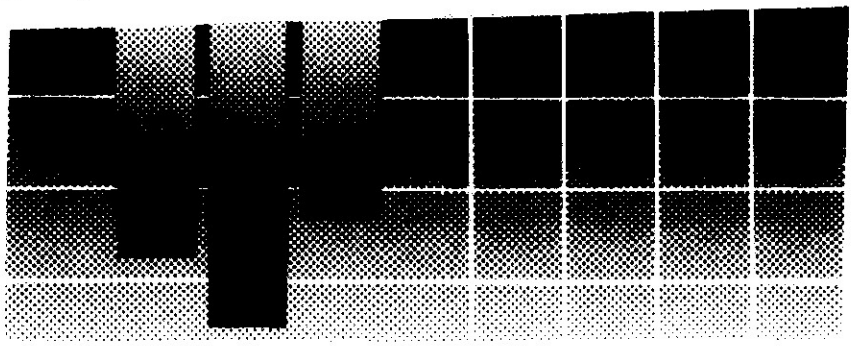

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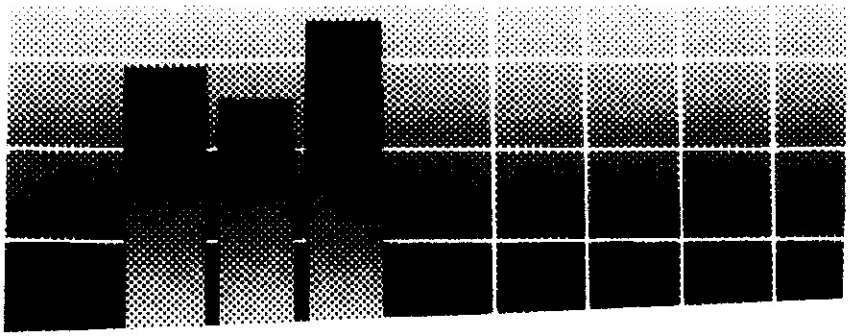

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Monocrystalline silicon subjected to multi-asperity sliding: nano-wear mechanisms, subsurface damage and effect of asperity interaction

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Abstract: Nano-sliding between two surfaces often involves the interaction of many asperities. With the aid of molecular dynamics analysis, this study uses a three-asperity model to investigate the effects of the relative orientation and position of the asperities on the nano-wear mechanism of silicon. It was found that when the first asperity has created a damaged layer, the material would deform differently under subsequent sliding. A thin amorphous layer always remains and there is also an absence of dislocations when the depth of asperity penetration is small. On the other hand, when the asperities are not traversing a damaged zone, the forces experienced by the asperities are independent of their relative positions. The results suggest that the microstructural changes are localized and the initial sliding affects the subsequent deformation over a damaged region.

Keywords: amorphous silicon, asperity interaction, cutting force, diamond cubic silicon, molecular dynamics, multi-asperity, nano-sliding, nano-wear, phase transformation, subsurface damage.

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1 Introduction

The micro-/nano-tribological studies are needed to develop fundamental understanding of interfacial phenomena on a small scale and to study the interfacial phenomena in micro- and nano-structures used in magnetic storage systems, MEMS, and other industrial applications. The components used in micro- and nano-structures are very light (on the order of a few micrograms) and operated under the loads on the order of a few micrograms to a few milligrams. As a result, friction and wear on a nanoscale of lightly loaded micro-/nano-components are highly dependent on the surface interactions among few atomic layers.

Emerging technologies such as atomic force microscopy and other surface force methods have opened the possibility to study friction and wear phenomena on a molecular scale and to measure frictional forces between contacting molecules at the nano-newton level. Increased computational power has also made it possible to study nano-friction and the associated phenomena by molecular dynamic simulations and to investigate the atomic-scale contact mechanisms. Some aspects of these complex nano-physical phenomena have been investigated. An example is the friction that arises from slippage between solid-to-solid interfaces and between closely packed films in contact sliding. However, we are only at the very beginning of the understanding of the nano-mechanical tribological origin.

At the interfaces of technological innovations, contact occurs at multiple asperity contacts. Previous studies of a single sliding asperity using molecular dynamics simulation has provided us with important knowledge on the deformation mechanisms of friction and wear of monocrystalline materials [1–3]. Results obtained, however, are not sufficient to provide a complete understanding of the mechanism of deformation in many processes, because in a nano-system, a surface subjected to contact sliding is actually under multi-asperity interactions. When the first interaction has created a damaged zone, the material may deform differently in subsequent operations. The present study tends to take the previous research a step further by considering not only the effects of sliding over a damaged region but also the extent of the effects due to different configurations of the sliding asperities.

