Anisotropic character of atoms in a two-dimensional Frenkel–Kontorova model*

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The dynamics of a certain density of interacting atoms arranged on a two-dimensional square lattice, which is made to slide over a two-dimensional periodic substrate potential with also the quare lattice symmetry, in the presence of dissipation, by an externally applied driving force, is studied. By rotating the misfit angle θ, the dynamical behaviour displays two different tribological regimes: one is smooth, the other becomes intermittent. We comment both on the nature of the atomic dynamics in the locked-to-sliding transition, and on the dynamical states displayed during the atom motion at different values of the driving force. In tribological applications, we also investigate how the main model parameters such as the stiffness strength and the magnitude of the adhesive force affect the static friction of the system. In particular, our simulation indicates that the superlubricity will appear.

Keywords: nanotribology, Frenkel–Kontorova model, phase transitions

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1. Introduction

Driven dynamics of a system of interacting atoms is an interesting physical problem. It has important applications in mass and charge transport phenomena in solids and crystal surfaces. One of the important applications has emerged in tribology studies, where a thin atomic layer is confined to appear between two substrates which move with respect to one another.[1,2] Fundamental understanding of friction is vitally important in many areas of science and technology, ranging from nanotribology to crack propagation to earthquake dynamics.[3] Progress has also been made on how to tune the intrinsic frictional forces between a sliding object and the underlying substrate, through interface modification down to the molecular or atom scale.[4−6] Such an important understanding at the microscopic level, in turn, is expected to serve as important guidance in the design of smart materials with desirable lubricant properties for industrial and biomedical applications.[3,7]

Shinjo and Hirano[8] and Hirano[9,10] predicted the existence of a state of extremely low friction between two solids in contact at the beginning of the last decade. This state was named superlubricity. In these studies, it was argued that when mechanical contact took place between two incommensurate crystals, the forces lying in the contact plane are likely to be cancelled in a systematic fashion. Such a cancellation results in an adiabatic motion of the atoms in contact. If the above condition holds, friction is always zero in the limit of zero sliding velocity. The phenomenon of superlubricity started to receive increasing attention after a series of experiments had reported that friction coefficients could be reduced below a resolution of 10^{-3}, which were 3–4 orders of magnitude smaller than that previously measured. Recently, motivated by the potential technological applications of superlubricity in microelectromechanical systems, a large new set of theoretical[11−14] and experimental studies[15−19] have been conducted.

Two of the experimental studies showed how to switch between a superlubric regime and a finite friction regime.[16,17] It was reported by Dienwiebel *et al.*[16] that such a transition could be realized after

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rotating a graphite flake attached to a tungsten tip with respect to a graphite surface under dry contact condition. A second group of experiments focused on diamond-like carbon films and hydrogen-terminated diamond surfaces.[15,18,20,21] Hydrogen-terminated carbon films appear as the most promising candidates of superlubric materials for industrial purposes. Because hydrogen treatment effectively reduces or eliminates sigma bonds, these compounds have very smooth and nonreactive surfaces. Moreover, the property of such a compound to form layered structures appear to be a key ingredient in achieving ultralow friction.

Theoretically, special attention has been paid to understanding the roles of the surface roughness and the dimensionality in superlubricity or ultralow friction.[12,13,22,23] There are many processes that can break the superlubric regime, including plastic deformation, adsorbed layers, and cold welding.[24,25] Although slight plastic deformation and surface contamination are unavoidable in the majority of the cases, frequently it is assumed that the aforementioned friction mechanisms can be neglected. This leaves the competition between elastic interactions and interfacial forces as the a main source of friction induction.

One of the explanations for how this competition can produce friction at low velocity is given by the Frenkel–Kontorava (FK) model. In its simplest form, the standard FK model consists of a one-dimensional(1D) chain of atoms coupled by a harmonic nearest neighbour interaction under the influence of an external spatially periodic potential.[9,10,26] The essential physical feature of the model consists in the competition between these two types of interactions: one is to favour a uniform separation among particles, the others is to tend to pin the atom positions to the bottom of the substrate wells. This competition results in a rich complexity of spatially modulated structure.[27] Some important generalizations of 1D FK model have already been carried out by studying more general types of substrate potentials, as well as anharmonic interactions in the chain.[28,29]

The simple 1D FK model, being very useful in understanding many physical aspects of friction, has been qualitatively explained.[10,30−32] However, in practice, the friction is sensitively dependent on the atomic structure of the mating interface. In order to reproduce this feature more adequately and to include subtler details which can be realized in experiments, it is necessary to generalize this model to the two-dimensional (2D) case, where it would be possible for the sliding particles to avoid passing over a highest barrier in the substrate potential, which they has to overcome in the 1D case.

