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Friction and Wear Simulation of Suspended Silicon Asperity Moving over a Plate at Microscale

Sung-San Cho, Jung Soo Kim and Seungho Park*

Department of Mechanical & System Design Engineering, Hongik University, Seoul 121-791, Korea

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Abstract : A suspended hemispherical silicon asperity moving over a silicon plate was simulated. The simulation results on friction and wear in the interface between the two can help obtain more durable miscroscale structures. Silicon structures were constructed with Tersoff three-body potential. Dependence of friction and wear of the asperity on both the atomic arrangement in the plate and the moving direction was investigated under the condition that the asperity is subject to the attractive normal force due to the plate. The results show that the variation of friction force with the movement of asperity, and the occurrence of adhesive wear are attributed to the formation and rupture of adhesive junction between the asperity and the plate. The friction force and wear are smaller when the asperity is incommensurate with the plate, and they also depend on the moving direction of the asperity over the plate.

Key words: commensurate surface, friction, molecular dynamics simulation, silicon asperity, tersoff potential, wear

1. Introduction

Friction and wear adversely affect the performance and durability of micro systems such as MEMS [1-3], and can lead to premature failure, thus compromising safety. In micro systems that are characterized as large surface-to-volume ratio and extremely light contact load, friction and wear depend significantly on surface interaction forces at the atomic level rather than the contact load. Hence, in-depth understanding of the atomic-scale friction and wear are needed for development of micro systems.

Experimental studies have revealed some interesting characteristics of atomic-scale friction and wear. Friction forces can be generated even at zero normal load [4], indicating the significance of surface interaction forces in atomic-scale friction. Meanwhile, friction forces completely vanish when sliding contact occurs between atomically clean incommensurate surfaces [5]. However, significant friction forces are produced in air because of absorbed layers on the contact surfaces [6].

Theoretical studies have been conducted using molecular dynamics (MD) simulation that overcomes the difficulties in performing experiments under controlled conditions. These studies confirmed the experimental observations [7-9], and provided further knowledge as follows. When the indentation depth of asperity is extremely small so that the substrate is deformed elastically, wear does not occur although friction forces are generated [10]. At appreciable indentation depths, friction forces depend on substrate orientation and sliding direction [11]. When an asperity slides on incommensurate substrate, structural transformation occurs at the adhesive junction, leading to wear [12].

In most previous studies the material of asperity or tip differs from that of substrate, and the contact load is compressive or almost zero. However, micro systems are usually made of single material such as silicon. Moreover, some moving components are designed to suspend over the adjacent surfaces with a narrow gap so that the components are subject to the attractive normal force. Unfortunately the friction and wear in this case has been scarcely investigated.

With the assumption that surfaces of microstructures consist of atomic-scale asperities whose shape can be modeled as hemispheres, this paper investigates the friction and wear of a suspended atomic-scale hemispherical asperity moving over the plate using the classical MD simulation technique. The simulation intended to reveal the dependence of friction and wear of the asper-

*Corresponding author: spark@hongik.ac.kr

ity on both the atomic arrangement in the plate and the moving direction under the condition that the attractive normal force acts between the asperity and the plate.

2. Molecular Dynamics Simulation Model

A classical MD simulation model has been constructed for a suspended hemispherical silicon asperity moving over a silicon plate as shown in Fig. 1. The asperity of diameter 53 Å is composed of 2080 atoms and is attached to the lower part of upper plate that is parallel to the lower plate. There is a gap between the asperity and the lower plate such that the lower plate exerts attractive force on the asperity. The plane in the upper plate and the asperity that is parallel to the top surface of the lower plate is (001) while the top surface of lower plate is either (001) or (111). That is, the asperity is commensurate with the lower plate when the lower plate is (001), and incommensurate when the lower plate is (111). It is assumed that both the lower and upper plates are rigid in order to focus on the friction and wear associated with the asperity.