2 Modelling

The present mechanics model consists of three spherical diamond Asperities, A, B and C, sliding on an atomically smooth silicon surface, as illustrated in Figure 1.

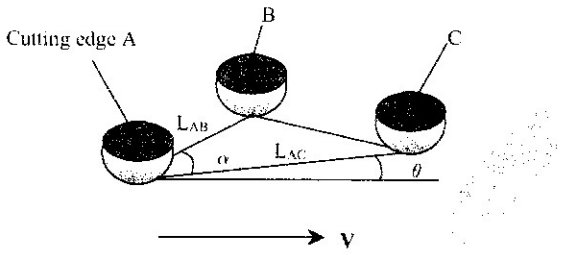


Figure 1 General mechanics model for multi-asperity cutting.

Their relative positions and orientations are defined by their distances, L_{AB} and L_{AC}, and angles with respect to the sliding direction, α and θ. Three cases are of our particular interest. These are (I) $\alpha = \theta = 0°$ with $L_{AB} < L_{AC}$, representing a repeated single-asperity sliding so that the effect of residual subsurface damage can be understood, (II) $\alpha = 0°$ and $\theta = 90°$ with $L_{AB} = L_{AC}$, standing for the interaction of two parallel asperities, and (III) $\alpha = 45°$ and $\theta = 45°$, indicating the case with parallel sliding asperities coupled with an interaction from a third asperity. Since diamond is much harder than silicon, the asperities are modelled as rigid spheres. These spheres slide across the silicon surface at a specified velocity 40 m/s. The maximum depth of cut is 1.0 nm.

Figure 2 shows a molecular dynamics representation of the three configurations described above. The dimensions of the moving control volume of the silicon specimen in Figures 2(a), 2(b) and 2(c) are chosen respectively as 24.435 nm × 9.231 nm × 4.34 nm containing 60, 446 silicon atoms, 13.575 nm × 19.791 nm × 4.34 nm containing 57,007 silicon atoms and 19.005 nm × 14.661 nm × 4.34 nm containing 63,433 silicon atoms. These control volume sizes are large enough to eliminate the boundary effect. Boundary and thermostat atoms are used to cancel rigid body motion of the silicon specimen and ensure reasonable heat conduction from the moving control volume respectively. Layers of boundary atoms and thermostat atoms are arranged to surround the Newtonian atoms of silicon in the control volume except its top surface that is subjected to asperity sliding.

For covalent systems such as silicon, the directionality of bonding is important. Tersoff [4, 5] proposed a simple pair-like potential where the bond order of the atoms is affected by its local environment. This replaces the two- and three-body potential conventionally employed when directionality of bonding is a concern. Based on empirical data, Tersoff [5] also verified that the Tersoff potential is capable of predicting stable phases of diamond cubic silicon and body-centred tetragonal

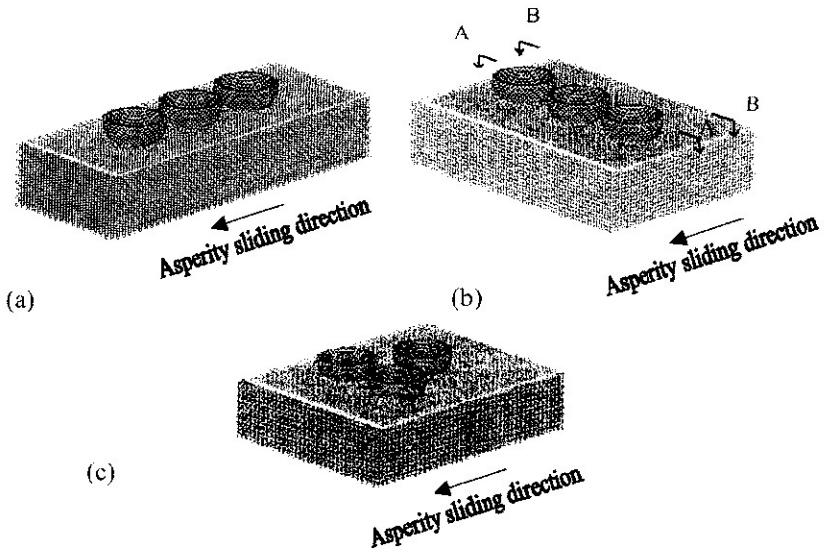


Figure 2 Molecular dynamics representation of the models (a) Configuration I, (b) Configuration II, and (c) Configuration III.

