Hysteresis phenomenon in commensurate structures with an asymmetric deformable substrate potential

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Abstract. Hysteresis is studied in an asymmetric deformable substrate potential. When the upper atom chain is driven by an external force, the average velocity of the upper atom changes from zero to non-zero. The force at this point is defined as the maximum static friction force. When external driving forces continue to increase, at some value, the external driving force is reduced slowly. The average velocity of the upper atom changes from non-zero to zero, this critical force is defined as the maximum kinetic friction force. The static friction and kinetic friction force have been analyzed for the shape parameter.

1. Introduction

The Frenkel–Kontorova model is widely used in the study of nonequilibrium properties and other physical fields, especially in condensed matter physics [1, 2, 3]. Because it is a theoretical tool for in-depth study of complex problems in the field of nanotribology, it can make it easier for people to understand the mechanism of nanotribology [4, 5, 6].

In the recent experimental studies in the measuring of the friction force between two contacting layers, the influence of the misfit angle on the friction force has been studied. According to results, superlubricity (the state of vanishing friction) may appear for certain values of the misfit angle [7].

Hysteretic phenomenon is studied by Li ru tao et al. in the 2D Frenkel-Kontorova model system. The influence of four critical forces on the system parameters such as stiffness coefficient, misfit angle, winding number is investigated [8]. However, hysteretic phenomenon is seldom studied in the 1D Frenkel-Kontorova model system with an asymmetric deformable substrate potential.

In this paper, hysteresis is studied in an asymmetric deformable substrate potential. When the upper atom chain is driven by an external force, the average velocity of the upper atom changes from zero to non-zero, the force at this point is defined as the maximum static friction force. When external driving forces continue to increase, at some value, the external driving force is reduced slowly. The average velocity of the upper atom changes from non-zero to zero. The force at this point is defined as the maximum kinetic friction force. The static friction and kinetic friction force have been analyzed for the shape parameter.

2. Model

We consider the one-dimensional lattice of particles with harmonic interaction (upper layer) coupled to a static pinning potential (lower layer). The upper layer is driven by an external driving force $F_{ext}$ where the neighbors of each particle are fixed. The asymmetric deformable substrate potential [9] is given as follows:
\[
V(u) = \frac{K}{(2\pi)^2} \frac{(1-r^2)[1-\cos(2\pi u)]}{[1+r^2+(2r \cos(\pi u))^2]}, \quad (1)
\]

Where \( K \) is the pinning strength and \( r \) is the shape parameter \((-1 < r < 1)\). In Fig. 1, we plotted the asymmetric deformable substrate potential for different values of \( r \).

![Substrate potential for different values of the shape parameter](image)

**FIG. 1.** Substrate potential for \( K = 4 \) and different values of the shape parameter \( r \).

The particles are driven by the force \( F_{\text{ext}} \). The system satisfies the following equation of motions:

\[
m u_i = -\gamma u_i + g(u_{i+1}+u_{i-1}-2u_i) + \frac{dV}{du_i} + F_{\text{ext}}, \quad (2)
\]

Where \( u_i (i = 1,2,3,...N) \) stands for the coordinates of \( N \) chain particles. The damping \( \gamma \) terms in Eqs. (1) describe the dissipative forces that are proportional to the relative velocities of the particles with substrate. The coefficient \( \gamma \) represents degrees of freedom inherent in the real physical systems (e.g., substrate phonons and electronic excitations) (we choose \( \gamma = 0.1 \) in our numerical examples, so that it is an underdamped system). Simulations have provided indirect evidence that such phenomenological viscosity terms serve this purpose. We have used dimensionless units with chain atom mass \( m = 1 \) and substrate period \( a = 1.0 \). The fourth terms in Eqs. (2) represents the on-site interaction between the particles and the substrates. The interparticle chain interaction [third term in Eq. (2)] is harmonic with strength \( g \) and equilibrium spacing \( b \).

Eqs. (2) has been using the fourth-order Runge–Kutta method. The time step used in the simulations is 0.02s, and a time interval of 100s is used as a relaxation time to allow the system to reach the steady state. The force is varied with the step of \( 10^{-4} \).

3. Results and discussion

In fig. 2, the variation of the average atomic velocity of the upper layer with the driving force \( F_{\text{ext}} \) for \( K = 4 \), and different values of the shape parameter \( r \) : (a) \( r = 0.0, g = 1.0 \); (b) \( r = 0.5, g = 1.0 \) is presented. In the pinning-depinning transition the average velocity of particles is zero. When the external driving force increased, the average velocity of the upper atom \( \dot{v} \) changes from zero to non-zero. The force at this point is defined as the maximum static friction force \( F_s \). When external driving forces continue to increase, at some value, the external driving force is reduced slowly. The
average velocity of the upper atom changes from zero to non-zero. It is defined that the critical force at this point as the maximum kinetic friction force $F_k$.

![Graph showing average velocity as a function of the average driving force $F_{ext}$ for different values of the shape parameter $r$.](image)

FIG. 2. Average velocity $v$ as a function of the average driving force $F_{ext}$ for $K = 4$, and different values of the shape parameter $r$: (a) $r = 0.0, g = 1.0$; (b) $r = 0.5, g = 1.0$;

It is found that different $r$ has a great influence on the maximum static $F_s$ and kinetic friction force $F_k$ of the system. The maximum static $F_s$ and kinetic friction force $F_k$ as a function of the shape parameter $r$ for $K = 4$ are presented in Fig. 3(a) and Fig. 3(b). When $r$ increases, the maximum static friction increases to a certain value first, and then presents a chaotic form. The maximum kinetic friction also shows the same trend. It can be seen that when $r$ is fixed, the maximum static friction force is greater than the maximum kinetic friction force, which also corroborates the physical law.
FIG. 3. (a) the maximum static friction force $F_s$ as a function of the shape parameter $r$ for $K = 4$.

(b) the maximum kinetic friction force $F_k$ as a function of the shape parameter $r$ for $K = 4$.

4. Conclusions
In this paper, it is studied that the interaction of a simple harmonic interaction atomic chain subjected to an asymmetric deformable substrate potential. The harmonic interaction atomic chain is driven by external force. When the external driving force increases, the average velocity of the upper atom changes from zero to non-zero. The force at this point is defined as the maximum static friction force. When external driving forces continue to increase, at some value, the external driving force is reduced slowly. The average velocity of the upper atomic chain changes from non-zero to zero. The force at this point is defined as the maximum kinetic friction force. It is presented that the maximum static and kinetic friction force as a function of the shape parameter. It is concluded that when $r$ increases, the maximum static friction increases to a certain value first, and then presents a chaotic form. The maximum kinetic friction also shows the same trend. It can also be seen that when $r$ is fixed, the maximum static friction force is greater than the maximum kinetic friction force, which also corroborates the physical law.

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