The diamond structure of silicon was constructed with the Tersoff three-body potential [13] that incorporates the cut-off function into Morse potential for two-body system and modifies the repulsive term to consider three-body interaction. The Tersoff potential function is given as follows:

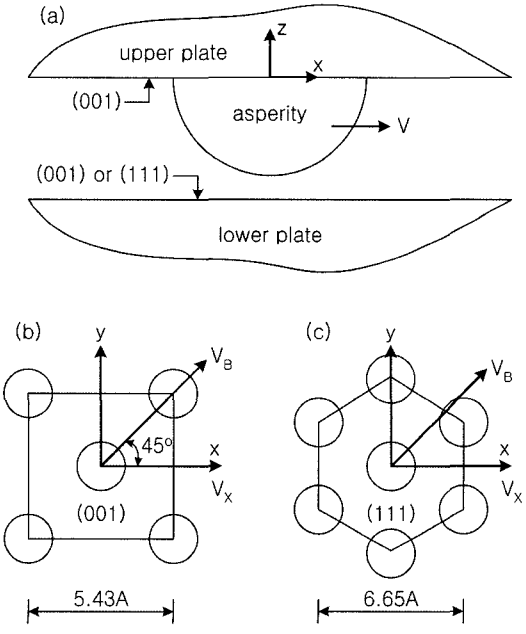


Fig. 1. (a) Schematic representation of an asperity moving over a plate. The asperity moves in either V_X or V_B direction over (b) (001) or (111) lower plate.

$$\Phi_{ij} = f_C\left[f_R(r_{ij}) + b_{ij}f_A(r_{ij})\right] \tag{1}$$

$$f_R(r_{ij}) = A_{ij}\exp(-\lambda_{ij}r_{ij}) \tag{2}$$

$$f_A(r_{ij}) = -B_{ij}\exp(-\mu_{ij}r_{ij}) \tag{3}$$

$$f_C(r_{ij}) = \begin{cases} 1 & :r_{ij} \le R_{ij} \\ \frac{1}{2} + \frac{1}{2}\cos\left[\frac{\pi(r_{ij}-R_{ij})}{S_{ij}-R_{ij}}\right] & :R_{ij} < r_{ij} < S_{ij} \\ 0 & :r_{ij} \ge S_{ij} \end{cases} \tag{4}$$

$$b_{ij} = \chi_{ij}(1 + \beta_i^n\zeta_{ij}^n)^{-1/(2n)} \tag{5}$$

$$\zeta_{ij} = \sum_{k \ne i,j} f_C(r_{ij})g(\theta_{ijk}) \tag{6}$$

$$g(\theta_{ijk}) = 1 + \frac{c_i^2}{d_i^2} - \frac{c_i^2}{d_i^2 + (h_i - \cos\theta_{ijk})^2} \tag{7}$$

where r_{ij} is the distance between two silicon atoms, i and j, and q_{ijk} is the angle made by the third atom k with atoms i and j. The constants in the Tersoff potential function for silicon are A_{ij}=1830.8eV, B_{ij}=471.18eV, λ_{ij}=0.24799 nm^{-1}, μ_{ij}=0.17322 nm^{-1}, χ_{ij}=1.0, β_{ij}= 0.0000010999, n=0.78734, c_i=100390, d_i=16.217, h_i= -0.59826, R_{ij}=0.27 nm, and S_{ij}=0.30 nm. Fig. 2 shows variation of Tersoff potential energy with both the distance r_{ij} and the angle θ_{ijk}. It is noted that the equilibrium distance between two atoms is significantly influenced by the position of the adjacent atom.