The aim of the present work is to perform a detailed study of quantities of relevant physical interest such as the average mean (centre of mass) velocity and frictional force in an underdamped 2D FK model with a square substrate potential. Transitions between the different dynamical states are studied and related to the details of motion of atoms. Our results are especially important for tribological systems, where the mechanism of the locked-to-sliding transition determines frictional properties of a lubricant film.[33,34]

The remainder of the present paper is organized as follows. In Section 2, technical details enclosed within the implementation of the model are reviewed. Simulation results are presented in Section 3. Finally, conclusions are drawn in Section 4.

2. Methodology

In this paper, to model more real physical systems, we consider that a certain density of interacting atoms arranged on a 2D square lattice (the upper layer), is made to slide over a 2D periodic substrate potential (the lower layer) with also the square lattice symmetry,[35] in the presence of dissipation, by an external applied force. For simplicity, the substrate potential is taken as a sinusoidal function,

$$V = \frac{f}{2\pi}\left[\cos\frac{2\pi x'}{b} + \cos\frac{2\pi y'}{b}\right],$$

where f is the magnitude of the adhesive force between the two layers, and the length b determines the shape of the substrate potential. In order to investigate the general case of the system, in which the orientations of the two layers of lattices do not match, we rotate one of the two layers with respect to the remaining one by an arbitrary misfit angle θ. This must satisfy,

$$x' = x\cos(\theta) - y\sin(\theta),$$

$$y' = x\sin(\theta) + y\cos(\theta).$$

Considering that an arbitrary atom, for example the (n,m)th atom, that interacts only with the nearest and next nearest neighbours, the interatomic interaction is chosen to be of the simple harmonic form

$$U = \sum_{i,j}\frac{K}{2}[(x_{i,j} - x_{n,m} - l)^2 + (y_{i,j} - y_{n,m} - l)^2],$$

with a stiffness strength K, a natural equilibrium spacing $l = a$ between the nearest neighbour atoms, $l = \sqrt{2}a$ between the next nearest neighbour atoms of the upper lattice, and the position vector of the (n, m)th atom being expressed as $\boldsymbol{r}_{n,m} = (x_{n,m}, y_{n,m})$.

Thus, the displacement vector $\boldsymbol{r}_{n,m}$ of the (n, m)th atom satisfies the following equation of motion:

$$\ddot{\boldsymbol{r}}_{n,m} + \gamma\dot{\boldsymbol{r}}_{n,m} + \frac{\partial(U+V)}{\partial \boldsymbol{r}_{n,m}} = \boldsymbol{F}_{\rm ext}, \qquad (1)$$

where $\boldsymbol{F}_{\rm ext} = (F_{\rm ext}\cos\alpha, F_{\rm ext}\sin\alpha)$ is the external driving force, with α being the angle between $\boldsymbol{F}_{\rm ext}$ and the unit vector of x axis; γ is a phenomenological viscous damping coefficient and chosen such that it is in the damped regime, and can be thought of as degree of freedom in real physical systems which are not explicitly included in our model (e.g., vibrational or electronic excitations in the substrate). The damping coefficient used in our simulations is $\gamma = 0.7$. Throughout the paper we use dimensionless system of units, where identical mass $m = 1$ is assigned to each atom, the natural equilibrium spacing $a = 1$. The frequencies of atomic vibrations at the minima of the substrate potential are isotropic, i.e., $\omega_x = \omega_y = \sqrt{2\pi f/b}$, the characteristic time scale that we use in the model is determined in terms of the oscillation period of an atom in the substrate potential, $\tau_0 = \sqrt{2\pi b/f}$.

A fourth-order Runge–Kutta algorithm[31,35] is adopted to solve numerically Eq. (1). The atoms are fixed at the minima of the substrate potential, then the force $F_{\rm ext}$ is increased adiabatically in steps of $\mathrm{d}F_{\rm ext} = 0.005$, allowing a sufficiently long time $t = 300$ (time step $\mathrm{d}t = 0.006$) to equilibrate at each new value of $F_{\rm ext}$. In order to discuss the mobility of the system, the averaged velocity is defined as $\overline{\boldsymbol{V}} = (1/N \times M)\sum_{i=1,j=1}^{i=N,j=M}\langle\dot{\boldsymbol{r}}_{i,j}\rangle$, where $\langle\ \rangle$ denotes the time average. The interparticle equilibrium length a, not entering explicitly Eq. (1), appears only via the boundary condition, $x_{N+1} = x_1 + Na$ and $y_{M+1} = y_1 + Ma$ (N and M are integers), to enforce a fixed density condition for the system.[31,32,35]

3. Results and discussion

In the following, restricting the system to the atomic layer $N \times M = 12 \times 12$ atoms placed, we analyse the behaviour of the system motion for the different values of model parameters such as misfit angle θ, direction angle of external driving force α, magnitude of the adhesive force f and stiffness strength K, commenting both on the nature of the atomic dynamics in the locked-to-sliding transition, and on the dynamical states displayed during the atom motion at different values of the driving force. In this way, to allow the identification of the scenario of the transition, the atomic trajectories are examined.

