Molecular dynamics simulation of lateral ultrasonic excitation in atomic-scale friction

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Abstract

The normal and lateral (in the sliding direction) vibration can achieve ‘dynamic superlubricity’ at the atomic scale which has been studied and proved by other researchers. In this study, we have found that the lateral excitation (perpendicular to the sliding direction) which has rarely been studied before can also reduce the average friction force greatly. By utilizing the tip path on the interaction potential energy surface and plotting the interaction potential energy as a function of support position, we elucidated the reason of dynamic superlubricity caused by lateral excitation. The details of the lateral excitation at the atomic scale friction have been demonstrated by molecular dynamics simulations and numerical computation based on the Prandtl-Tomlinson model. This study can increase the understanding of the ultrasonic vibration excitation at atomic scale friction.

1. Introduction

Tribology is an ancient and important discipline, which involves friction, adhesion, lubrication and wear between surfaces or interfaces in relative motion. Controlling friction and reducing dissipation have long been pursued for many researches [1–5]. At the macro scale, gears and bearings and liquid lubricants can reduce friction, but these methods may fail at the micro- or nanoscale [5]. Ultrasonic excitation has been proven to reduce friction at the macroscale [6–10] and the nanoscale [5, 11–20]. However, the studies on the ultrasonic vibration at the nanoscale are still insufficient [6]. Therefore, more investigations about it should be taken.

Dinelli et al [11] carried out experiments in ambient conditions by using the friction force microscopic (FFM) and the ultrasonic force microscopic (UFM) to study dynamic friction dependence on normal ultrasonic vibration (out-of-plane) of a sample. They reported that friction reduces and even vanishes as the excitation amplitude increases. However, they ascribed this effect to ‘dilation’, which is different from the work and explanation of Socoliuc et al [5, 12]. Socoliuc et al [5] demonstrated that friction can be switched on and off by exciting normal vibration in ultrahigh vacuum (UHV) conditions. Their subsequent work found that the ‘dynamic superlubricity’ can also be observed in the ambient conditions [12]. They introduced the dimensionless parameter $\eta = \frac{2\pi^2 E_0}{ka^2}$ in the prandtl–Tomlinson (PT) model [13] to account for the suppression of the atomic stick-slip friction. Moreover, there are other experimental studies on the normal ultrasonic excitation at the atomic scale have been carried out [14–16]. Numerical simulations based on one dimension [17, 18] and two dimension [19] PT model have been used to study the mechanism and the condition of superlubricity. The effect on the dynamic superlubricity of the temperature, velocity and damping coefficient were also investigated. Zaloj et al [21] investigated the coupled lateral-normal response to a lateral external drive in the nanoscale. However, as an important method of studying atomic friction, molecular dynamics (MD) simulations on the reduction of friction by ultrasonic vibration excitation are really scarce. Gao et al [22] performed MD simulations and demonstrated that friction can be suppressed in thin-film boundary lubricated junctions by normal vibration with small amplitudes. Recently, MD simulations were carried out to study the
Boundary atoms are substrate includes three kinds of atoms, namely, Newtonian atoms, Thermostat atoms and Boundary atoms. The MD simulation model comprising of a hemispherical silicon tip and a silicon substrate is shown in Figure 1. In this sliding system, there are four atoms types which are Loaded atoms, Newtonian atoms, Thermostat atoms and Boundary atoms respectively.

In addition, periodic boundary conditions are applied in the dimensions of 168 Å, 120 Å and 52 Å corresponding to the x, y and z directions respectively. The tip contains 2889 silicon atoms with a radius of 30 Å. The substrate which contains 53196 silicon atoms has a radius of 80 Å. Figure 1 only shows the total spring force for a virtual atom called 'dynamic superlubricity'. To the best of our knowledge, ultrasonic vibration excitation in the lateral (y direction in our study) which is perpendicular to the sliding direction (x direction in our study) has rarely been studied at the atomic scale before. In this work, we performed MD simulations and numerical calculation based on PT model to investigate the influence of the y-direction vibration on the atomic-scale friction.