Motion of atoms is determined with the Tersoff potential function and the Newton's equations of motion

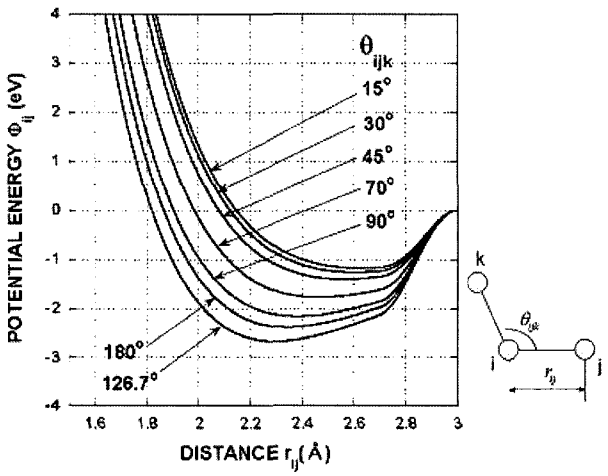


Fig. 2. Tersoff 3-body potential model for silicon.

given by,

$$F_i = -\sum_{j \neq i}^{n} \frac{\partial \Phi(r_{ij}, \theta_{ijk})}{\partial r_i} = m_i \frac{d^2 r_i}{dt^2} \quad (8)$$

In this study equation (8) was solved numerically using the Gear Predictor-Corrector algorithm[14] with a time step of 2 fs and average temperature of the structure is kept constant (300 K) by the momentum scaling method. In order to examine the accuracy of the silicon model, elastic modulus was calculated through a simple tension test. The results was 130.186, 169.103, and 187.810GPa in <100>, <110> and <111> directions, respectively, which are in good agreement with the published results [15], 130.608, 167.791, and 187.105GPa. This implies that the present silicon model is reliable to investigate the various microscopic phenomena.

3. Results and Discussion

3.1 Adhesion

Since the adhesion strength between the asperity and the lower plate has strong influence on the friction and wear of the asperity, the dependence of adhesion strength on the atomic arrangement in the lower plate is investigated. Fig. 3 shows the variation of forces exerted on the asperity by the lower plate while the lower plate approaches and then draws away from the asperity. The lower plate moves 10Å during the approach and then 30Å during the withdrawal at a speed of 1Å/ps. The normal force F_z varies drastically while the forces in the x-y plane F_x and F_y vary marginally. The marginal variations of F_x and F_y are attributed to the axisymmetric shape of asperity. There is no normal force at the beginning of approach because the gap between the asperity and the lower plate is greater than the cut-off distance. During the approach the asperity is subject to the attractive (positive value) normal force for a very short period of time, and then subject to the repulsive (negative value) force, the strength of which increases rapidly. During the withdrawal, the magnitude of repulsive force diminishes rapidly and then the force becomes attractive. The attractive force increases to a maximum value and then vanishes.

In addition, Fig. 3 shows the difference in the forces for (001) and (111) lower plates. When the lower plate is (001), i.e., when the lower plate is commensurate with the asperity, the repulsive force during the approach is weaker and the attractive force during the withdrawal is stronger than when the lower plate is (111). Hence, it is concluded that the adhesion is stronger when the asperity is commensurate with the lower plate.

Fig. 4 shows the snapshots of molecular distribution at the elapsed time of 30ps (displacement of –10Å) in Fig. 3 for two different lower plates. Adhesive junction between the asperity and the lower plate is being ruptured with a formation of neck, and some atoms of the asperity transfer to the lower plate. Both the number of atoms in the adhesive junction and the number of transferred atoms are greater when the lower plate is (001) than (111). These snapshots are evidences for the strong adhesion between the commensurate surfaces.

