Evaluation of friction transition for metal-semiconductor interfaces using model potential comprising three-body contributions

Motohisa Hirano¹, Hiroki Murase¹, Takahiro Nitta¹, and Tomonori Ito²

¹Department of Mathematical and Design Engineering, Gifu University, 1-1 Yanagido, Gifu, 501-1193, Japan
²Department of Physics Engineering, Mie University, 1577 Kurima-Machiya, Tsu 514-8507, Japan
E-mail: hirano@gifu-u.ac.jp

Abstract.
Whether or not the friction transition [1, 2] occurs in the frictional systems of W(011) and Si(001) atomically clean surfaces has been examined in relation to a previous ultrahigh vacuum scanning tunneling microscopy experiment investigating friction transition. This examination takes into account of empirical inter-atomic potentials with three-body interactions. To obtain equilibrium atomic arrangements of the frictional system for evaluating friction transition, the parameters of the interatomic potential applicable for tetrahedrally bonded materials were examined. From studying the criterion of the friction transition for the frictional systems of W(011) and Si(001), it has been concluded that friction transition does not occur for the real systems, which supports the experimental results of a previous ultrahigh vacuum scanning tunneling microscopy experiment.

1. Introduction
The total energy of contacting surfaces is invariant for sliding distance $Q$ as in the case of incommensurate interfaces, resulting in vanishing frictional force. The increase in interfacial interactions, on the other hand, leads to the discontinuous motion of constituent atoms, resulting in the appearance of friction. We thus see that the frictional force changes from vanishing to finite due to increased interfacial interactions. This is called friction transition [1]. Whether the friction transition occurs in real systems is unknown. The occurrence of the friction transition has been examined by deriving its condition in various inter-metallic systems by using pairwise inter-atomic potentials [1, 3]. A related experiment has been conducted using a scanning tunneling microscopy technique in the frictional systems of W(011) tips and Si(001) atomically clean surfaces. The conclusion was that the friction transition does not occur in a frictional system [4, 5]. This paper, in relation to that experiment, theoretically examines whether or not friction transition occurs in the frictional systems of W(011) and Si(001) atomically clean surfaces, by taking into account empirical inter-atomic potentials with three-body interaction [6].
Figure 1. Schematic illustration of STM friction measurement system in an ultra-high vacuum with base pressure of $10^{-9}$ Pa. Cleanliness and crystal orientation of W(011) surface of tungsten tip were determined by a field emission microscope, and that of Si(001) surface by low energy electron diffraction and Auger electron spectroscopy.

2. Experiments for W(001) and Si(001) interfaces in ultrahigh vacuum

Ultrahigh vacuum scanning tunneling microscopy (STM) technology has been used to study friction between atomically clean, well-defined crystal surfaces equivalent to theoretical models [4]. In an ultra-high vacuum ($10^{-9}$ Pa), the W(011) surface of a tungsten (W) tip is brought close to a Si(001) surface (Sb-doped, n-type, 0.01 Ω·cm) (Fig. 1). Then, while the tunnel gap between the two surfaces is kept constant, the Si(001) surface is one-dimensionally scanned by the tip and the friction force between the surfaces is measured from the deflection of the tip at the time of scanning (Fig. 1). Quantum tunneling was used to prevent plastic deformation caused by contact between the tip and the surface. In contrast to ordinary STM, the tungsten tip is not sharpened on purpose and the minute surface, as shown in Fig. 1, prepared on the tip is used as a friction surface.

Experimental results agreed with theoretical predictions, and a friction force equivalent to the theoretical one was observed for commensurate contact [4]. A friction force of 0.8 nN was obtained for a tip elastic modulus of 1.5 N/m and tip deflection of 50 nm in agreement with theoretical values. On the other hand, friction force could not be observed for incommensurate contact at an observation accuracy of 3 nN. In the above manner, the experimental results for clean surfaces at the atomic level agreed with the theoretical prediction. It was concluded that friction forces equivalent to theoretic values can be observed for commensurate contact while friction forces cannot be observed for incommensurate contact at a measurement resolution of 3 nN.