The most relevant concept of the FK model is the so-called commensurability. Namely, the periodicity of the substrate potential b coincides with the natural equilibrium distance between the atoms a. In such a case, we model the sliding between two identical perfectly aligned crystalline workpieces. Figure 1 shows the corresponding mapping of the average mean system velocity as a function of external driving force $F_{\rm ext}$.

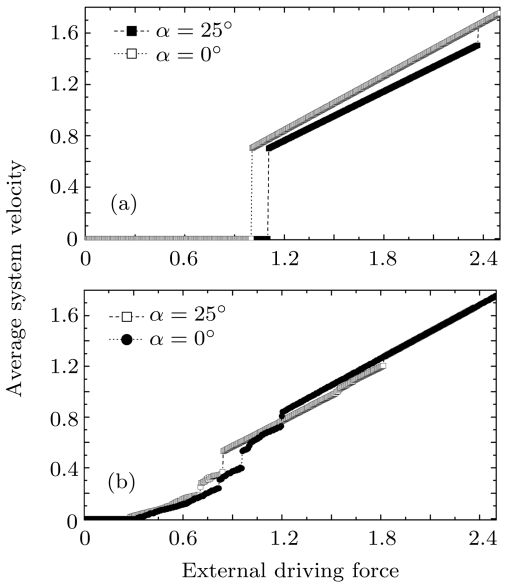


Fig. 1. Corresponding mappings of average mean system velocity $\overline{V}$, each as a function of the external driving force $F_{\rm ext}$, for $f = 1$, $a = b = 1$, $K = 1$ and two values of the misfit angle θ: (a) $\theta = 0°$ and (b) $\theta = 40°$.

As force $F_{\rm ext}$ increases, in the case of perfect matching of the two layers, i.e., the misfit angle $\theta = 0°$ (see Fig. 1(a)), the system undergoes a sharp transition from the locked phase to the moving crystal phase. For example, when the system is dragged along the direction $\alpha = 25°$, the system transfers directly from the locked state to the sliding state without passing through any intermediate steady-state regimes.[34] At a fixed value of driving force that corresponds to the critical depinning force $F_{\rm ext} = 1.105$, we observe the whole process of transition. The system is pinned by the substrate and begins to move when the external driving force $F_{\rm ext}$ exceeds the critical value. The transition, occurring at the critical depinning force, from

a pinned state with zero velocity to a moving state with nonzero velocity is called the locked-to-sliding transition. From the examination of the atomic trajectories (shown in Fig. 2(a)), one can see that in the locked state, almost all atoms lie nearly at the substrate potential minimum, where they are trapped due to the stronger interatomic interaction with respect to the substrate potential. Starting from the locked state, as the driving force $F_{\rm ext}$ increases, the system spreads mainly in the x axis direction (see Fig. 2(b)). Finally, under the larger driving force, for example $F_{\rm ext} = 2.46$, one can observe from Fig. 2(c) that the atomic structure in the moving regions becomes more and more crystalline. The ordering spreads over the whole lattice and the system reaches the higher sliding state of a moving crystal.

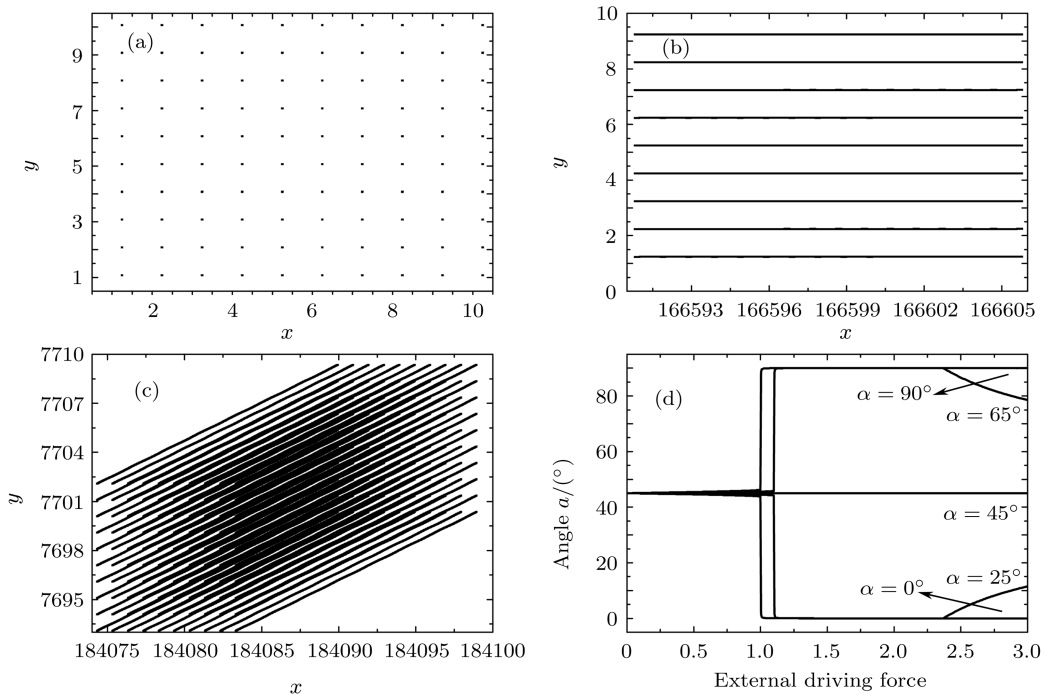


Fig. 2. Atomic trajectories with $\theta = 0°$ under different values of force $F_{\rm ext} = 0.8$ (a), 1.37 (b) and 2.46 (c). Panel (d) shows angle α' as a function of driving force. Other parameters are the same as those in Fig. 1.