3.2 Friction and Wear

Fig. 5 shows the variation of forces acting on the

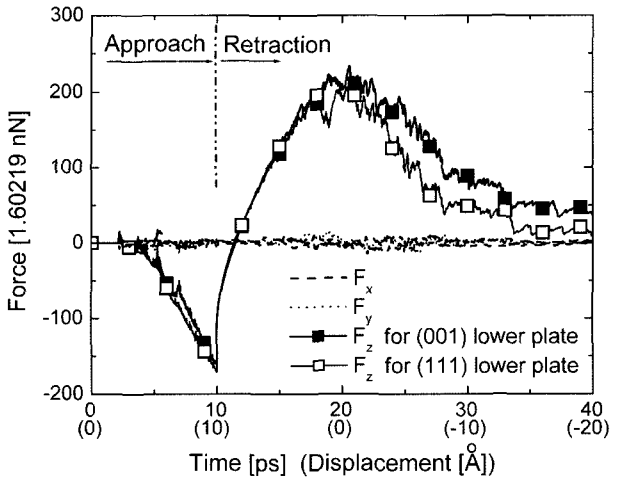


Fig. 3. Interaction forces during approach and withdrawal.

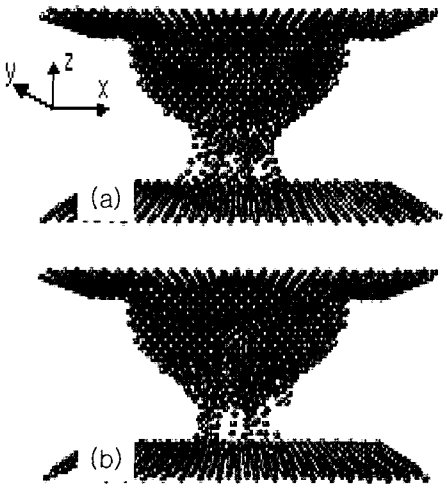


Fig. 4. Snapshots of molecular distribution during withdrawal. Top surface of lower plate is (a) (001) and (b) (111).

(001) asperity while the asperity moves horizontally over the stationary (001) lower plate. The asperity moves in the x-axis direction, i.e., [100] direction in the (001) plane (direction V_X in Fig. 1(b)). There is a gap (2.0Å or 2.4Å) between the asperity and the lower plate at the beginning of horizontal movement such that the lower plate exerts the net attractive normal force on the asperity. This simulation was conducted with the following steps. At the first step, the silicon structure of the asperity and the plates were constructed, and then an equilibration period of 100ps was allowed. At the second step, the lower plate was approached to the asperity until the gap reached the desired value (2.0Å or 2.4Å), and then an additional equilibration period of 100ps was allowed. At the final step, the asperity was moved horizontally while the lower plate is at rest.

The asperity is subject to the attractive normal force F_N during the horizontal movement of the asperity. Its magnitude, although it fluctuates, increases during the early period, and then decreases with the horizontal movement of the asperity. The traction force in the moving direction F_T exhibits the similar variation to the force F_N. Meanwhile, the lateral force F_L, which is normal to F_T in the x-y plane, keeps changing its direction although its variation is marginal. These characteristic variations of forces are not altered with the change in the initial gap, but the magnitude of forces are affected.

Fig. 6 shows the snapshots of molecular distribution at various moving distances in Fig. 5. At the beginning of movement, the atoms of asperity are clearly distinguished from those of the lower plate. At the moving distance of 10Å, however, the adhesive junction is formed so that the distinction is somewhat vague near the bottom of the asperity. At the moving distance of 20Å, larger gap is observed at the leading edge, and some atoms of the asperity are transferred to the lower plate at the tailing edge. With farther movement, the region of larger gap extends from the leading edge to the tailing edge, and more atoms are accumulated at the tailing edge. The result of atom transfer is the adhesive wear. Hence, it is argued that the initial increase in the normal and traction forces are associated with the formation of adhesive junction, and the decrease in the forces results from the extension of area with larger gap with the movement of asperity. Meanwhile, it is conjectured that the marginal variation of the lateral force is due to the almost symmetric arrangement of atoms in the adhesive junction with respect to the x-z plane (refer to Fig. 1(a)).

