

## Effect of repeated nano-indentations on the deformation in monocrystalline silicon

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The study of a single nano-indentation using molecular dynamics simulation has provided us with much important knowledge on the deformation mechanisms in monocrystalline silicon indentation [1–3]. Previous simulations have shown the phase transformation of silicon from diamond cubic structure to the metallic phase and finally to the amorphous phase during a nano-indentation [2]. A failure criterion to predict this transformation has been laid down [1]. Studies have also achieved an understanding of the overall response of silicon in a complete loading–unloading cycle of nano-indentation. These include the load–displacement relationship, the load–contact area relationship, the number of silicon atoms that have transformed from its original diamond cubic structure to other forms, the volume of the transformed zone, the ratio of the average density of transformed silicon to the density of crystal diamond cubic silicon and the average temperature rise in the specimen during indentation [1].

However, the results obtained from a single indentation are not sufficient to provide a complete understanding of the mechanism of deformation in many processes. For example, in grinding and polishing silicon wafers, the material is actually subjected to repeated tool–workpiece interactions. When the first interaction has created a damaged zone, the material may deform differently under subsequent operations. The purpose of this short paper is to understand how monocrystalline silicon will behave under repeated indentations.

Using the same conditions as the previous simulation [1–3], the molecular dynamics method is used to simulate the behavior of silicon monocrystal under three indentations repeated at the same location with the same speed and maximum indentation depth. Further details about carrying out adequate molecular dynamics simulation can be found elsewhere [1–5].

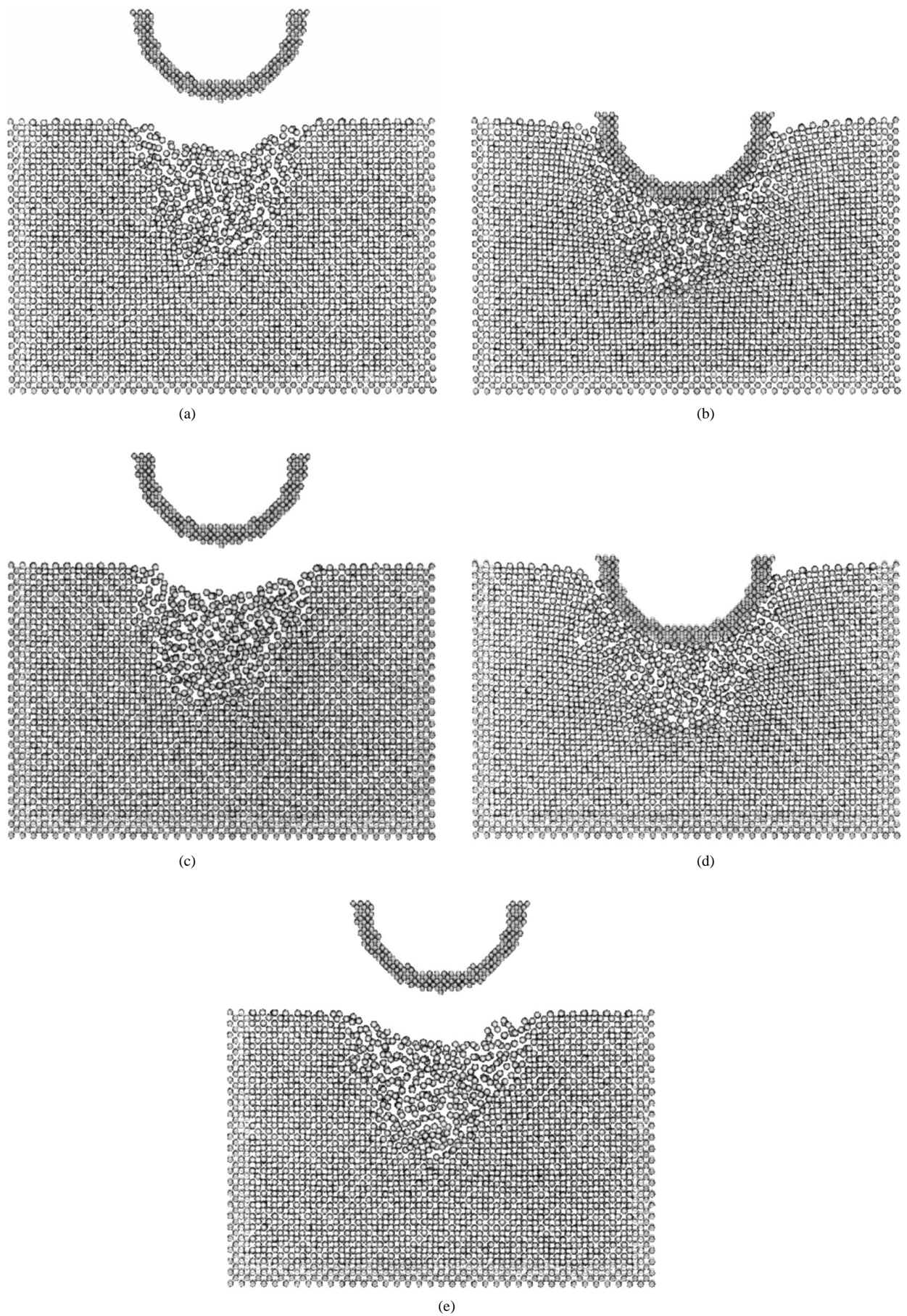
Fig. 1 shows the location of the atoms of a silicon specimen at different stages during the second and third indentations. The big spheres represent the silicon atoms while the smaller ones represent the carbon atoms of the hemispherical diamond indenter. The residual amorphous zone after the first indentation seems to remain amorphous throughout the second and third indentations. There is no significant change in size of the amorphous zone. The residual indentation depths also appear to be consistent after the first, second and third indentations. Fig. 2 shows the volume of the transformed zone during indentation. The loading