For the better identification of the differences between the direction of the external driving force and the direction of motion of the centre of mass, we define a parameter α' to represent the angle between the direction of motion of the centre of mass and the unit vector of the x axis. The dependency of α' with $F_{\rm ext}$ for $\theta = 0°$ is displayed in Fig. 2(d).

As one can see from Fig. 2(d), in the locked state, the direction of motion of the centre of mass is always consistent with the direction of $\alpha' = 45°$ for different values of angle α. Things become more interesting once the system transfers sharply to the sliding state. As shown in Fig. 2(d), the direction of the motion of the centre of mass is aligned with the direction of the external driving force for the cases $\alpha = 0°$, $45°$ and $90°$. However, in the cases of $\alpha = 25°$ and $\alpha = 65°$, for example, the motion starts first in the x and the y directions, respectively, and then broadens gradually in the direction of the driving force. It is also noted that due to the symmetry of the system, α' is symmetric about $\alpha' = 45°$.

In order to produce the orientations of the two layers latices which do not match, one of the layers is rotated with respect to the remaining one by an arbitrary misfit angle θ. The dependency of the average mean system velocity with the external driving force $F_{\rm ext}$ for the misfit angle $\theta = 40°$ is shown in Fig. 1(b).

On the contrary to the case $\theta = 0°$, within our simulations (see Fig. 1(b)), note that the change of the misfit angle θ can produce a series of dynamical mode-locking phases. Tekic *et al.*[34] have also shown a similar behaviour for the 2D triangular substrate potential. Moreover, a remarkable difference between misfit angles $\theta = 40°$ and $\theta = 0°$ is that the critical depinning force may be reduced. For example, in the case of misfit angle $\theta = 40°$, when the external driving

force is in the direction $\alpha = 25°$, as far as the locked-to-sliding transition is concerned, there exists a lower critical depinning force $F_{\rm ext} = 0.28$. Below the critical value, the external driving force is too low and the atoms, trapped by the external substrate potential, do not move. The system is in the locked (or pinned) state with a zero mobility. The atomic structure in this state is shown in Fig. 3(a). As observed, when the system lies in the locked state, e.g., $F_{\rm ext} = 0.1$, all atoms are trapped near the minimum of the substrate potential.