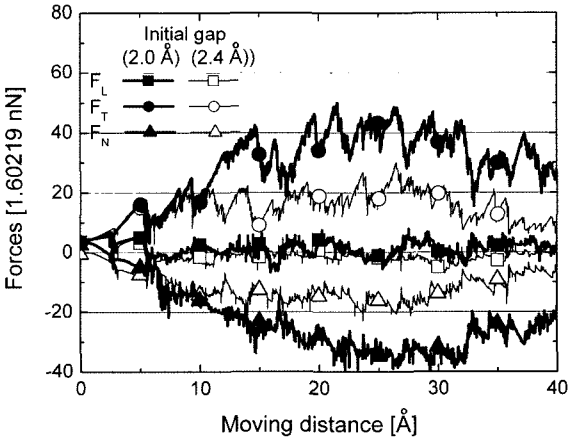


Fig. 5. Variation of forces while the asperity moves in the x-axis direction over (001) lower plate.

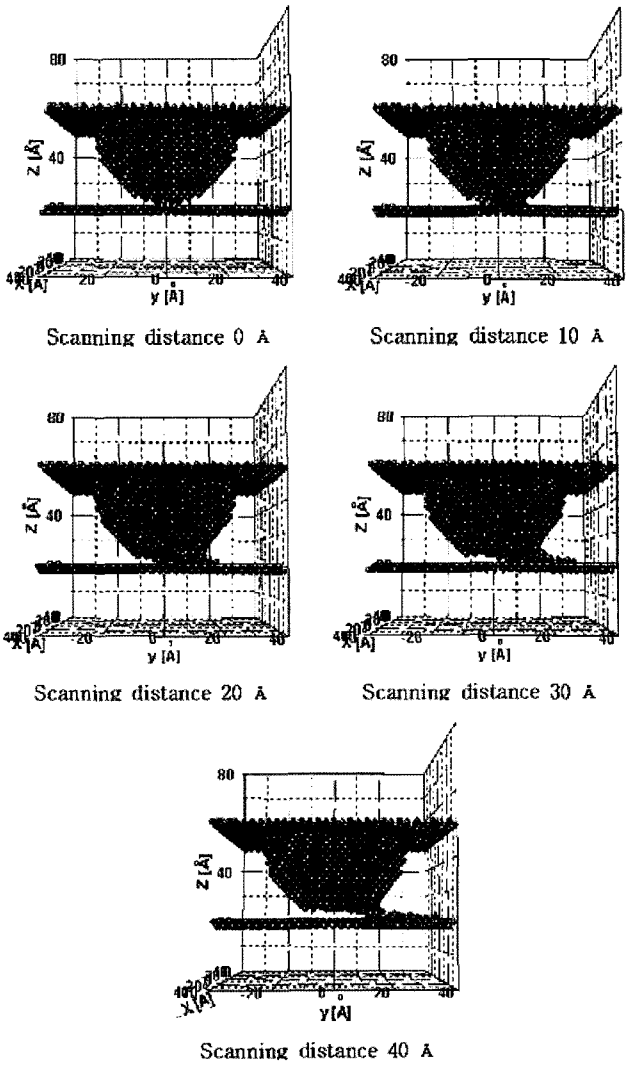


Fig. 6. Snapshots of molecular distribution while the asperity moves in the x-axis direction over (001) lower plate with an initial gap of 2Å.

Fig. 7 shows the variation of forces acting on the asperity at the same condition as Fig. 5 except that the asperity is rigid. All the three forces exhibit periodic variations. The normal force is always attractive while the traction and lateral forces change their direction periodically. The change in the direction of traction force is an evidence for Tomlinson's friction mechanism, and that of the lateral force is known as the zigzag walk [16]. Since the movement of atoms in the asperity is allowed in Fig. 5 but not in Fig. 6, it is claimed that Tomlinson's mechanism and the zigzag walk occurs when the cohesive force is stronger than the adhesion force.

