Theoretical study of friction: One-dimensional clean surfaces

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Another method has been proposed to evaluate the frictional force in the stationary state. This method is applied to the one-dimensional model of clean surfaces. The kinetic frictional force is seen to depend on velocity in general, but the dependence becomes weaker as the maximum static frictional force increases and in the limiting case the kinetic friction becomes only weakly dependent on velocity as described by one of the laws of friction. It is also shown that there is a phase transition between a state with vanishing maximum static frictional force and a state with finite static frictional force. The role of randomness at the interface and the relation to the impurity pinning of the sliding charge-density wave are discussed.

I. INTRODUCTION

The study of friction has been carried out for a long time.[1] Recently, developments of new technologies enable us to investigate the friction in a situation that was not considered before.[2–10] It is well known that the three laws of friction hold well in a usual situation:[1] (i) The frictional force does not depend on the apparent area of contact surfaces. (ii) The frictional force is proportional to the normal load, where the proportionality constant is called the coefficient of friction. (iii) The kinetic frictional force does not depend on the relative velocity of the contact surfaces and is less than the maximum static frictional force. It is also known that there are cases where these laws of friction no longer hold. The limitation of the laws and the possible new laws which hold beyond such limitation have, however, not been clarified to the best of our knowledge. Actually, even though there exist attempts at the theoretical explanation of the laws of static friction as discussed below, a concrete explanation of the laws of kinetic friction is lacking. This paper is our first step to study these basic questions on friction theoretically.

Theoretical explanations of the laws of static friction have been as follows.[1] Due the the surface roughness the area of actual contacting points is much less than the apparent contact area, and the pressure there reaches the yield pressure. Thus the total area of actual contact points is proportional to the normal load. The two surfaces adhere to each other by intermolecular forces at the contact. The maximum static frictional force is equal to the shear strength of the contact times the total area of contacting points, and is thus proportional to the normal load.

This view cannot be applied to a clean surface without surface randomness.[6] For example, as the interatomic force between two bodies works among all atoms at surfaces, the frictional force is expected to survive even for vanishing normal load and to be proportional to the contacting area, and then the first and second laws of friction will no longer hold.

Recently Hirano and Shinjo[6,8] pointed out another peculiar feature of the friction of clean surfaces. That is the frictional transition, which is the phase transition between states with and without finite maximum static frictional force. In the simplest case of one dimension (1D) where the atoms of the one body are fixed, the model reduces to the Frenkel-Kontorova model.[11] In that model such a phase transition is known to exist when the ratio of mean atomic distances of the two bodies is irrational, i.e., in the incommensurate case. This transition is called Aubry's breaking of analyticity transition.[12] When the strength of the interatomic potential is less than a critical value, the spatial configuration of atoms in the ground state is smooth and the maximum static frictional force vanishes. Above the critical value the configuration has a discommensurate structure and the maximum static frictional force is finite. Hirano and Shinjo have claimed the existence of such a frictional transition even in a 3D model where the atoms of the lower body are fixed, and that the static frictional force can vanish between pure metals with incommensurate clean surfaces, e.g., (111) and (110) surfaces of α-iron.[6,8]

All of these studies are, however, based on the model where atoms in one of the interfaces are held fixed. Nothing is known about the frictional transition in a more realistic model where both atoms can relax. The behavior of kinetic friction has also not been explored yet.

Deferring detailed studies on rough surfaces until future publications, we study in this paper the static and kinetic frictional forces of the 1D model of clean surfaces, where atoms on both sides of the interface can relax. In the theoretical study of friction, it is not clear even what should be calculated as the frictional force, and a method of calculation has not been established.

We first propose a method to calculate the kinetic frictional force in a stationary state and then apply it to a 1D model of clean surfaces. We derive the explicit velocity dependence of the kinetic friction of the present microscopic model. It is seen that the velocity dependence is appreciable in general. This dependence becomes weaker as the maximum static frictional force increases, and eventually the kinetic friction becomes almost velocity independent, as described by the third law of friction. At the same time we also find the frictional transition in the present model.

This paper is organized as follows. In Sec. II we address ourselves to the method to calculate the frictional force. In Sec. III we define the 1D model of clean surfaces and discuss the relationship of the present model with the Frenkel-Kontorova model. Then the numerical results based on the model are presented. Finally in Sec. IV we summarize the present results and discuss the effects of randomness and the relation to the impurity pinning of the sliding charge-density wave.

II. WHAT SHOULD BE CALCULATED AS A FRICTIONAL FORCE?

First let us consider what we should calculate in order to obtain the frictional force theoretically. We discuss the static and kinetic frictional forces between two bodies which are in contact. We assume that the contacting surfaces are on the average horizontal in order to simplify the problem and the external force is applied to the upper body. The extension of the present model to other cases is quite easy. Each body consists of atoms considered as classical point particles. Their equations of motion are expressed as follows.