2. Methods

The MD simulation model comprising of a hemispherical silicon tip and a silicon substrate is shown in figure 1. The tip contains 2889 silicon atoms with a radius of 30 Å. The substrate which contains 53196 silicon atoms has dimensions of 168 Å, 120 Å and 52 Å corresponding to the x, y and z directions, respectively. The silicon substrate includes three kinds of atoms, namely, Newtonian atoms, Thermostat atoms and Boundary atoms. Boundary atoms are fixed in space to eliminate the rigid body motion of the substrate. Thermostat atoms are used to maintain a constant temperature by Langevin thermostat and dissipate the heat generated from friction. In addition, periodic boundary conditions are applied in the x and y directions in order to eliminate the boundary effect while free boundary condition is enforced in the z direction. Tersoff potential is applied to depict the interaction of silicon atoms within the tip and the substrate [25]. The interaction between tip atoms and substrate atoms is modeled by the Lennard-Jones pair potential (with the parameters $\varepsilon = 17.44$ meV, $\sigma = 0.3826$ nm [26]). The MD simulations are performed by the LAMMPS with a time step of 1 fs [27] and the Velocity-Verlet [28] integration algorithm is used in MD simulations.

We apply spring force coupling a virtual atom (support A) at a constant velocity of 5 m s$^{-1}$ along the sliding (x-direction) direction. The spring stiffness $k_x$ is 32 N m$^{-1}$. Some discussion about applying harmonic springs in MD simulations can refer to [29]. The constant normal load (40nN) is applied on each Loaded atom. In addition, y-direction spring force is applied to each Loaded atom to replace the stiffness of the support in the y direction. Meanwhile, the set of paralleling springs can restrain the rotation of the tip around the z-axis. The y-direction spring force for $i_{th}$ Loaded atom at time $t$ is $F_{y,t} = k_y (y_t^i - y_t^i) / N_t$. Here, $N_t$ is the number of the Loaded atoms and $y_t^i$ is the original position of the $i_{th}$ Loaded atom and $y_t^i$ is the position of the $i_{th}$ Loaded atom at time $t$. Figure 1 only shows the total spring (the total spring stiffness $k_y$ is 80 N m$^{-1}$) in the y direction. The spring force is distributed to each Loaded atom in both x and y directions.
In this study, numerical calculation based on PT model is also performed. The y-direction excitation needs a two-dimensional potential to describe the interaction between the tip and the silicon (001) surface. Since the silicon (001) surface has square periodicity, the corrugation potential has the form \[ V_{\text{int}}(x, y) = -\frac{E_0}{2} \cos \left( \frac{2\pi x}{a} \right) \cos \left( \frac{2\pi y}{a} \right), \] where \( a = 0.543 \text{ nm} \), and \((x, y)\) is the tip position. The total potential energy including the elastic energy stored in the springs and the potential from the interface between the tip and the substrate are given by \[ V_{\text{tot}}(x, y) = V_{\text{int}}(x, y) + \frac{1}{2} k_x (R_x - x)^2 + \frac{1}{2} k_y (R_y - y)^2, \] where \( R_x = v t \) and \( R_y = A \sin(2\pi f t) \) are the positions of the support in the x and y directions respectively, \( v \) is the speed of the support in the x direction, \( A \) is the excitation amplitude and \( f \) is the excitation frequency, \( k_x \) and \( k_y \) are the effective stiffness in the x and y directions respectively. In order to obtain expediently the response of the tip influenced by the substrate, the substrate is assumed as a rigid body and the energy dissipation is only caused by the tip [31]. The dynamics of the tip can be described by the modified Langevin equation [32, 33],

\[
\begin{align*}
\frac{m}{2} \frac{d^2x}{dt^2} + m \gamma_x \left( \frac{dx}{dt} - v \right) + \frac{\partial V_{\text{tot}}(x, y)}{\partial x} &= \xi_x(t), \\
\frac{m}{2} \frac{d^2y}{dt^2} + m \gamma_y \left( \frac{dy}{dt} - 2\pi f A \cos(2\pi f t) \right) + \frac{\partial V_{\text{tot}}(x, y)}{\partial y} &= \xi_y(t).
\end{align*}
\]