Fig. 8(a) shows the variation of forces acting on the asperity at the same condition as Fig. 5 except that the asperity moves in the direction bisecting the angle between the x- and y-axes (direction V_B in Fig. 1(b)) instead of x-axis direction. Only the results at the initial gap of 2Å are presented because the characteristics in the force variation are not altered with the initial gap. The variations of the forces are similar to those in Fig. 5. However, the normal and traction forces are weak, the decrease in the force magnitude following the initial increase is small, and the characteristic variation occurs in a shorter moving distance.

Fig. 8(b) shows the snapshot of molecular distribution at a moving distance of 40Å. In comparison with Fig. 6, the gap at the leading edge is relatively small, and the fewer number of atoms is transferred to the lower plate, implying the weaker adhesion between the asperity and the plate. Hence, it is conjectured that the forces are relatively weak owing to the weak adhesion, the marginal decrease following the initial increase in the magnitude of normal and traction forces is attributed to the relatively small gap, and the rapid variation of

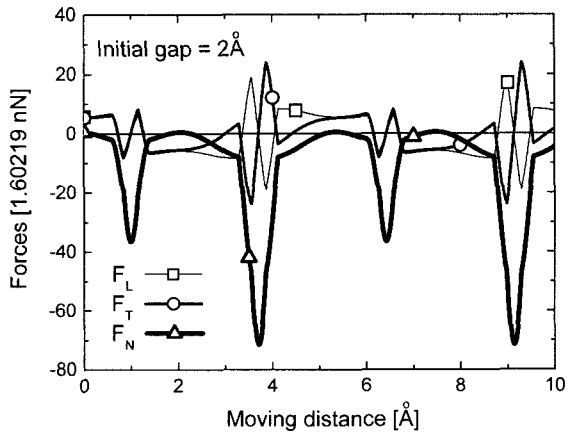


Fig. 7. Variation of forces with the movement of rigid asperity in the x-axis direction over (001) lower plate.

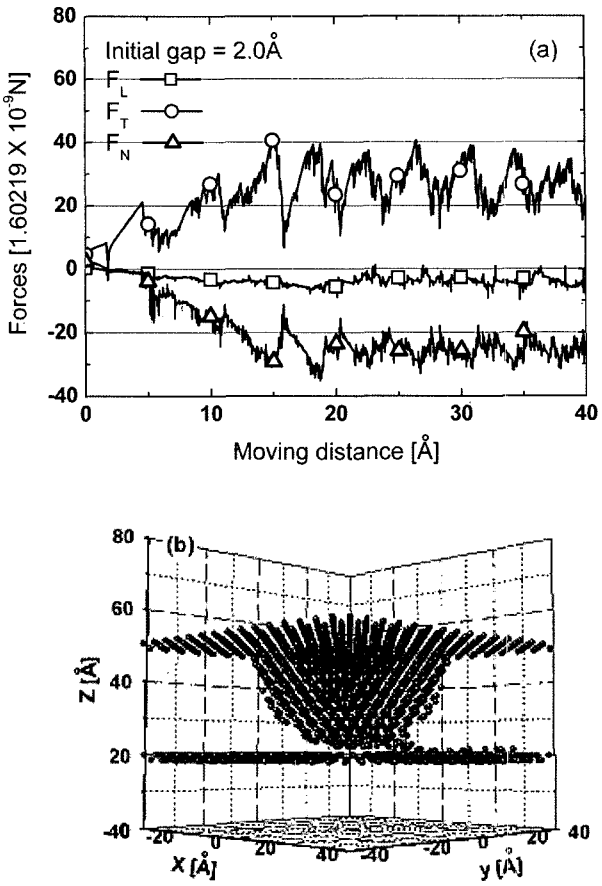
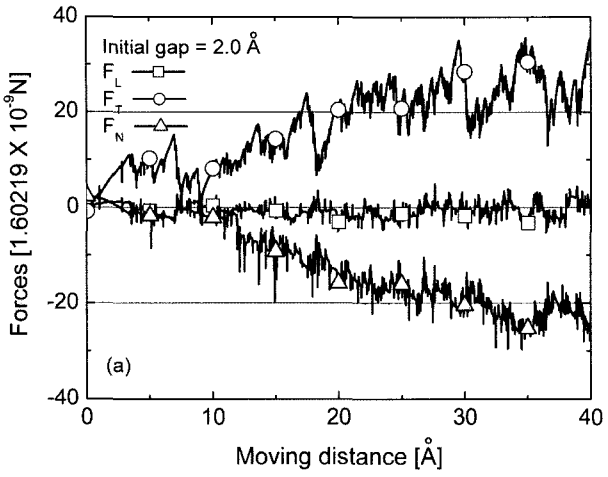