and unloading curves for the first, second and third indentations are almost identical to that of the number of transformed silicon atoms during indentation. There is only a small increase in the volume of amorphous silicon owing to the second and third indentations. This supports our earlier claim that the amorphous zone does not increase very much in size even after the second and third indentations.

However, by considering the number of the nearest neighbor atoms, it is observed that there is an increase of atoms with six nearest neighbors during the loading phase of each indentation. This suggests the recovery of the metallic phase from the amorphous phase, mentioned in greater detail in a previous paper [2].

Fig. 3 shows the load–displacement curves for all three indentations. The indentation depths are taken from the same reference, which is the initial untouched surface of the monocrystal silicon. This explains why both the load–displacement graphs for the second and third indentations start at the indentation depth of about 0.6 nm that is the residual depth after the first indentation. The behavior of the second and third indentations are similar to the first in the sense that they too consist of an initial attractive phase between the silicon and carbon atoms when the indenter is brought near the work-piece. This is followed by a phase of increasing load with increasing indentation depth. On unloading, the graphs given by the second and third indentations are also very similar to that of the first indentation. Despite the similarities mentioned above, there are however, significant differences between the load–displacement curve of the first indentation and those of the second and third. Firstly, there is a marked increase in the resistance to the indentation during the loading phase of the second and third indentation because the gradient of the load–displacement curve increases. This is due to the residual stresses acting within the residual amorphous zone after the first indentation to resist the second and subsequent indentations, as shown in Fig. 4.

Secondly, though all three indentations start with an initial attractive phase as mentioned before, it must be noted that the attractive forces between the work-piece and indenter during the second and third indentations are considerably greater than that of the first. This shows that the amorphous silicon atoms experience greater attraction to the diamond indenter compared to diamond-cubic silicon atoms. It should also be noted that the contact area between the work piece and the indenter



*Figure 1* Positions of atoms in a silicon specimen at different stages of the second and third indentations: (a) before the start of the second indentation; (b) at the maximum indentation depth of the second indentation; (c) before the third indentation; (d) at the maximum indentation depth of the third indentation; (e) after the third indentation.

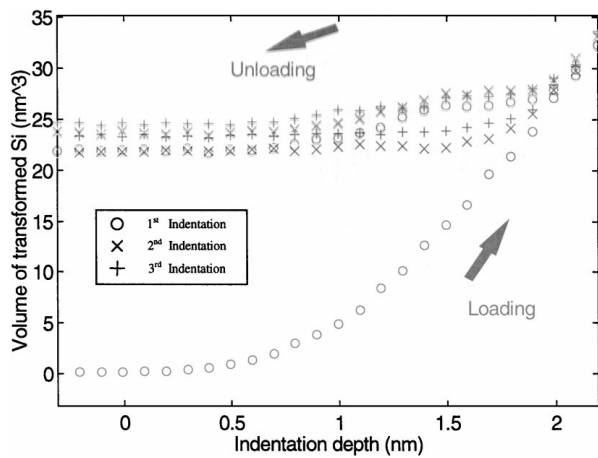


Figure 2 Volume of transformed silicon against indentation depth during repeated indentations.