β-silicon. Hence Tersoff potential is used in the present simulation to dictate the interaction between the silicon atoms. Morse potential is employed to describe the interactions between silicon and diamond atoms [1, 6]. In addition, based on careful considerations, it was found that the most appropriate equations for temperature conversion from the kinetic energy of an atom are the Debye equation for silicon and Einstein equation for diamond [7]. These equations are therefore used correspondingly in the present temperature conversion. As in previous simulations of silicon workpiece with carbon tool or asperity [1, 6, 8], the time step used for the molecular dynamics simulation is 2.5 fs.

3 Results and discussion

For each configuration of the asperities mentioned in the previous section, the following factors will be examined and discussed: (i) Mechanism of wear of silicon workpiece and, (ii) Phase transformation.

3.1 Mechanism of wear

The general mechanisms of wear of silicon specimens under all the asperity configurations are found to be the same as those described by Zhang and Tanaka [1, 2] when only a single asperity was involved. That is, as the penetration depth of an asperity increases, the mechanism of wear progresses from no-wear to adhering, ploughing and finally cutting. Deformation without wear happens at an extremely small penetration depth when the atomic lattice of silicon deforms purely elastically. By increasing the penetration depth, adhering takes place. Some surface atoms stick to the asperity surface and move together with it to cause wear. When the penetration depth is further increased, ploughing, characterized by an atomic cluster being pushed to move with the asperity, is observed. Finally cutting occurs upon further increment in the penetration depth, characterized by chip formation. Figure 3 shows these general wear characteristics obtained from present simulation.

3.1.1 Configuration II and III

In the cases of Configurations II and III, the asperities do not retrace the damaged zones. At the depth of cut of 1.0 nm, the wear mechanism observed is that of cutting. The plastic deformation due to the sliding asperities is very localized. Figure 4(a) shows a cross-section of the silicon workpiece through the centre of the asperities (Section A-A of Figure 2(b)). It can be seen that there is almost no subsurface damage to the silicon workpiece between the two asperities. Figure 4(b) shows a cross-section of the damaged zone of the silicon workpiece behind the asperities (Section B-B of Figure 2(b)). It is obvious that plastic deformation on the nanoscale is very localized and occurs beneath the asperities. There is little plastic deformation to the sides of the Asperities and therefore little interaction among Asperities A, B and C in terms the mechanism of wear.

As in nano-indentation [8], the sliding Asperities A, B and C also create trails of subsurface amorphous layer in the damaged zones, see Figure 5. Phase transformation of silicon occurs at the leading edge beneath the sliding asperity resulting in the formation of amorphous chips and an amorphous trail along the path traversed by

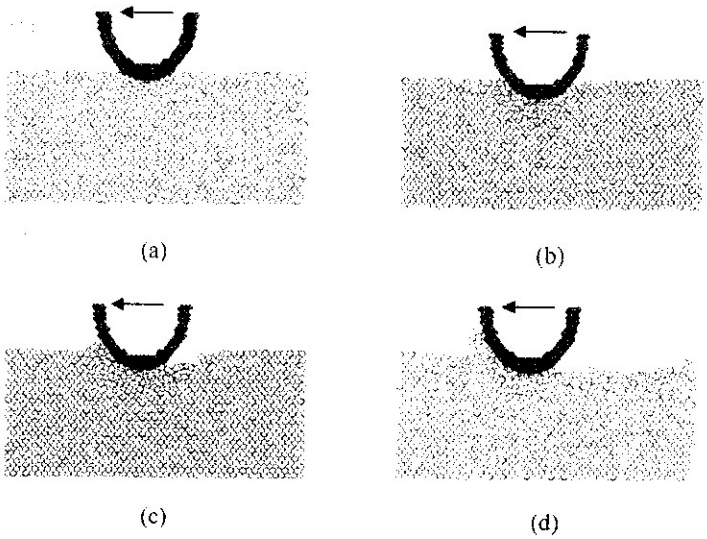


Figure 3 General wear characteristics of an diamond asperity sliding on the (100) silicon surface. (a) No wear, (b) Adhering, (c) Ploughing, and (d) Cutting.

