Sliding Friction in the Frenkel-Kontorova Model

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Abstract

A two-dimensional Frenkel-Kontorova model under a steady external force is used to study the nonlinear sliding friction between flat macroscopic surfaces with a lubricant layer in between. The nonequilibrium properties of the model are simulated by a Brownian molecular dynamics and results are obtained as a function of temperature and a microscopic friction parameter $\eta$. 
1 Introduction

The behavior of an adsorbed layer under an external force in the plane is a fundamental problem for understanding the mechanisms responsible for friction and lubrication between two flat macroscopic surfaces [1, 2]. Because of the lubricant, the friction between the surfaces is essentially determined by the force required to shear the adsorbed layer. For small external force, this is just the familiar study of the collective diffusion of the overlayer. However, for strong external fields, even a pinned layer can acquire significant mobility at low temperatures due to the lowering of the diffusion barrier by the external field. Moreover, the steady state effective temperature of the overlayer can be significantly higher than that of the substrate. Thus we can actually be dealing with the flow of a liquid layer rather than simple diffusion in the solid phase. Recently, there have been a great deal of interest in the study of this problem in regards to boundary lubrication. In particular, Persson [2] has made a series of studies based on a model of adatoms interacting with Lennard-Jones pair interaction. It is found that the response of the overlayer can develop hysteresis. This means that the threshold field $F_a$ required to initiate the motion of the adlayer is significantly larger than the threshold force $F_b$ below which an initially sliding layer will be pinned again. In fact, based on general hydrodynamical considerations, it is argued that the ratio of $F_a$ to $F_b$ should be 2 for all systems with sizable frictional coupling to the substrate. This hypothesis was tested for the Lennard Jones system by direct numerical simulation and seem to be satisfied [2]. The universality of this relation between sliding friction and static friction still remains an open question. Even the existence of a hysteresis effect is not necessarily true for other models of adsorbed layers.

We introduce a simple model for sliding friction based on a two dimensional version of the Frenkel-Kontorova model [3], where particles are coupled to each other by elastic springs and to a periodic potential. The equilibrium properties of this model are well understood both in one and two dimensions, largely in relation to the study of commensurate and incommensurate transitions [4]. It has also been a standard model in the study of mobility of charge density waves [5]. The infinite range of the harmonic interaction in the model leads to a disordered (fluid) state very different from the conventional one where atoms interact via short range forces. Even in the fluid phase, the atoms cannot diffuse around and will maintain their original neighbours.
Thus it is of particular interest to test whether the universality of hysteresis and the relation between static and kinetic friction still applies to this simple model.

2 Model and Simulation

The simplest version of the Frenkel-Kontorova model in two dimensions is to limit the displacements of the individual atoms in one direction only. Thus the Hamiltonian is of the form

\[
H = \sum_{i,j} \left\{ \frac{p_{ij}^2}{2m} + \frac{K_x}{2}(x_{i+1,j} - x_{ij} - b)^2 + \frac{K_y}{2}(x_{i,j+1} - x_{ij})^2 - U_0 \cos(2\pi x_{ij}/a) \right\}
\]  

(1)

which can be taken to represent a system of coupled linear harmonic chains of particles, each of mass \(m\) moving in a periodic potential of period \(a\) and amplitude \(U_0\). The second term represents the elastic interaction within a chain and the third term represents interaction between adatoms on different chains. The index \(i, j\) labels the particle with integer \(i (i = 1, ..., N_x)\) and the chain with integer \(j (j = 1, ..., N_y)\), so that the system consists of \(N_x \times N_y\) adsorbates at positions \(x_{i,j}\). We have considered \(N_x = N_y = N\) and \(K_x = K_y = K\).

Most of our results are obtained assuming periodic boundary conditions which means that the \(N + 1, j\) particle is a periodic image of particle \(1, j\) in each chain, so that \(x_{N+1,j} = x_{1,j} + N_s a\), where \(N_s\) is the number of local minima of the periodic substrate in the \(x\)-direction. In the other direction, periodic boundary condition means that \(x_{i,N+1} = x_{i,1}\). The average distance between particles, \(b\), in each chain is determined through the boundary condition and is given by \(b = N_s a/N\) and the overlayer coverage can be defined as \(\theta = N/N_s\). With this setup, \(b\) and \(\theta\) cannot be changed independently and the ratio \(b/a\) is forced to be rational. We have also performed few calculations with free boundary conditions in the \(x\)-directions. In this case, the ratio \(b/a\) can assume arbitrary nonrational values. The system now can remain commensurate for a given \(\theta\) only up to a critical value \(\delta_c\) of the misfit parameter \(\delta = (b - a)/a\).
To study sliding friction in the model we assume that the substrate acts as a heat bath at an equilibrium temperature $T$ and that an external force $F$ acts on each of the adsorbates. The equation of motion for the particle coordinates are described by Brownian dynamics

$$m\ddot{x}_{ij} + m\eta\dot{x}_{ij} = -\frac{\partial V}{\partial x_{ij}} - \frac{\partial U}{\partial x_{ij}} + F + f_{ij} \tag{2}$$

where $U$ is the periodic potential, $V$ is the adsorbate-adsorbate harmonic interaction potential and $f_{ij}$ is a random force that is related to the microscopic friction parameter $\eta$ by the fluctuation dissipation theorem

$$< f_{ij}(t) f_{i'j'}(t') > = 2\eta m k_B T \delta_{i,i'} \delta_{j,j'} \delta(t-t') \tag{3}$$