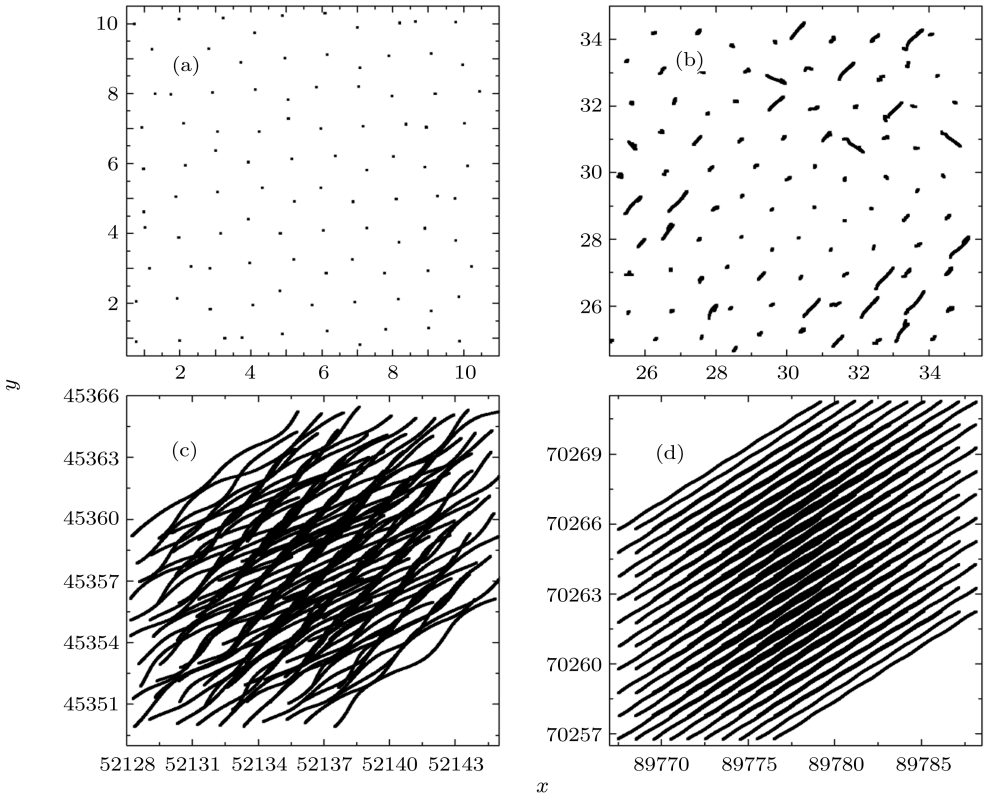


Fig. 3. Atomic trajectories with $\theta = 40°$ under the values of force: $F_{\rm ext} = 0.1$ (a), 0.3 (b), 1.5 (c) and 1.84 (d).

Above the critical value, the spontaneous square symmetry will be broken, and the various dynamical behaviours may be observed during the system motion. These regimes correspond to rearrangements of atomic configurations (spatial inhomogeneities) with distinct periodicities and amplitudes.

As one can see from Fig. 1(b), in the case of $\alpha = 25°$, staring from the locked phases, as the force varies in a range $0.28 < F_{\rm ext} < 0.8$, the system transfers smoothly. The atomic trajectory configuration for $F_{\rm ext} = 0.3$ is shown in Fig. 3(b). Note that different portions of the upper layer are moving along different directions, or some are moving while the others remain pinned. Meanwhile, the motion starts via the formation of a small number of isolated, narrow defects (kinks) on the edge of the system. In the context of tribological process, the most important object in the FK model is the kink excitation. The kink describes a configuration with one extra atom inserted into the system.[27] Each run of the kink through the system results in the shift of the whole system. In the case of the finite system, the onset of sliding is initiated by the creation of a local compression zone at the boundary of the system. Physically, the reason why kinks are so important is that they can move along the system much easily than the atoms themselves. The activation energy for kink motion is always smaller or much smaller than the amplitude value of the substrate potential. Because the kinks correspond to extra atoms, their motion provides a mechanism for mass transport along the system.

The number of these kinks grows and spreads gradually in the driving direction $\alpha = 25°$ (shown in Fig. 3(c)) as the driving force increases, until they begin to overlap. The phenomena, combined with Fig. 1(b), reflects the fact that the higher the concen-

tration of kinks is, the higher will the average mean system velocity $\overline{V}$ become. All of these states correspond to an intermediate sliding regime. In the rearrangement of atomic configurations, the more detailed study of the atom trajectories indicates a stick-slip behaviour. That is, from the viewpoint of total potential energy (the harmonic interaction and the substrate potential), under the low driving force $F_{\rm ext} \geq 2.8$, the potential energy landscape is characterized by different metastable positions, giving rise to the stick-slip behaviour.[36] The energy of the mobile atoms dissipates via the damping γ-term in Eq. (1). Then, they rapidly drop to the next nearest meta stable minimum, where they are locked again. Contrary to the mobile atoms, the immobile atoms are locked in their minima of the potential energy until the barrier is overcome.

Finally, under a higher driving force, the system dynamics changes to a high driving regime and kinks disappear. In this case, the flow of the system becomes more and more ordered and its structure with the square symmetry is preserved during motion. All the atoms slide almost uniformly over the substrate potential. Hence, the state corresponding to crystalline flow of atoms (shown in Fig. 3(d)), is characterized by the largest average sliding velocity $\gamma\overline{V} = F_{\rm ext}$.

It is also worthwhile to investigate how the variations of misfit angle θ in different states affect the direction of the centre of mess. Figure 4 exhibits the dependency of α' varying with $F_{\rm ext}$ for $\theta = 40°$. A comparison between Fig. 4 and Fig. 2(d) shows that in the case of the misfit angle $\theta = 40°$ the symmetry of α' is broken as $F_{\rm ext}$ increases, the direction of the motion of the centre of mass tends to the direction of driving force.

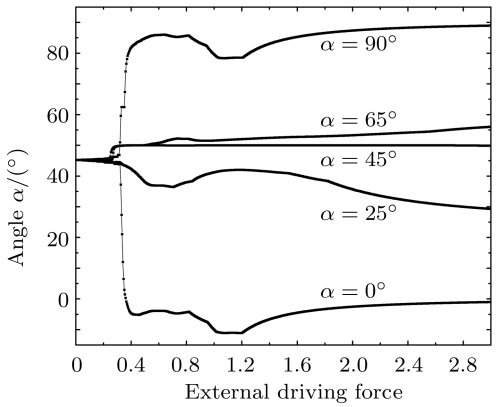


Fig. 4. Angle α' between the direction of motion of the centre of the mass and unit vector of x axis as a function of the magnitude of the external driving force $F_{\rm ext}$ for $\theta = 40°$.