3. Criterion for friction transition

According to Tomlinson’s mechanism[2], atoms at contacting surfaces discontinuously (abruptly) change their positions when solids slide against each other. The occurrence of the discontinuity means that the atoms can not take the arbitrary equilibrium position. This is equivalent to a condition that the second derivatives of the total potential energy $V(Q,r)$ with respect to
the coordinates of the atom \( r \) becomes be negative at the position where \( d^2V^l(r)/dr^2 \) takes the largest negative value (see Fig. 2). A simple case involving a one-dimensional system is shown, in which only \( V^l(r) \) and \( V^u(r) \) operate (Fig. 2). When \( V^l(r)=0 \), the atoms occupy positions that correspond to the lowest minima of \( V^u(r) \). For a weak \( V^l(r) \) limit, the atoms slightly change their positions towards the minimum positions of \( V^l(r) \). For a strong \( V^l(r) \) limit, the atoms occupy positions that correspond to the lowest minima of \( V^l(r) \). In the intermediate case, does the critical atom, shown in Fig. 2, sits an arbitrary position without showing the discontinuous motion of atoms? The criterion for the occurrence of the discontinuous motion is given in Ref. [1] as

\[
\frac{d^2V(Q, r_{\text{max}})}{dr_{\text{max}}^2} = \frac{d^2V^u(Q - r_{\text{max}})}{dr_{\text{max}}^2} + \frac{d^2V^l(r_{\text{max}})}{dr_{\text{max}}^2} < 0 \quad \text{for a certain } Q,
\]

where \( V^l(r) \) is the interaction from the atoms of the lower body. \( V^u(r) \) is the interaction from the atoms of the second, third, ... layers of the upper body. \( r_{\text{max}} \) stands for the position defining the largest negative value of \( d^2V^l(r)/dr^2 \), and \( Q \) stands for the displacement coordinate of the sliding upper body against the lower one.

Note that there is the case where discontinuous motion does not occur. This result suggests that the discontinuous motion is likely to occur only when the interaction or adhesion between two bodies becomes strong and successive discommensuration [7] occurs. This suggestion is generally valid since the equilibrium positions of atoms of the upper body are slightly disturbed by the lower body for the weak case of adhesion [8, 9]. It has been thus shown that the frictional force changes from vanishing to finite due to increased interfacial interactions in incommensurate systems. This is called “friction transition” [1]. Friction transition is the same as the transition of analyticity-breaking, often called Aubry transition [7]. Aubry studied the Frenkel-Kontorova model [10], which is a one-dimensional system to describe the movement of defects or dislocations. Analyticity-breaking corresponds to the discontinuous change of the relaxed particle positions.

The domains where the atom can take its equilibrium position when the adhesion increases between the upper and lower bodies [5] are shown in Fig. 3. The difference from the one-
Figure 3. Topological property of the whole domain, where the atom can take its equilibrium position. Figures show the cases where the contacting surface of the lower body has the oblique-square crystalline symmetry.

dimensional case is that the path where the atom can slide by continuously changing its equilibrium position depends on the direction of sliding displacement coordinate $Q$. The atom can slide towards an arbitrary direction by continuously changing its equilibrium position, as in the case shown in Figs. 3(a) and (b). In the case shown in Fig. 3(c), the atom can slide continuously in the $x$-direction, but can slide in the $y$-direction only by discontinuous transformation. The atom can slide only by discontinuously changing its equilibrium position in any direction for the case shown in Figure 3(d). As seen in these figures, the frictional property depends on the topological property, i.e., the disconnectedness or connectedness of the domains where the atom can take the equilibrium position.

4. Friction transition for metal-semiconductor interfaces

The main concern here is whether or not friction transition occurs in the frictional systems of W(011) and Si(001) atomically clean surfaces, which were measured by a ultrahigh vacuum STM technology [4]. It is necessary to assess the interatomic potential for tetrahedrally bonded materials. The empirical interatomic potentials proposed by Khor and Das Sarma [6] have been adopted for evaluating the frictional system. This potential, which uses very few parameters, is useful, particularly for surface studies, including the surface reconstruction of Si surfaces. The potential is given by

$$V_{ij} = A \exp[-\beta(r_{ij} - R_i)] \left[ \exp(-\theta r_{ij}) - \frac{B_0}{Z_i^{\alpha}} \exp(-\lambda r_{ij}) G(\eta) \right],$$

where $r_{ij}$ is the interatomic distance, $R_i$ is the minimum interatomic distance of the neighbors, and $A, B_0, \theta, \beta, \gamma, \lambda$ are respectively constants. The effective coordination number of atoms...
is