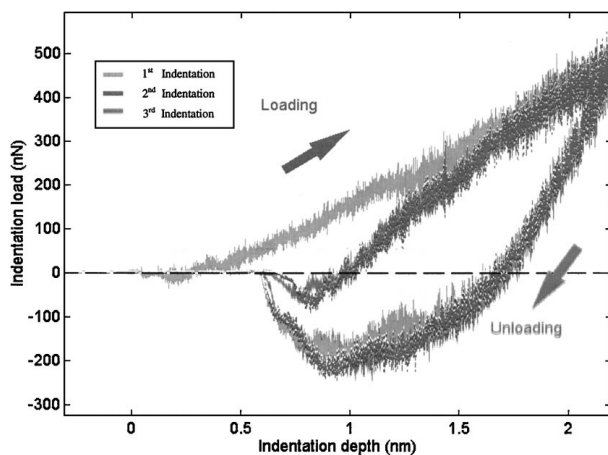


Figure 3 Load-displacement curves of repeated indentations.

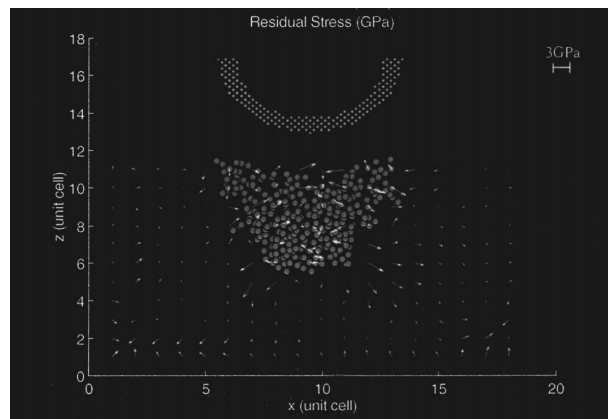


Figure 4 Residual stresses in silicon generated by the first indentation. The larger spots are amorphous silicon atoms and the smaller ones are carbon atoms of the diamond indenter.

is greater for the second and third indentation than that of the first. The load-contact area curves for the three indentations are shown in Fig. 5.

The unloading phases of the load-displacement graphs from the second and third indentations are almost identical to that of the first indentation. This is consistent with a previous claim that there is almost no increase in the residual indentation depth after the second or third indentation.

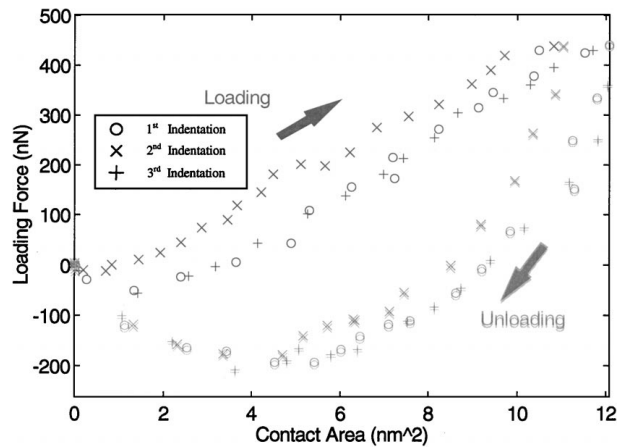


Figure 5 Indentation force against contact area between indenter and silicon specimen.

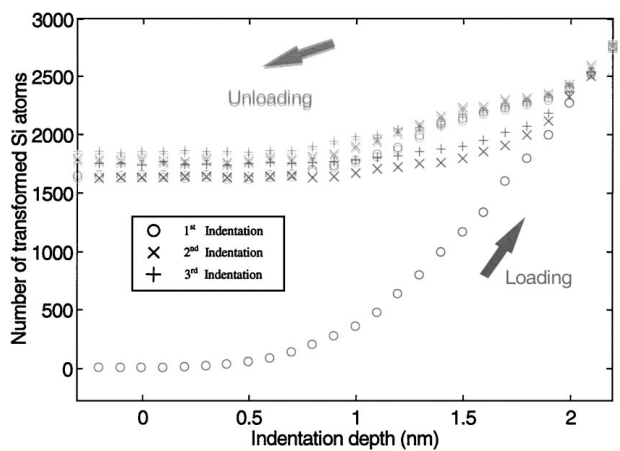


Figure 6 Number of silicon atoms that have transformed from its diamond cubic to other structures against indentation depth.

Fig. 6 shows the number of silicon atoms that have transformed from its original diamond cubic structure to other forms during indentation. Compared to the first indentation where the number of amorphous silicon atoms increases from 0 to 1624, the increase in the number of amorphous silicon atoms in the second and third indentations is very small. For the second indentation, there is merely an increase of 8.6% in the number of amorphous silicon atoms (from 1622 to 1761) and for the third indentation, an increase of only 4.9% (from 1748 to 1834). In fact, considering the loading and unloading graphs shown in Fig. 6, the loading and unloading paths of the second and third indentations almost follow the unloading path of the first. This shows that once the atoms have already transformed to its amorphous state, further indentation does little to change it. The amorphous zone does not change much.