In the following paragraphs, we may gain an insight into the fundamental tribological concept, the static friction which is probably already encountered in some early stage during courses on classical mechanics or general physics and defined as the minimal threshold force needed to drive the relative motion. On the other hand, in numerous experimental and theoretical studies, it was found that the static friction of the system depends strongly on the main model parameters such as the stiffness strength K, the magnitude of the adhesive force f and the effective elastic constant $g_{\rm eff} = a^2 V''_{\rm int}(r_0)/\pi f$,[34] where $r_0 = a$ (or $\sqrt{2}a$). This single dimensionless number gives an indication of the strength of the elastic constant of the atomic layer relative to the strength of the substrate potential f and the stiffness strength K. A value of $g_{\rm eff} \leq 1$ indicates a relatively weakly coupled layer (or a very strong pinning potential of the substrate). This scenario may correspond, for example, to a monolayer adsorbed on a crystal surface. On the contrary, a value $g_{\rm eff} > 1$ describes a stiff atomic layer. For example, the case of dry friction between two blocks of material corresponds to this limit. Also we study how the variations in the magnitude of the adhesive of force and the stiffness strength affect the static friction of the system, in particular, whether the superlubricity appears.

As observed in Fig. 1, variations in the direction of driving force α, affect the critical depinning force (known as the static friction $F_{\rm s}$ in tribology), from which we have determined the static fiction from our simulation as the external driving force at which the system first has nonzero velocity. The $F_{\rm s}(\alpha)$ dependencies are plotted in Fig. 5 for the different vales of misfit angle θ and the model parameters.

As clearly shown in Fig. 5(a), the static friction, $F_{\rm s}$, in the case of $\theta \neq 0°$, is much less than that in the case $\theta = 0°$. Especially, note that the case of $\theta = 0°$ and $\alpha = 0°$ corresponds strictly to 1D case. It suggests that there are great differences between 1D case and 2D case. The reason for this may be as follows: the magnitude of static friction $F_{\rm s}$ depends on the atomic arrangement of the two solid layers that are in contact with each other. For the 1D commensurate case where $\theta = 0°$ and $\alpha = 0°$, the contact between the two layers where their lattice spacing ratio is an rational number ($\beta = b/a = 1$) and the magnitudes of the force received by atoms, namely, the friction forces are not zero. In order to make the upper layer slide, all atoms must climb over the potential peak of

the other solid simultaneously. We can compare this situation to a tug-of-war between many atoms and an external driving force. Hence, each atom receives a force, i.e., resistance to motion, in the direction opposite to the external driving force. In order to make all of the atoms move together in this situation, the external driving force must be larger than the total sum of resistance forces of atom. This mechanism is one source of friction and called atomistic locking.[10] In contrast, for the 2D case of $\theta \neq 0°$, the directions of the forces received by atoms do not line along the direction of sliding at all. Thus, for an infinite system, the sum of the forces received by the atoms may be much smaller than of the case of $\theta = 0°$ and $\alpha = 0°$, or even zero, in which case superlubricity takes place.

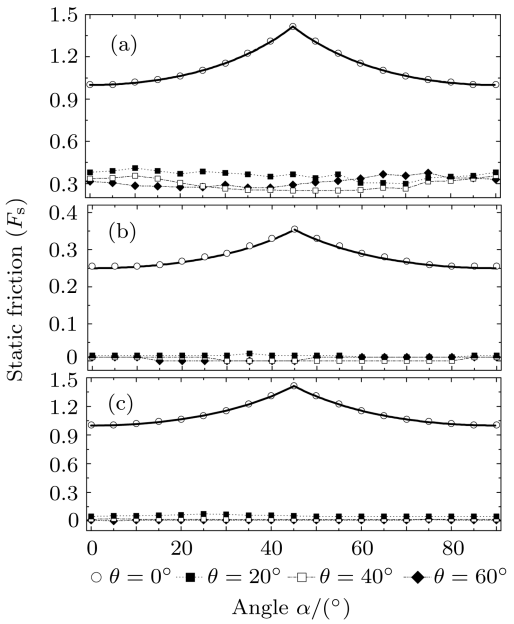


Fig. 5. Static frictions, as a function of α for different vales of misfit angle θ, with the parameters being (a) $f = 1$, $K = 1$ and $\beta = 1$; (b) $f = 0.25$, $K = 1$ and $\beta = 1$; (c) $f = 1$, $K = 10$ and $\beta = 1$. The solid lines are the analytical results of Eqs. (2) and (3).

In addition, the case of $\theta = 0°$ in Fig. 5 grabs our attention. Note that the curves are symmetric about $\alpha = 45°$. Meanwhile, the maximum static frictions are reached when $\alpha = 45°$. They are consequences of the symmetry of the system. Particularly, in the case of $\theta = 0°$, the variation in stiffness strength K cannot affect the static friction (comparing Fig. 5(a) with Fig. 5(c)). We have also carried out more simulations for other choices of the stiffness strength K. All our simulations are in accordance with the regulation. To further understand how the particular feature arises in our system, a more detailed explanation is discussed in the next paragraph.