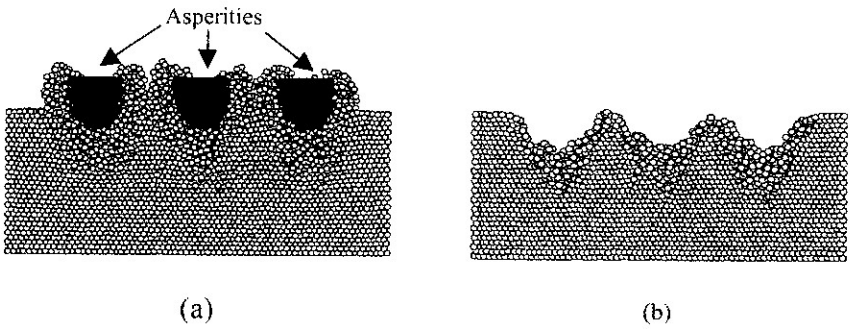


Figure 4 Subsurface damage. (a) Cross-section of the silicon workpiece (Section A-A of Figure 2(b)), and (b) Cross-section of the damaged zone of the silicon workpiece (Section B-B of Figure 2(b)).

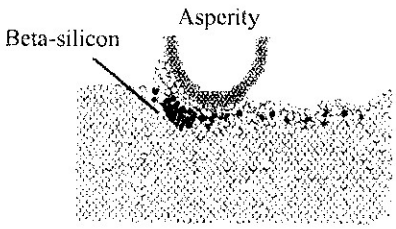


Figure 5 A typical cross-sectional view of Asperities A, B and C in Configuration II. The light coloured circles represent atoms with coordination number 4 and the dark ones represents β-silicon atoms with coordination number 6.

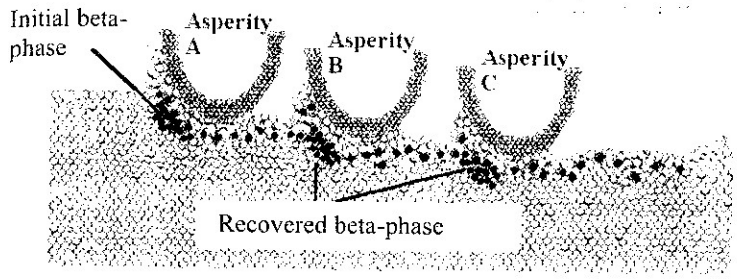


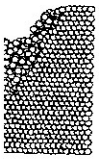
Figure 6 The cross-sectional view of Asperities A, B and C in Configuration I. The light coloured circles represent atoms with coordination number 4 and the dark ones represent β-silicon atoms with coordination number 6.

the asperities. Dislocations are absent at this particular depth of cut. This suggests that the plastic deformation is solely due to phase transformation that will be discussed later.

(100) silicon surface.

3.1.2 *Configuration I*

In this case, the second and third Asperities B and C retrace the damaged path caused by Asperity A (Figure 6). Therefore, the cutting mechanism involved in the first and the following two asperities are very different. Asperity A cuts the silicon workpiece in the same manner as the case of a single sliding asperity, causing phase transformation of the original diamond cubic silicon. Asperity B, however, ploughs through the residual amorphous layer in the wake of Asperity A. No further phase transformation occurs but the amorphous silicon atoms are pushed away as the asperity ploughs through. It should also be noted that the depth of cuts of Asperities A, B and C are maintained as a basis for comparison. The effects of this differing sliding mechanism will be discussed in the following sections.



A-A of Figure 2(b)).
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3.2 *Phase transformation*

As mentioned, something apparent in the silicon workpiece in all the three configurations is the formation of an amorphous subsurface layer in regions traversed by the diamond asperities. This is analogous to the amorphous damaged zone due to nano-indentation. Hence it is worthwhile to draw comparisons and predict the process of phase transformation based on results obtained from nano-indentation [8].

3.2.1 *Configurations II and III*

Wear of silicon via cutting is achieved by chipping the amorphous silicon. By considering the exact coordinates of the silicon atoms, it is found that the transformation mechanism is similar to that of nano-indentation [8–10]. Diamond cubic silicon first transforms into its β-silicon and then upon the removal of stresses, the β-silicon transforms into an amorphous phase. This explains the trail of subsurface amorphous silicon in the damaged zone behind each sliding asperity. The mechanism of phase transformation is reflected in the coordination numbers

