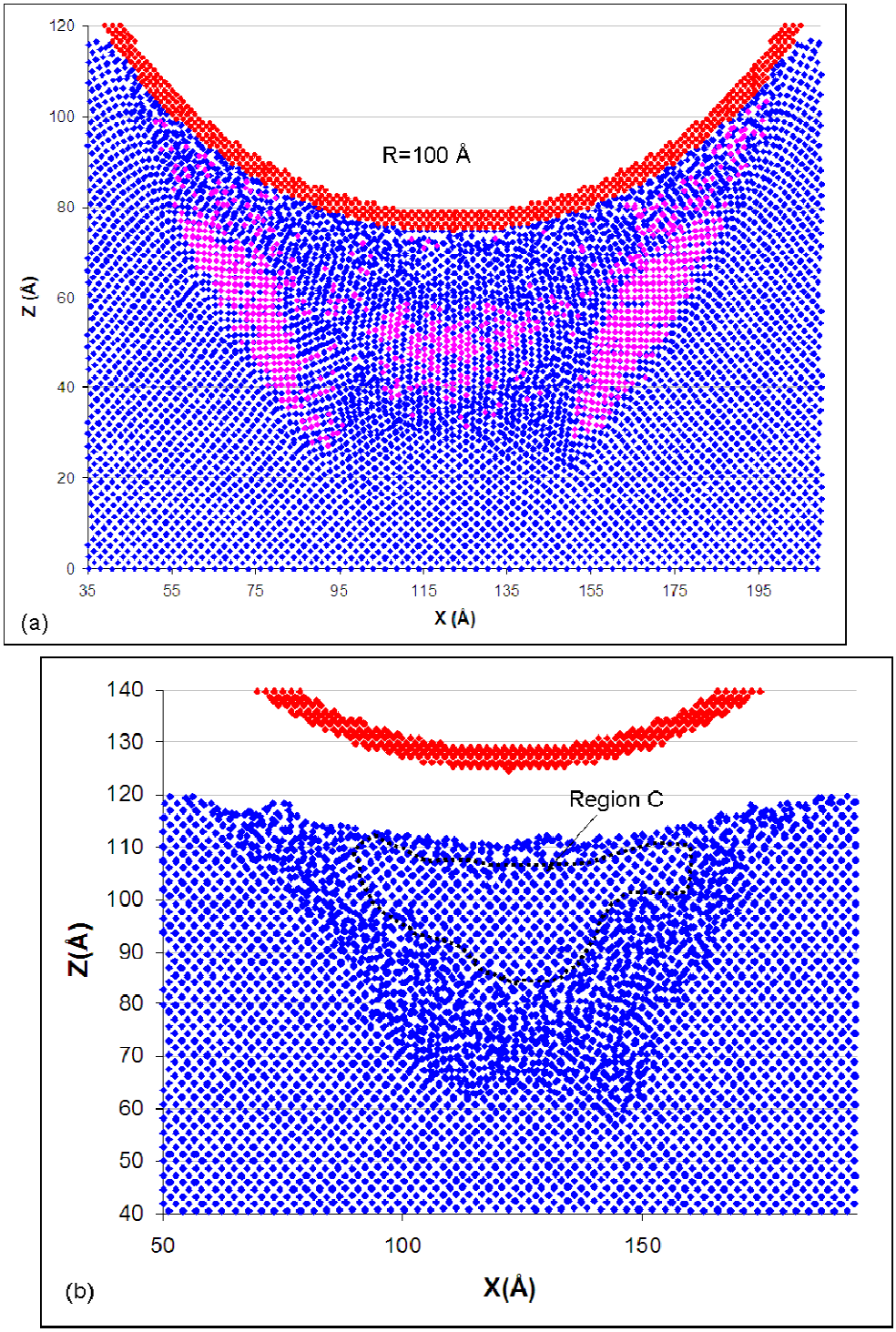

Figure 5. A portion of the cross-sectional view of the atomic positions (a) on indenting big silicon work piece with a 100 Å radius indenter tip; six coordinated atoms are shown in pink colour, (b) after unloading.

Conclusions

The present study on the scale effect of indenter size on the deformation in silicon has shown new mechanisms:

(i) A new six coordinated silicon phase different from β-silicon appears on loading.

(ii) A diamond-like phase of silicon is observed under the indenter on unloading.

Acknowledgement
The authors thank the Australian Research Council for its continuous financial support. This work was also supported by the Australian partnership for advanced computing.

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Advances in Abrasive Technology XI
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