Here, \( m \) is the mass of the tip, \( \gamma_x \) and \( \gamma_y \) are the damping coefficients, \( \xi_x(t) = \xi(t) \cos(\theta) \) and \( \xi_y(t) = \xi(t) \sin(\theta) \), and \( \theta \) is subject to uniform distribution \([0, 2\pi]\) [34], \( \xi(t) \) is a Gaussian distributed random noise satisfying the fluctuation-dissipation theorem

\[ \langle \xi(t) \xi(t') \rangle = 2 m \gamma_x k_B T \delta(t - t'), \]

where the angular brackets denote the ensemble average, \( k_B \) is the Boltzmann constant, \( T \) is temperature, \( \delta \) is Dirac delta function. The Langevin equation is solved by Runge–Kutta algorithm [35]. For the parameter values, we took \( E_0 = 2.5 \text{ eV}, k_x = 10 \text{ N m}^{-1}, k_y \) varies between \( 5 \text{ N m}^{-1} \) and \( 80 \text{ N m}^{-1} \), \( v \) varies between \( 1 \text{ m s}^{-1} \) and \( 15 \text{ m s}^{-1} \), \( m = 1.35 \times 10^{-22} \text{ kg} \) corresponding to the MD simulations in this paper.

### 3. Results and discussion

The foremost question for this work is whether y-direction excitation can reduce friction like normal and lateral (in the sliding direction) excitation. We firstly selected the natural frequency of the tip in the y direction \( f_{\text{tip}} = \sqrt{k_y / m} / (2\pi) = 122.6 \text{ GHz} \) as the excitation frequency in the MD simulations. Figure 2 shows the relation between the lateral force and support position. The lateral force has the typical characteristic of stick-slip without excitation (in figure 2(a)). When the support A starts to move forward, the spring coupling to the tip stretches and the spring force increases. Once the spring force is larger than the resistance, the tip rapidly slips to the next energy minimum and the energy dissipates. Here, we can see the maximum instantaneous lateral force appears at the first sliding period which indicates the static friction force. However, when the excitation is applied on the tip with \( A = 0.08 \text{ nm} \) and \( f = 122.6 \text{ GHz} \) (in figure 2(b)), the stick-slip motion is suppressed and the average friction becomes negligible. We then performed numerical computation based on PT model as shown in figures 2(c), (d). The qualitative results of MD simulations and numerical computation are the same.

In order to reveal the reason of the dynamic superlubricity caused by lateral excitation, we plotted the interaction potential energy as a function of support position as depicted in figure 3. The interaction energy for MD simulations and PT model are the Lennard–Jones pair potential and the corrugation potential (equation (1)) respectively. For better showing the periodicity (corresponding to figure 2(a)), the support position plotted in figures 3(a), (b) is from 1.57 nm for MD simulations. The interaction potential energy is low at most time in a period of sliding which results in stick-slip phenomenon when the excitation is off. However, with the excitation on, the potential energy changes continuously around \( y = 0 \) many times in a period of sliding which leads to continuous sliding and the average friction force becomes negligible. In addition, we plotted the interaction potential energy surface and the tip path for both MD simulations and PT model as shown in figure 4. The interaction potential energy surface for MD simulations is obtained by a constant-velocity scan with the thermostat temperature \( T = 0 \text{ K} \) and the substrate is not rigid. Therefore, the interaction potential energy surface is a bit different from PT model which is normal for more realistic simulations (MD simulations). The excitation frequency is \( f = \sqrt{k_y / m} / (2\pi) = 122.6 \text{ GHz} \) and the excitation amplitude \( A = 0.08 \text{ nm} \). The vibration amplitude of the tip in the y-direction is about 0.2 nm for PT model (figure 4(d)) due to the resonance when the excitation is on, however, the value is about 0.8 nm for MD simulations (figure 4(b)). From
figures 4(a), (c), we can find that the tip path (red line) without excitation was restricted in the y-direction. The tip spent much time jumping over a potential barrier and arrived at the next minimum potential point. However, when the excitation is on, the tip can easily find the low potential points which can help the tip to slide (figures 4(b), (d)) to reduce the friction.

To further investigate the influence of the y-direction excitation on the atomic friction, we performed more MD simulations with different amplitudes and frequencies of excitation. As shown in figure 5(a), for the case of $f = 122.6$ GHz, the excitation frequency equals the natural frequency of the tip, the lateral resonance occurs while the average friction force decreased rapidly with the increasing amplitudes. In this situation, the excitation of the support can result in a larger amplitude of the tip to damage the structure of the tip in our MD simulations, so the results with excitation amplitudes below 0.1 nm at the frequency $f = 122.6$ GHz are shown in figure 5(a). In addition, the average friction has a tendency to gradually reduce with the increasing amplitudes at the frequencies above 4 GHz. However, at the frequency $f = 4$ GHz, the y-direction excitation has little effect on reducing friction with the amplitudes below 0.4 nm. Moreover, small amplitudes (e.g., 0.02 nm) of the vibration can hardly reduce the average friction force dramatically.