We have studied the sliding friction of the adsorbate by simulating the above equations using standard methods of Brownian molecular dynamics [6]. We use units in which $a = 1$, $m = 1$ and $U_o = 1$. Typically, the time variable was discretized with time step $\delta t = 0.02\tau$ to $0.06\tau$ where $\tau = (ma^2/U_o)^{1/2}$ and $4 \times 10^5$ time steps were used in each calculation allowing $10^5$ time steps for equilibration. The elastic constant was set to $K = 10$ and calculations were performed as function of temperature, external force and coverage for a system containing $N \times N$ adsorbate particles where $N = 10$. The system was allowed to evolve into a steady state such that the time average of physical quantities approached a constant.

3 Results and Discussion

When the external $F = 0$, the drift velocity $v_d$ of the adsorbate center of mass is zero independent of the temperature with each particle performing a Brownian motion. At $T = 0K$, the velocity remains zero for any applied force less than a critical value $F_o$ where the effective potential minima disappears, $F_o = 2\pi U_o$, the same result as for the one-dimensional case [4]. From now on, we will normalize the external force by this critical value. If a small force is applied at higher enough temperature, in addition to the irregular motion of the particles, one expects an overall drift in the direction of the force with a speed $v_d$ proportional to the external force, $v_d = F/m\bar{\eta}$ in the linear regime, where $\bar{\eta}$ is an effective sliding friction. Fig. 1 shows the results of the inverse of the normalized linear sliding friction, $\eta/\bar{\eta}$, calculated as a
function of temperature for a small value of the external force, $F/F_0 = 0.035$ and $b/a = 2$. At low temperatures the adlayer is in a pinned state at small forces, and $\eta/\bar{\eta}$ is essentially zero. As the temperature is increased $1/\bar{\eta}$ remains zero until $T = T_c$, beyond which $\eta/\bar{\eta}$ increases significantly and should approach 1 at higher enough $T$. The value of $T_c$ correspond to the commensurate solid-fluid transition where the overlayer at high temperatures become disordered and is effectively depinned from the substrate. Figs. 2 and 3 shows snapshot pictures of the adsorbate in the commensurate solid and the fluid state respectively. From Fig. 1 we estimate that $T_c \approx 2.3$. We have also performed similar calculations with different boundary conditions. In Fig. 4 we show the results for the structure factor at low and high temperatures for $b/a = 1.9$ with free boundary condition. At low $T$ the structure factor has a sharp peak at $q = \pi$ and the overlayer is commensurate with the substrate with lattice vector $2a$. At high $T$ the structure factor is much broader corresponding to a fluid state. For $b/a = 1.9$ it peaks at an incommensurate value which is temperature dependent and limited by $q = 2\pi/b$. The corresponding result for $b/a = 2$ and p.b.c is similar except that the structure factor at high temperature remains peaked at $q = \pi$.

In the nonlinear regime, the relation between $v_d$ and $F$ is expected to depend strongly the initial phase. If the adsorbate, when $F = 0$, is a fluid, $v_d$ will be nonzero for arbitrarily small external force. This result is also true for the present model. In the fluid phase above $T_c$, the overlayer is essentially depinned and any small force leads to nonzero $v_d$. Moreover, the relation $v_d = f(F)$ shows no hysteresis. For $T < T_c$ however, where a commensurate (solid phase) prevails when $F = 0$, a critical force $F_a$ is necessary to depin and initiate sliding. It is expected that in this case the nonlinear sliding friction exhibit hysteresis as a function of $F$, i.e., the relation between velocity and external force depends on whether $F$ increases from zero or decreases from a high value and this in turn implies a stick and slip motion.