$$Z_i = \sum_j \exp[-\beta(r_{ij} - R_i)^\gamma],$$

(3)

where the summation is carried over all neighbors of $i$. The parameters $\beta$ and $\gamma$ can be fitted to give the correct effective coordination numbers of crystal structures of materials. $G(\eta)$ is given by

$$G(\eta) = 1 + \sum_{k \neq i,j} [\cos(\eta \Delta\theta_{jik}) - 1],$$

(4)

where $\eta$ is a parameter for the bond-bending force constant, and the summation is carried out over the nearest-neighbor atoms. $\Delta\theta_{jik}$ is expressed as

$$\Delta\theta_{jik} = |\theta_{jik} - \theta_i|,$$

(5)

where $\theta_i$ is the equilibrium angle between nearest-neighbor bonds for a regular structure with the coordination number $Z_i$ (i.e., 109.47° for a diamond structure). $\theta_{jik}$ is the angle between bonds $ij$ and $ik$, $\eta$ is a parameter to be fitted to the bond-bending force constant, and the summation is to be carried out only over nearest-neighbor atoms whose bonds $ik$ are the nearest to $ij$. $\theta_i$ is given by

$$\theta_i = \frac{2}{3} \pi + A_2 x^2 + A_3 x^3 + A_4 x^4 + A_5 x^5,$$

(6)

$$x = \ln(Z_i) - \ln(3),$$

(7)

where $A_2, A_3, A_4, and A_5$ are parameters given by $A_2=-4.137495128948$, $A_3=8.5530372320793$, $A_4=-7.1599649270085$, and $A_5=2.0627878449403$ respectively.

In Table 1, we give the values of the parameters of Eqs.(2)-(4) for the three pairs Si, W, and W-Si, respectively. These are fitted to the measured bulk modulus and the cohesive energy shown in Table 2.

| Parameters | Si       | W       | W-Si     |
|------------|----------|---------|----------|
| $A$        | 2794.2386| 3798.6189| 38444.1675|
| $B_0$      | 0.08251716| 0.251094 | 0.169645 |
| $\theta$   | 3.13269  | 2.68935  | 2.79434  |
| $\lambda$  | 1.34146  | 1.52280  | 1.70172  |
| $\alpha$   | 0.6249096| 0.548241 | 0.285641 |
| $\beta$    | 25.44123 | 20.75723 | 25.42105 |
| $\gamma$   | 3.38218  | 3.26327  | 3.39927  |
| $\eta$     | 0.90084597| 0 | 0 |

The friction transition calculation follows the same procedures as described elsewhere [1]. Figure 4 shows the atomistic model of Si(001) and W(011) for evaluating friction transition. The upper body shows the Si diamond structure, and the lower body shows the W face-centered tetragonal lattice.

It is assumed that only the atoms of the upper body are allowed to change their positions while the atoms of the lower body remain fixed. To satisfy this assumption, the closed packed
crystal planes (hard planes), such as the W(011) planes for tungsten lattices, are taken as the contact surfaces of the lower bodies. The atoms of the upper body Si lattice were relaxed by operating the interatomic force given by Eqs. (8)-(12).

\[
\frac{\partial V_{ij}}{\partial r_{ij}} = -A\beta\gamma(r_{ij} - R_i)\gamma^{-1}\exp[-\beta(r_{ij} - R_i)] \left[ \exp(-\theta r_{ij}) - B_0 \exp(-\lambda r_{ij}) \frac{G(\eta)}{Z_i^\alpha} \right] \\
+ A \exp[-\beta(r_{ij} - R_i)] \left[ -\theta \exp(-\theta r_{ij}) - \left\{ -\frac{B_0\alpha}{Z_i^{\alpha+1}} \nabla_j(Z_i) \exp(-\lambda r_{ij}) G(\eta) \right\} \right].
\]

(8)

\[
\nabla_j(Z_i) = \sum_j -\beta\gamma(r_{ij} - R_i)\gamma^{-1}\exp(-\beta(r_{ij} - R_i)\gamma). 
\]

(9)

\[
\nabla_j \{ G(\eta) \} = \sum_k \frac{\eta \sin(\eta \Delta \theta_{ijk})}{\sin \theta_{ijk}} \nabla_j(\cos \theta_{ijk}) + \eta \sin(\eta \Delta \theta_{ijk}) \nabla_j(Z_i). 
\]