To elucidate the reason and study more details of dynamic superlubricity caused by y-direction excitation, we performed numerical computation based on the two-dimensional PT model. In order to correspond to the MD simulations, the parameters of the PT model are in the same order of magnitude with those of the MD simulations. The value of $k_x$ (PT model) is $10$ N m$^{-1}$ which is smaller than the value of $k_x$ (32 N m$^{-1}$ in MD simulations). The reason is that the value of 32 N m$^{-1}$ cannot lead to stick-slip phenomenon (in PT model) and the average friction force would be very small.

The average friction force varying with the excitation amplitudes at different excitation frequencies is plotted in figure 5(b). Applying the excitation at $f = 122.6$ GHz (lateral resonance frequency), the average friction decreases rapidly and vanishes with the increasing amplitude. This result demonstrates that the y-direction excitation can achieve dynamic superlubricity with high-frequency vibration like normal and lateral (sliding direction) excitation. For the lower frequencies ($f = 4$ GHz and $f = 8$ GHz), the average friction decreases...
Figure 3. The interaction potential energy as a function of support position for both MD simulations (a), (b) and PT model (c), (d) without lateral excitation (a), (c) and with excitation (b), (d). The $k_s = 80$ N m$^{-1}$ and the excitation frequency $f = \sqrt{k_s / m / (2\pi)} = 122.6$ GHz and the excitation amplitude $A = 0.08$ nm. The temperature is 300 K and $v = 5$ m s$^{-1}$. The parameters above are the same for both MD simulations and PT model.

Figure 4. Tip path on the interaction potential energy surface for both MD simulations (a), (b) and PT model (c), (d) without lateral excitation (a), (c) and with excitation (b), (d). The $k_s = 80$ N m$^{-1}$ and the excitation frequency $f = \sqrt{k_s / m / (2\pi)} = 122.6$ GHz and the excitation amplitude $A = 0.08$ nm. The temperature is 300 K and $v = 5$ m s$^{-1}$. The parameters above are the same for both MD simulations and PT model.
non-monotonically with the increasing amplitude and cannot be negligible. When the excitation frequency is too high (e.g., \( f = 367.8 \) GHz), the average friction force can hardly be decreased. The reason is that high excitation frequency above a critical value cannot lead to high vibration amplitude of the tip in the \( y \)-direction. Therefore, we can conclude that excitation frequency needs to satisfy the condition

\[
\frac{V}{a} \ll f \ll \frac{4\pi \Gamma_{nt}^2}{\Gamma_{nt}}
\]

where \( \Gamma_{nt} = \gamma_y / m \) for dynamic super lubricity which is same as the case of normal ultrasonic excitation [16]. In addition, we need to illustrate that the results of the PT model cannot exactly correspond to the results of MD simulation. For example, the average friction force (the value of PT model) without excitation is about one-tenth of the value of MD simulation. This is normal and reasonable because MD simulations (in our study) considering three dimensional cases and the tip is not rigid.

**Figure 5.** The variation of the average friction force with the excitation amplitude \( A \) at different excitation frequencies for both MD simulations (a) and PT model (b). The excitation frequencies are \( f = 4 \) GHz (red line), \( f = 8 \) GHz (blue line), \( f = 61.3 \) GHz (yellow line), \( f = 122.6 \) GHz (green line), \( f = 245.2 \) GHz (purple line) and \( f = 367.8 \) GHz (grey line). The speed of the support \( v = 5 \) m s\(^{-1}\), and the temperature \( T = 300 \) K. The washboard frequency \( f_{\text{washboard}} = v/a = 9.2 \) GHz.
Since the excitation is sensitive to the washboard frequency, which is determined by sliding velocity, studying the velocity dependence of friction with lateral excitation becomes essential. Figure 6 depicts the velocity dependence of friction both in MD simulations and PT model. The stiffness of the $y$-direction springs in both MD simulations and PT model are $80 \text{ N m}^{-1}$ and the temperature is 300 K and the excitation frequency is $122.6 \text{ GHz}$ (resonance frequency). In the MD simulations (figure 6(a)), the average friction force decreases with the increasing velocity of the support without excitation (i.e., $A = 0$). However, as we can see from the results of the PT model (figure 6(b)), the average friction force for the excitation amplitudes below 0.8 nm increases with the increasing velocity of the support. Therefore, we can find that the results of the velocity dependence of friction for MD simulations and PT model are different. The reason for this phenomenon has not been clear which needs further investigations.