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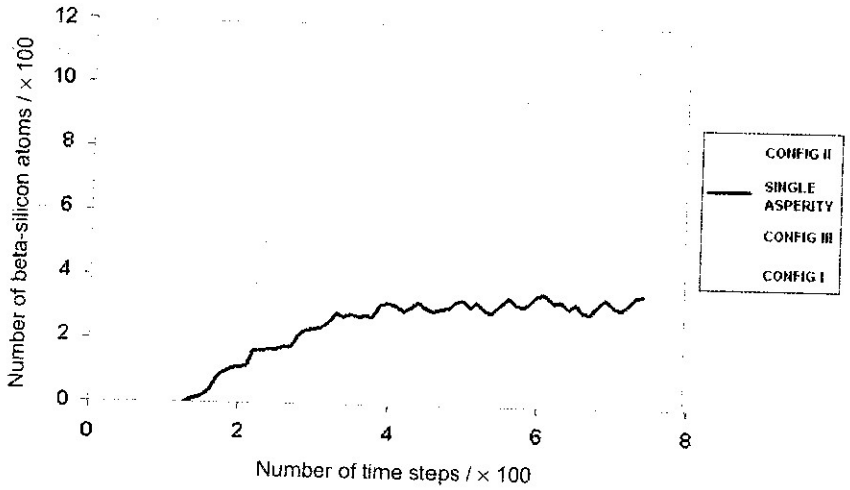


Figure 7 The number of 6-coordinated β-silicon atoms in Configurations I, II and III compared to that with a single asperity.

of atoms near the regions beneath the asperities. It can be seen that a cluster of six-coordinated body-centred tetragonal β-silicon atoms indicated by darken circles (Figure 5) forms near the leading edge beneath each asperity. Four-coordinated diamond cubic silicon transforms to its six-coordinated β-silicon form due to the stresses induced by the asperity. When the stresses are removed as the asperity slides past, the atoms transforms into an energetically more favourable amorphous form. The coordination number of the silicon atoms in the trailing amorphous region is mostly equal to four. Therefore, as the asperity slides across the silicon workpiece, diamond cubic silicon continuously transforms into β-silicon beneath the asperity and then transforms into amorphous silicon when the asperity passes, leaving a layer of subsurface amorphous silicon in its wake.

Figure 7 shows the number of β-silicon atoms formed during the cutting process with asperity Configurations I, II and III. The number of β-silicon in Configurations II and III are three times that of a single asperity cutting process. This indicates that the formation of β-silicon is highly stress state dependent [12] and occurs only beneath the three asperities. Although regions between the asperities are compressed due to the proximity of the asperities, it is likely that β-silicon do not form because of the absence of the required stress states and that is why there is no amorphous silicon in the zone between asperities.

3.2.2 *Configuration I*

Asperity A in this configuration cuts the silicon workpiece in very much the same way as in the other two configurations described above. The asperity cuts through the diamond cubic silicon leaving behind a trail of subsurface amorphous silicon. However there is a vast difference in the silicon phase tranformation involved due to Asperities B and C, which represents subsequent cuts into the amorphous zone. In the present case, the six-coordinated atoms also form beneath Asperities B and C (dark circles in Figure 6). This implies that the β-silicon phase is recoverable from the

amorphous phase provided that the required stress field is achieved. It must be noted that only some of the β-silicon is recovered as Asperity B and C retraces the amorphous damaged zone. That is why the number of β-silicon atoms in Configuration I is slightly less than that of Configuration II and III (Figure 7). This agrees with the authors' previous findings on nano-indentation that the transformation of silicon from its β-phase to the amorphous phase is reversible [8, 11, 12].

3.3 Cutting force

Figure 8 shows the force experienced by each asperity in different configurations.

3.3.1 Configurations II and III

In Configuration II and III, there is no interaction between the cutting zones around the asperities in the direction of cut. This is because the mechanism of wear on the nanoscale is very localized as explained before. As a result, the cutting force experienced by the Asperities A, B and C is similar to that of a single sliding asperity, averaged at around 150 nN (Figure 8(a)). Similarly, in Configuration III, all asperities behave like that of single sliding asperity as there is no interaction between the cutting zones (Figure 8(b)).