We sum over all $N \times M$ atoms in the system from Eq. (1) when the system is pinned. $\sum_{n=1,m=1}^{n=N,m=M} \partial V_{\rm sub}/\partial \boldsymbol{r}_{n,m} = (N \times M)\boldsymbol{F}_{\rm ext}$. For a large enough K, the atoms are nearly equally separated, i.e., $x_{n,m} = na + \Delta_x$, and $y_{n,m} = ma + \Delta_y$, where $\mid \Delta_x \mid < a$ and $\mid \Delta_y \mid < a$ are uniform shifts for all atoms. If $\theta \neq 0°$, for most choices of the parameters, the sums above will be zero valued for large enough N and M, i.e., for a classical finite area of the layer. So there is no possible stable solution for $F_{\rm ext} > 0$ and the static friction will vanish. However, when $\theta = 0°$, then sum will not vanish and a nonzero static friction will appear. As a result, for the case of $\theta = 0°$, the static friction is obtained as follows:

$$F_{\rm s} = f\sqrt{1 + \tan^2 \alpha} \tag{2}$$

for $0° \leq \alpha \leq 45°$, and

$$F_{\rm s} = f\sqrt{1 + \tan^2(45° - \alpha)} \tag{3}$$

for $45° \leq \alpha \leq 90°$.

As a final remark, note that from Eqs. (2) and (3), in the locked state, the static friction $F_{\rm s}$ is essentially relevant to the magnitude of the adhesive force f and angle α. The trend is clear according to the above discussion. Consequently, the simple analysis, combined with the simulation results, points out that the theoretical analytical results are in good agreement with numerical ones (see Fig. 5). By the way, based on a simple mechanical model called the 1D FKT model, which combines the FK model with Tomlinson model, Weiss and Elmer[37] also pointed out that in the commensurate case, zero kinetic friction does not imply zero static friction. Furthermore, they also found out that the static friction $F_{\rm s}$ is always unequal to zero in the commensurate structure.

Comparing Figs. 5(a) and 5(b), one can see that the static friction for the case of $f = 0.25$ is smaller than that the case of $f = 1$. It is also noted that except for the case of $\theta = 0°$, the static friction for the case of the smaller f is very small ($\sim 10^{-2}$) or even zero, in which case superlubricity may take place. A few earlier experiments provided indications of superlubricity. Hirano *et al.*[38] found a modest reduction in friction between two mica sheets from 8×10^{-4} to 2×10^{-4} N, caused by rotating the two sheets with respect to each other. By the calculation of the dependency $F_{\rm s}$ in a higher value of $K = 10$ (shown in Fig. 5(c)), we find that the static friction $F_{\rm s}$ decreases with the increase of interatomic strength K. Especially, the choice for $\theta \neq 0°$ can also give rise to superlubricity. A similar phenomenon can be obtained in

the pioneering work.[31,32,37] In a word, the two aforementioned phenomena are explained as follows. For a very stiff layer, for example $f = 0.25$, $\beta = 1$, and $K = 1$ (or $f = 1$, $\beta = 1$, and $K = 10$), the system is unpinned and begins to slide under a small driving force.

In conclusion, variations in the magnitude of the adhesive force f and stiffness constant K affect the system dynamics. Especially, for a very stiff atomic layer, the superlubricity will appear.

4. Conclusions

We have presented a detailed numerical study of the locked-to-sliding transition in the underdamped 2D FK model with a square substrate potential for an arbitrary misfit θ. Our results show that the system parameters, particularly misfit angle θ, stiffness constant K, adhesive force f, direction of driving force α and geometry of the substrate each play a crucial role in the scenario of the locked-to-sliding transition and the determination of the structure of the sliding state.

In the case of sliding between two identical perfectly aligned crystalline workpieces (i.e., $\beta = 1$), by rotating a misfit angle θ, the dynamical behaviour displays two different tribological regimes. At high rates(larger values of the mean velocity or of the external driving force $F_{\rm ext}$), the system slides smoothly. In contrast, at low rates the motion becomes intermittent, with the system alternately sticking and slipping forward. In this situation, energy is stored, while atoms are trapped in metastable states (sticking), and it is converted into kinetic energy as the atoms pop in the next metastable state (slipping). Moreover, the locked-to-sliding transition, observed during the adiabatic increase of the external driving fore $F_{\rm ext}$, is driven by the moving topological local compression (kinks), leading to the growth of a domain of running atoms, finally bringing the system to a running state. On the other hand, investigating frictional processes on the atomic scale, our simulations show that when the two contact solids are not matched with each other (the misfit angle $\theta \neq 0°$), the static friction of the system can also be reduced which is similar to the result in Ref. [37], in particular, for very stiff layers, superlubricity can arise. Our simulations can provide quantitative interpretations of the underlying tribological processes.[37−40]

As a final statement, it is important to stress that the study on the mechanism of the locked-to-sliding transition could make a great contribution to the understanding of the phenomena of friction and lubrication between two flat macroscopic surfaces on the atomic scale. Since the microscopic friction began to be investigated only recently, new experimental and theoretical studies need to be conducted in order to further understand the relevant phenomena.