Due to the fact that the increase in the volume of the transformed silicon and the increase in the number of transformed silicon atoms is proportional. The relative density of the amorphous silicon remains almost constant. From Fig. 7, which shows the relative density of the transformed silicon, it can be seen that the relative density of the transformed silicon during the second and third indentation varies in a manner very similar to the unloading phase of the first indentation. This again shows that the second and third indentations do not do much to change the existing residual amorphous region.

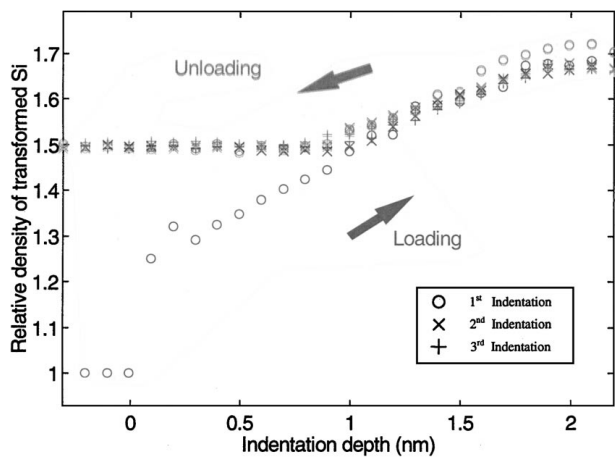


Figure 7 Relative density of transformed silicon against indentation depth.

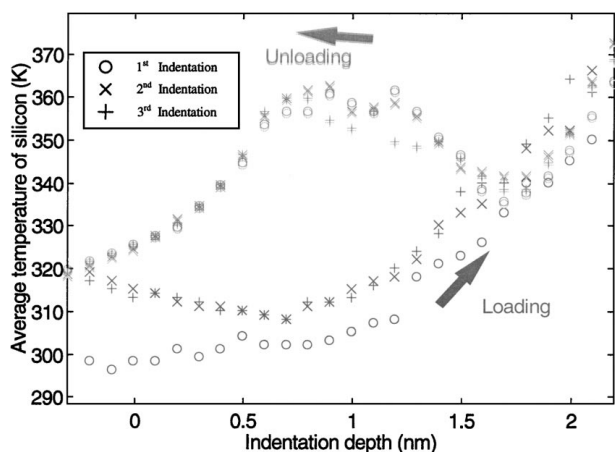


Figure 8 Average temperature of silicon specimen against indentation depth.

Fig. 8 shows the average temperature variation of the silicon work-piece during indentation. Note that the initial drop in temperature is due to the fact that the indenter does not touch the work-piece until it reaches the indentation depth of 0.6 nm (with respect to the reference frame of the first indentation). Once the indenter comes into contact with the work-piece, there is an increase in the temperature of the work-piece due to the micro-structural changes occurring to the silicon work-piece (suspected to be the phase change from amorphous to metallic phase silicon). Upon unloading, the temperature drops initially followed by another increase in temperature. This could be due to micro-structural changes within the silicon as it changes reversibly from the metallic phase back to the amorphous form. The graphs for the first, second and third indentations do not differ greatly from one another.

It has also been found that irreversible plastic deformation in monocrystalline silicon only occurs with

the initiation of the phase transformation from diamond cubic to metallic silicon. The monocrystalline silicon recovers elastically when the indenter is unloaded before the onset of the metallic phase. However, once the transformation occurs, there will be a residual indentation due to the dense amorphous phase that results from the metallic phase upon unloading of the indenter.

**Conclusion.** The above discussion leads to the following understanding of the deformation of silicon under repeated indentations.

1. Repeated indentations of the same depth and speed hardly increase the volume of the residual amorphous zone formed during the first indentation.
2. The relative density of the amorphous zone remains almost constant with repeated indentations.
3. The increase in the number of amorphous silicon atoms due to the second and third indentations is small.
4. Similarities in temperature changes in the silicon specimen suggest that the microstructural phase transformations that occurred during the first indentation may also occur during the second and third indentations.
5. The maximum contact area between the indenter and silicon specimen is greater for the second and third indentations.
6. Residual stresses within the amorphous zone after the first indentation act to resist subsequent indentations.
7. Irreversible plastic deformation in monocrystal silicon only occurs with the initiation of the metallic phase. If the indenter is unloaded before that, the deformation in silicon specimen will recover completely elastically.

## Acknowledgments

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