3.2.2 Configuration I

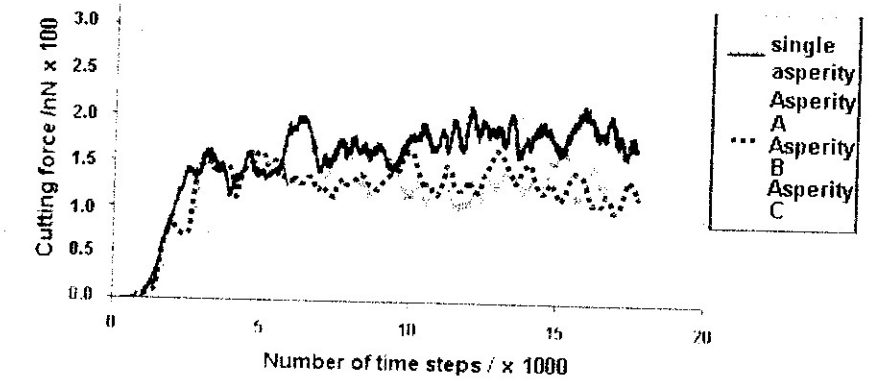
In this case, however, Asperities B and C experience a lower cutting force, around 125 nN, compared to that of Asperity A, which is around 150 nN. This shows that the asperity cutting through amorphous silicon experience less resistance compared to the cutting through diamond cubic silicon. It is interesting to note that in the case of repeated nano-indentations, residual stresses within the amorphous zone after the first indentation act to resist subsequent indentation [11]. However, this is not the case in the present sliding simulation, where subsequent cuts experience less resistance. Nevertheless, there is little difference in the cutting forces experienced by Asperities B and C which represent the second and third cuts respectively (Figure 8(c)).

4 Conclusions

The above discussion leads to the following understanding of the wear of monocrystalline silicon under multi-asperity sliding on the nanometre scale:

1 The mechanism of cutting proceeds from no-wear to adhering, ploughing and finally cutting as the depth of asperity penetration increases. This is aligned with single asperity sliding.

2 The effect of asperity and workpiece interaction is very localized at the asperity penetration depth of 1.0 nm and hence interactions between the asperities do not affect the mechanism of wear. The only situation where the mechanism of wear of asperities affect each other is when they retrace a damaged zone traversed by a previous asperity.



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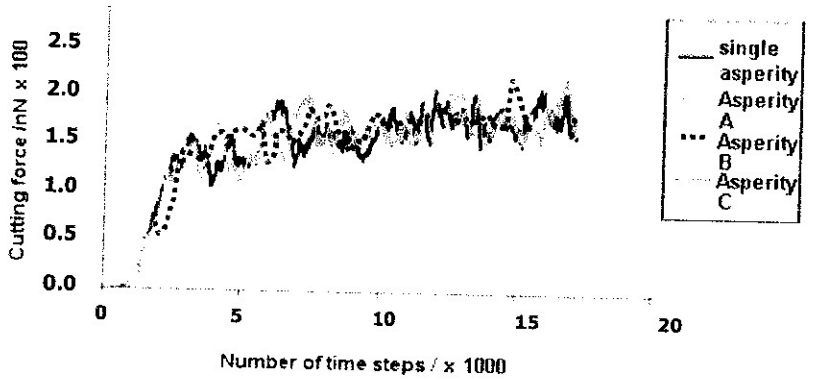

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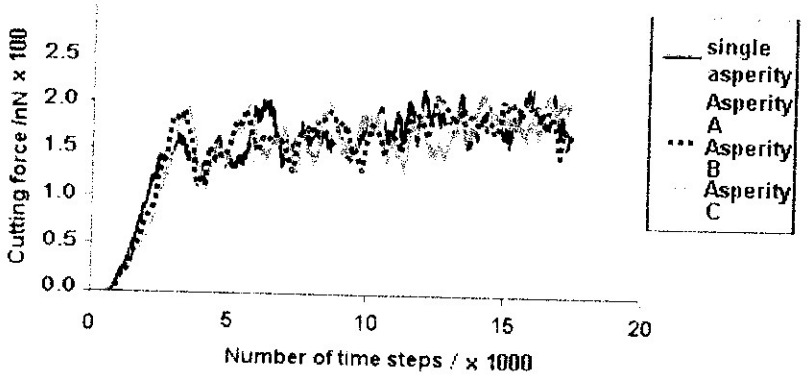

(c)

Figure 8 Cutting force vs. time. (a) Configuration I, (b) Configuration II, and (c) Configuration III.

3 Plastic deformation of silicon is a result of phase transformation. There are no dislocations observed. When an asperity cuts through diamond cubic silicon, stress-induced phase transformations occur and diamond cubic silicon transforms

to β-silicon beneath the asperity. At the trailing edge of the sliding asperity, the β-silicon transforms into amorphous silicon upon the removal of stresses as the asperity slides past. This results in a trial of subsurface amorphous layer in the damaged zone behind the asperity.

4 Asperities cutting through the amorphous layer in a damaged zone experience less resistance compared to the asperities cutting through diamond cubic silicon.

5 Acknowledgements

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