References

[1] Blatter G, Feigel'man M V, Geshkenbein G B, Larkin A I and Vinokur V M 1994 *Rev. Mod. Phys.* **66** 1125
[2] Marley A C, Higgins M J and Bhattacharya S 1995 *Phys. Rev. Lett.* **74** 3029
[3] Persson B N J 2000 *Sliding Friction* (Berlin: Springer) 2nd ed
[4] Daly C and Krim J 1996 *Phys. Rev. Lett.* **76** 803
[5] Gao J P, Luedtke W D and Landman U 1998 *J. Phys. Chem.* B **102** 5033
[6] Volokitin A I and Person B N J 2003 *Phys. Rev. Lett.* **91** 106101
[7] Persson B N J, Albohr O, Tartaglino U, Volokitin A I and Tosatti E 2005 *J. Phys.*: *Condens. Matter* **17** R1
[8] Shinjo K and Hirano M 1993 *Surf. Sci.* **283** 473
[9] Hirano M and Shinjo K 1990 *Phys. Rev.* B **41** 11837
[10] Hirano M 2003 *Wear* **254** 932
[11] Wenning L and Muser M H 2001 *Europhys. Lett.* **54** 693
[12] Lin M M, Duan W S and Chen J M 2010 *Chin. Phys.* B **19** 026201
[13] Tartaglino U, Samoliov V N and Persson B N J 2006 *J. Phys.*: *Condens. Matter* **18** 4143
[14] Jabbarzadeh A, Harrowell R and Tanner A I 2005 *Phys. Rev. Lett.* 2005 **95** 126103
[15] Erdemir A 2001 *Surf. Coat. Technol.* **146** 292
[16] Dienwiebel M, Verhoeven G S, Pradeep N, Frenken J W M, Heimberg J A and Zandbergen H W 2004 *Phys. Rev. Lett.* **92** 126101
[17] Socoliuc A, Bennewitz R, Gnecco E and Meyer E 2004 *Phys. Rev. Lett.* **92** 134301
[18] Erdemir A 2004 *Surf. Coat. Technol.* **188** 588
[19] Maier S, Sang Y, Filleter T, Grant M, Bennewitz R, Gnecco E and Meyer E 2005 *Phys. Rev.* B **72** 245418
[20] Kano M, Yasuda Y, Okamoto Y, Mabuchi Y and Hamada T 2005 *Tribol. Lett.* **18** 245
[21] Bec S, Tonck A and Fontaine J 2006 *Philos. Mag.* **86** 5465
[22] Muser M H 2004 *Europhys. Lett.* **66** 97
[23] Qi Y, Cheng Y T, Cağin T and William A 2002 *Phys. Rev.* B **66** 085420
[24] Muser M H, Urbakh M and Robbins M O 2003 *Adv. Chem. Phys.* **126** 187
[25] Muser M H, Wenning L and Robbins M O 2001 *Phys. Rev. Lett.* **86** 1295
[26] Braun O M, Bishop A R and Röder J 1997 *Phys. Rev. Lett.* **79** 3692

[27] Zheng Z G, Hu B and Hu G 1998 *Phys. Rev.* B **58** 5453

[28] Guo Y, Qu Z H and Zhang Z Y 2006 *Phys. Rev.* B **73** 094118

[29] Gao X X, Hong X R Wang C L and Duan W S 2008 *Chin. Phys.* B **17** 3378

[30] Tsironis G P, Bishop A R, Savin A V, Zolotaryuk A V 1999 *Phys. Rev.* E **60** 6610

[31] Vanossi A, Bishop A R, Franchini A and Bortolani V 2004 *Surf. Sci.* **566** 816

[32] Vanossi A, Röder J, Bishop A R and Bortolani V 2003 *Phys. Rev.* E **67** 016605

[33] Reichhardt C, Olson C J and Nori F 1997 *Phys. Rev. Lett.* **78** 2648

[34] Tekic J, Braun O M and Hu B 2005 *Phys. Rev.* E **71** 026104

[35] Wang C L, Duan W S, Chen J M and Hong X R 2008 *Appl. Phys. Lett.* **93** 153116

[36] Sasaki N, Kobayashi K and Tsukada M 1996 *Phys. Rev.* B **54** 2138

[37] Weiss M and Elmer F J 1996 *Phys. Rev.* B **53** 7539

[38] Hirano M, Shinjo K, Kaneko R and Murata Y 1991 *Phys. Rev. Lett.* **67** 2642

[39] Hirano M, Shinjo K, Kaneko R and Murata Y 1997 *Phys. Rev. Lett.* **78** 1448

[40] Dienwiehel M, Verhoeven G S, Pradeep N, Frenken J W M, Heimberg J A and Zandbergen H W 2004 *Phys. Rev. Lett.* **92** 126101