(10)

\[
\nabla_j(\cos \theta_{ijk}) = \frac{1}{r_{ij}} (\hat{r}_{ik} - \hat{r}_{ij} \cos \theta_{ijk}). 
\]

(11)

\[
\nabla_j(\theta_i) = (2A_2x + 3A_3x^2 + 4A_4x^3 + 5A_5x^4) \frac{1}{Z_i} \nabla_j(Z_i), 
\]

(12)

Table 2. Experimental data for determining potential parameters. \( r_e \) is equilibrium interatomic spacing, \( E_{coh} \) is cohesive energy, and \( B \) is bulk modulus.

| Material | Structure | \( r_e (\text{A}) \) | \( E_{coh} (\text{eV/atom}) \) | \( B(10^{11}\text{N/m}^2) \) |
|----------|-----------|---------------------|-----------------------------|-------------------------|
| W        | bcc       | 2.74                | 8.90                        | 3.232                   |
| W        | fcc       | 2.84                | 8.414                       | 1.087                   |
| W-Si     | Zinc blende | 2.44               | 5.308                       | 2.84                    |
| W-Si     | Rocksalt  | 2.55                | 6.214                       |                         |
| W-Si     | CsCl      | 2.68                | 6.667                       |                         |

The Si(001) plane is placed against the W(011) plane, as shown in Fig. 4. The upper body is composed of \( 5 \times 5 \times 5 \) diamond structure unit cells (1166 atoms), and the lower body is composed of \( 18 \times 18 \times 2 \) face-centered tetragonal unit cells (3423 atoms). The corresponding interfaces with misfit angles of 0 and 30° respectively are shown in Fig. 5.

The critical atom for each contact is placed at the point satisfying \( \partial V^l(r)/\partial r = 0 \) and \( \partial^2 V^l(r)/\partial r^2 < 0 \) along lines perpendicular to the ridge lines of \( V^l(r) \), where the local minimum of potential \( V^u(r_{min}) \) from the upper body and the local maximum of potential \( V^l(r_{max}) \) from the lower body exist. In the calculation, the atoms of the upper body, excluding the critical atoms, are three-dimensionally relaxed. After relaxation, second order derivative \( V_{\alpha,\beta} \) is calculated for the direction perpendicular to the ridge line of each critical atom.

Figure 6 shows the calculated \( V_{\alpha,\beta} \) as a function of the misfit angle at the contacting surfaces. The calculated \( V_{\alpha,\beta} \) values are positive for the misfit angle between 0 and 90°. This shows that friction transition does not occur in the frictional system of Si(001) and W(011) surfaces. The \( V_{\alpha,\beta} \) sign is actually determined by competition between a positive \( V^u(r_{min}) \) contribution from the upper body and a negative \( V^l(r_{max}) \) contribution from the lower body as seen in Eq. (1). A positive \( V^u(r_{min}) \) always defeats a negative \( V^l(r_{max}) \) in the frictional system. From studying the frictional properties of Si(001) and W(011) surfaces, it has been concluded that friction transition does not occur for real systems, which supports the experimental results of the ultrahigh vacuum STM experiment [4].
Figure 4. Atomistic model of Si(001) and W(011) for evaluating friction transition.

Figure 5. Interface model for friction transition in realistic systems of Si(001) and W(011).

5. Summary
Whether or not the friction transition occurs has been examined by studying the atomistic frictional systems of W(011) and Si(001). The interatomic potential, comprising three-body contributions, for tetrahedrally bonded material was used. The construction of the potential is based on the idea that bonding energies of many substances can be modeled by pairwise interactions moderated by the local environment. The friction transition was calculated by following the same procedures as described elsewhere [1]. From studying the frictional properties of Si(001) and W(011) surfaces, which were actually measured by STM techniques, the calculated $V_{\alpha,\beta}$ values were found to be all positive for various contacting conditions of W(011) and Si(001). This proves that friction transition does not occur for real systems, which supports the experimental results of the ultrahigh vacuum STM experiment [4]. Friction transition does not occur even for strong adhesion such as metallic bonding [1]. The case of weak adhesion has been discussed elsewhere [8, 9]. Thus, the present conclusion may hold true for a wider class of
Figure 6. Calculated $V_{\alpha,\beta}$ as function of misfit angle $\theta$ of contacting surfaces.

adhesion.

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