Fig. 8. (a) Variation of forces and (b) snapshot of molecular distribution at the moving distance of 40Å. The asperity moves in the direction bisecting the angle between x- and y-axes over (001) lower plate.

forces is associated with the smaller adhesive junction. Since only the difference between Fig. 8 and Fig. 5 is the moving direction, it is concluded that the moving direction affects the adhesion strength between the asperity and the plate, and thus both the interaction forces and the atom transfer.

Fig. 9(a) shows the variation of forces acting on the asperity when the (001) asperity moves in the x-axis direction over the (111) plate (direction V_X in Fig. 1(c)). It is noted that the asperity is incommensurate with the plate. Both the normal and traction forces increase and then are stabilized without appreciable decrease in the magnitude. Fig. 8(b) shows the snapshot of molecular distribution at a moving distance of 40Å. The region with the increased gap due to the atom transfer is much smaller in comparison with Fig. 6 where the asperity is commensurate with the asperity (??????). Since the adhesion is weaker when the contacting surfaces are incommensurate as in Fig. 9, it is conjectured that the stabilization of forces without



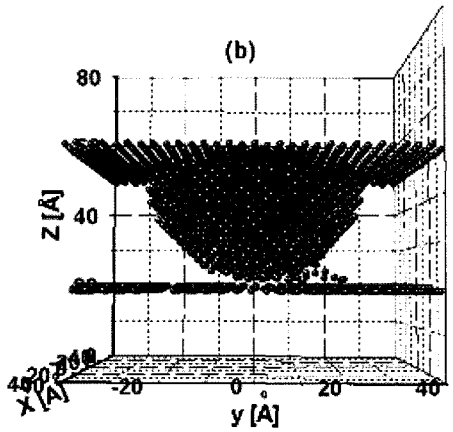
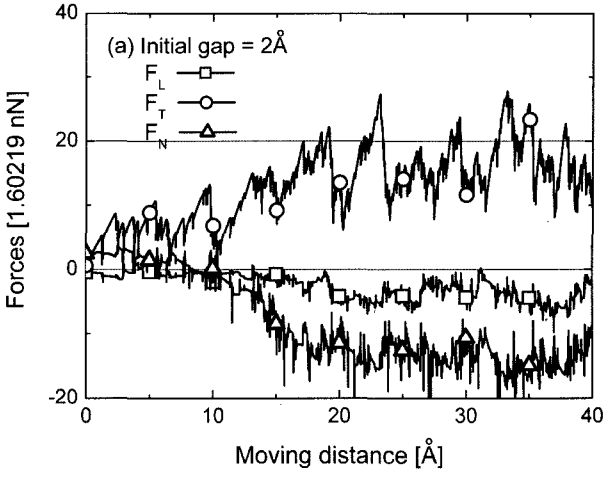


Fig. 9. (a) Variation of forces and (b) snapshot of molecular distribution at the moving distance of 40Å. The asperity moves in the x-axis direction over (111) lower plate.