There is a wide range of stiffness of AFM tip in experiments, which influences the resonance frequency of the system significantly. Therefore, a study of the dependence of friction on spring constants would help to understand this phenomenon better. We performed numerical computation based on PT model with different
as shown in figure 7. The excitation frequency is natural frequency for each $k_y$ respectively. For example, the excitation frequency selected for $k_y = 5 \text{ N m}^{-1}$ is $f = \sqrt{\frac{k_y}{m}} / (2\pi) = 30.6 \text{ GHz}$. The computation results of $k_y = 40 \text{ N m}^{-1}$ and $k_y = 80 \text{ N m}^{-1}$ are similar. For the lower values of $k_y$ ($5 \text{ N m}^{-1}$ and $10 \text{ N m}^{-1}$), the lateral excitation cannot lead to superlubricity with the excitation amplitudes lower than 0.1 nm. The reason for this

Figure 7. The spring stiffness dependence of friction with lateral excitation for PT model. The spring stiffness in $y$-direction $k_y = 5 \text{ N m}^{-1}$ (red line), $k_y = 10 \text{ N m}^{-1}$ (blue line), $k_y = 40 \text{ N m}^{-1}$ (yellow line) and $k_y = 80 \text{ N m}^{-1}$ (green line). The washboard frequency for all $k_y$ is $f_{\text{washboard}} = v / \alpha = 9.2 \text{ GHz}$. The temperature is 300 K. (results of PT model).

Figure 8. The temperature dependence of friction with lateral excitation. The temperature $T = 0 \text{ K}$ (red line), $T = 100 \text{ K}$ (blue line), $T = 300 \text{ K}$ (yellow line) and $T = 500 \text{ K}$ (green line). The velocity of the tip is $v = 5 \text{ m s}^{-1}$ and $k_y = 80 \text{ N m}^{-1}$.(results of PT model).
results is that the excitation frequencies (natural frequencies here) for \(k_x = 5 \, \text{N m}^{-1}\) and \(k_y = 10 \, \text{N m}^{-1}\) are not too higher than the washboard frequency \(f_{\text{washboard}} = v/a = 9.2 \, \text{GHz}\).

Beside the influence of the factors mentioned above, it’s well known that the temperature is also an important role in nanoscale friction. Therefore, the temperature dependence of friction for the studied system and its influence on the lateral vibration are worth studying. Figure 8 gives the temperature dependence of friction with lateral excitation for PT model. The average friction force decreases with the increasing temperature without lateral excitation, as previously reported \([34, 36]\). However, the temperature has little effects on the friction with excitation under these parameters selected in our modeling. More studies for temperature dependence of friction with ultrasonic excitation need to be performed in future.

4. Conclusion

In summary, we have studied the influence of \(y\)-direction excitation (in-plane and perpendicular to the sliding direction) on the atomic friction by using MD simulation and numerical computation based on PT model. We found that the \(y\)-direction excitation can also reduce the average friction force and achieve ‘dynamic superlubricity’ like the normal and lateral (the sliding direction) excitation. We utilized the tip path on the interaction potential energy surface and the interaction potential energy as a function of support position to elucidate the reason of dynamic superlubricity induced by \(y\)-direction excitation. When the excitation frequency equals the natural frequency of the tip, the average friction force will decrease deeply with the increasing of the excitation amplitude. In addition, the dynamic surperlubricity can be also achieved with large excitation amplitude at some excitation frequencies which do not equal resonance frequency. Moreover, we investigated the velocity dependence and spring constant dependence and temperature dependence of the friction with excitation at the resonance frequency. Although ultrasonic excitation may require more energy to achieve dynamic superlubricity, this method is still valuable for micro- and nanoelectromechanical systems (MEMS/NEMS) \([37]\). It is worth mentioning that the lateral excitation may be more suitable than normal excitation for the 2D materials (e.g., graphene sliding on another surface) to decrease the friction.

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