In Fig. 5, we show the results for $v_d$ as a function of $F$ for $\eta = 0.6$, $T = 0.5$. Note that in this case the temperature is considerably less than the activation energy barrier ($2U_0$) for particle diffusion. We found that this is an important requirement for hysteresis to appear. Initially, the adlayer is in a pinned state. Then the simulation was started with various external force strengths. An hysteresis loop is clearly seen, corresponding to a stick and slip motion. The effective temperature $T^*$ of the adlayer is shown Fig.
6. It is seen that the initial sliding phase when the applied force is increased beyond the static threshold $F_a$ has almost the same temperature as the substrate and the substrate potential provides no additional resistance. This is a sliding solid phase. It corresponds to the floating or incommensurate solid phase in the equilibrium situation. It is important to note that this phase is dynamically generated by the external field. With our present choice of parameters, the misfit is zero and the floating solid phase does not exist in equilibrium. Thus the external force induces a commensurate solid to sliding solid transition at $F = F_a$. As the force is decreased through $F_a$, there is a jump in $T^*$ accompanied by a simultaneous decrease in $v_d$. This corresponds to an overheating of overlayer to an effective temperature above $T_c$ (compare with Fig. 1), dynamically “melting” the sliding solid phase. This can be regarded as sliding solid to fluid transition. Finally at $F = F_b$, the fluid phase condenses into a commensurate solid phase and the temperature of the adlayer and the substrate become the same again. The fact that there is a condensation from the ”melted” phase is confirmed by noting that the temperature of the adlayer at this condensation is almost identical to the temperature $T_c$, the temperature where the pinned solid to fluid phase transition occurs. Thus there is already a rich variety of dynamical phase transitions manifested in this simple model. We note that Persson [2] has observed very similar phase transitions for Lennard-Jones systems, showing that these features are universal in the non-linear response of overlayers and not just for specific models. In addition the present results show that a conventional ”liquid” phase is not required and a high temperature disordered fluid phase with vanishing shear resistance is sufficient to show some of these effects.

We now consider the behavior of the nonlinear sliding friction at higher temperatures but still less than $T_c$. We find that at $T \approx U_o$, hysteresis disappears as indicated in Fig. 7 but $F_a$ can still be defined. This behavior is not specific to the present model and has also been found in the molecular dynamics simulation of the Lennard-Jones system [4]. This temperature is comparable to the energy barrier for center of the mass diffusion and for a given force $F$, within the range where hysteresis is observed at low $T$, the system is able to relax in a short enough time to a stable single velocity, independent of the history of force variation. This suggests that the hysteresis observed at low $T$ is due to metastability.

We have also studied the effects of varying the microscopic friction pa-
rameter $\eta$ and found that the ratio $F_b/F_a$ strongly depends on $\eta$ and converge to $F_b/F_a = 1$ for sufficiently large $\eta$ as shown in Fig. 8. This should be contrasted to the results obtained by Persson [2] for the Lennard-Jones system where $F_b/F_a$ is found to saturate for large $\eta$ at a universal value $\approx 0.6$. We suggest that this is due to the fact that the nature of the fluid phase in the two models are very different. The hydrodynamics arguments used by Persson [2] based on the existence of a drag force acting on a nucleating domain may not be valid in this case.

4 Conclusions

There are many questions that remains to be investigated. The most important one is probably to establish which features of the nonlinear transport are universal and model independent and which ones are model sensitive. Already, we have observed in the Frenkel-Kontorova model that under increasing values of the microscopic friction $\eta$, the hysteresis loop tends to disappear whereas it is stable in the Lennard Jones system. We suspect that this is related to the stability of the sliding solid phase as a function of $\eta$ as well as the dependence of the fluid-pinned solid transition on the nature of the fluid state. However, many features observed in the Lennard-Jones system also appear in the simple Frenkel-Kontorova model. The advantage of this model system is that the equilibrium property of the commensurate-incommensurate transition is well understood through a series of studies.

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Figure 1: Inverse of the normalized sliding friction $\bar{\eta}$ as a function of temperature $T$ for $\eta = 0.5$, $b/a = 2$.
Figure 2: Snapshot picture of the adsorbate in the commensurate solid phase, for $T = 0.5$, $b/a = 2$. 
Figure 3: Snapshot picture of the adsorbate in the high temperature phase, for $T = 3, b/a = 2$. 
Figure 4: Structure factor $S(q)$ as a function of reciprocal lattice vector $q$ at different temperatures, using free boundary conditions and $b/a = 1.9$. Open diamonds correspond to $T = 0.5$ and circles to $T = 3$. The large and small arrows indicate reciprocal lattice vectors $q = 2\pi/2a$ and $q = 2\pi/b$, respectively.
Figure 5: Drif velocity $v_d$ as a function of external force $F$ for $\eta = 0.6$ and $T = 0.5$. 
Figure 6: Effective temperature $T^*$ of the overlayer normalized to the substrate temperature $T$ as a function of the external force $F$ for $\eta = 0.6$ and $T = 0.5$. 
Figure 7: Drift velocity $v_d$ as a function of external force $F$ for $T = 1$ and $\eta = 0.5$. 
Figure 8: Ratio $\frac{F_b}{F_a}$ as a function of $\eta$ for $T = 0.5$