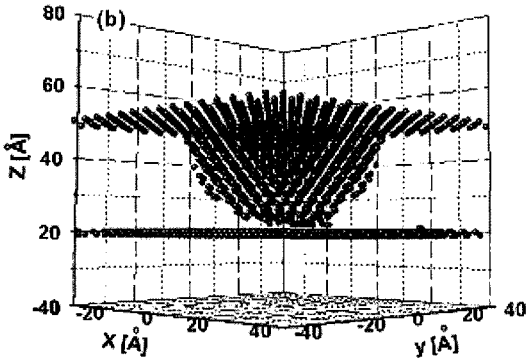


Fig. 10. (a) Variation of forces and (b) snapshot of molecular distribution at the moving distance of 40Å. The asperity moves in the direction bisecting the angle between x- and y-axes over (111) lower plate.

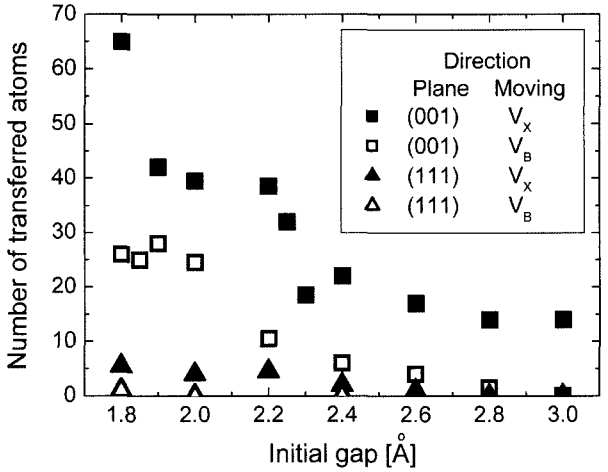


Fig. 11. The number of atoms transferred from asperity to lower plate.

appreciable decrease in the magnitude is associated with the difficulty in the formation of adhesive junction and the transfer of atoms between incommensurate surfaces.

Fig. 10 shows the variation of forces acting on the asperity with the snapshot of molecular distribution at a moving distance of 40Å when the (001) asperity moves over the (111) plate in the direction bisecting the angle between the x- and y-axes (direction V_B in Fig. 1(c)). In comparison with Fig. 9 where only the moving direction is different, the normal and traction forces are weak, and vary in a similar manner but more rapidly. The gap at the leading edge looks comparable but there is no transferred atom on the lower plate. Hence, the influence of moving direction stated in interpreting Fig. 8 is confirmed here again.

Fig. 11 shows the number of transferred atoms at various simulation conditions. It is noted that the number of transferred atoms means the amount of adhesive wear. The adhesive wear is reduced as the initial gap increases, or when the asperity is incommensurate with

the lower plate (when the lower plate is (111)). The moving direction affects the adhesive wear, and its effect is more significant when the asperity is commensurate with the lower plate. It is noted that no atom is transferred to the lower plate even at the initial gap of 1.8Å when the asperity moves over the incommensurate lower plate in the direction V_B.

4. Conclusions

Friction forces and wear of a suspended hemispherical silicon asperity moving over a silicon plate were investigated using molecular dynamics simulation. The friction and wear characteristics are important factors for determining durability in microscale devices. Various cases were simulated under the condition that the asperity is subject to attractive normal force, and the followings are observed.

The adhesive junction - formed between the asperity and the plate with the onset of movement - is ruptured with the increase in the moving distance. During the rupture, some atoms of the asperity are transferred to the plate and thus the gap between the asperity and the plate increases. The region with the increased gap extends with the movement of asperity so that the friction force varies as well as the normal force.

The friction force and wear are smaller when the asperity is incommensurate with the plate, and they also depend on the moving direction of the asperity over the plate. When the asperity is incommensurate with the plate, no transfer of atom that means no adhesive wear is observed at a specific moving direction even if the gap between the asperity and the plate is smaller than the equilibrium distance between silicon atoms.

Acknowledgement

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