$$m_a\ddot{\mathbf{u}}_i+m_a\gamma_a(\dot{\mathbf{u}}_i-\langle\dot{\mathbf{u}}_i\rangle_i)=\sum_{j\in a}\mathbf{F}_a(\mathbf{u}_i-\mathbf{u}_j)+\sum_{j\in b}\mathbf{F}_I^{(i,j)}(\mathbf{u}_i-\mathbf{v}_j)+\mathbf{F}_{\rm ex}+\mathbf{F}_{G_a}\ , \tag{1a}$$

$$m_b\ddot{\mathbf{v}}_i+m_b\gamma_b(\dot{\mathbf{v}}_i-\langle\dot{\mathbf{v}}_i\rangle_i)=\sum_{j\in b}\mathbf{F}_b(\mathbf{v}_i-\mathbf{v}_j)+\sum_{j\in a}\mathbf{F}_I^{(i,j)}(\mathbf{v}_i-\mathbf{u}_j)+\mathbf{F}_s(\mathbf{v}_i)+\mathbf{F}_{G_b}\ . \tag{1b}$$

Here $\mathbf{u}_i$ ($\mathbf{v}_i$) is the position vector of the ith atom of the upper (lower) body, m_α ($\alpha=a,b$) is the atomic mass, γ_α is the parameter of energy dissipation, the subscript a (b) refers to the upper (lower) body, and $\langle\cdots\rangle_i$ represents the average with respect to i. The four terms in the right-hand side of Eq. (1a) represent the interatomic force between atoms of the upper body $\mathbf{F}_a(\mathbf{u}_i-\mathbf{u}_j)$, that between the ith atom of the upper body and the jth atom of the lower body $\mathbf{F}_I^{(i,j)}(\mathbf{u}_i-\mathbf{v}_j)$, the external force $\mathbf{F}_{\rm ex}$, and the gravitational force $\mathbf{F}_{G_a}$, respectively. The first term on the left-hand side of Eq. (1a) is the inertial term. The second one represents the effect of the energy dissipation to the degrees of freedom, which are not considered explicitly here. Such degrees of freedom belong to the same body, so that the effect is proportional to the difference of the velocity of the ith atom and that of the center of gravity. The terms in Eq. (1b) are the same as those in Eq. (1a) except the third term in the right-hand side, $\mathbf{F}_s(\mathbf{v}_i)$, which represents the force between the ith atom of the lower body and the substrate and is necessary to keep the lower object from moving with the upper body. Hereafter we consider only the stationary state, sum up Eq. (1a) for all atoms, and average the equation with respect to time. Then the first term in the left-hand side vanishes by the time-averaging procedure and the second term in the left-hand side and the first term in the right-hand side vanish by summing the equation for i. Hence we obtain

$$-\sum_{i\in a}\sum_{j\in b}\langle F_{I\parallel}(\mathbf{u}_i-\mathbf{v}_j)\rangle_t=N_a\langle F_{\rm ex}\rangle_t\ . \tag{2}$$

Here $F_{I\parallel}$ is the component of $\mathbf{F}_I$ parallel to the external force, N_a is the number of atoms of the upper body, and $\langle\cdots\rangle_t$ represents the average with respect to t. With the total external force in the right hand side of Eq. (2) the upper body will either stop or be in constant-velocity motion. Hence the left-hand side, the total sum of the interatomic forces between atoms of the upper body and those of the lower body, is the frictional force, which should be calculated. It is to be noted that, under an external force greater than the maximum static frictional force, all the energy supplied by the external force flows into the lattice vibrations and then dissipates via the second terms with γ_a and γ_b in Eq. (1). Hence the stationary state is achieved. Since the dissipation is proportional to the difference of the velocities between each atom and the center of gravity, the expression of the total frictional force in the stationary state, Eq. (2), does not depend on γ_a and γ_b.

III. ONE-DIMENSIONAL MODEL OF FRICTION OF CLEAN SURFACES AND NUMERICAL RESULTS

A. The model

As mentioned in Sec. I it is known that the surface roughness plays an important role in friction under the usual situation and makes the laws of static friction work. Deferring studies on such realistic cases to further publications, we consider, in this paper, the friction between clean surfaces, i.e., surface without randomness even on an atomic scale. In that case the interatomic force between two bodies works among all atoms at the surfaces, and the gravitational force can be neglected since it is very small compared with the interatomic force, at least in the first approximation. The problem is to understand how the friction works in such a case. In order to simplify the problem we consider the 1D model of clean surfaces, where the atoms in both bodies make 1D rings and their degrees of freedom are also 1D. The equations of motion are given as follows.

$$m_a\ddot{u}_i+m_a\gamma_a(\dot{u}_i-\langle\dot{u}_i\rangle_i)=K_a(u_{i+1}+u_{i-1}-2u_i)+\sum_{j\in b}F_I(u_i-v_j)+F_{\rm ex}\ , \tag{3a}$$

$$m_b\ddot{v}_i+m_b\gamma_b(\dot{v}_i-\langle\dot{v}_i\rangle_i)=K_b(v_{i+1}+v_{i-1}-2v_i)+\sum_{j\in a}F_I(v_i-u_j)-K_s(v_i-ic_b)\ . \tag{3b}$$

Here we have adopted the harmonic approximation both for the interatomic force among atoms of the same body and for the force between atoms of the lower body and the substrate, and we take the forces only between nearest neighbors. In Eq. (3b) c_b is the mean atomic spacing of the lower body. K_a and K_b are the strengths of the interatomic force within the same body. K_s is the strength of the force between the lower atoms and their equilibrium positions on the substrate and controls the rigidity of the lower body. Here we assume the same F_I among all atoms. Periodic boundary conditions for u_i and v_i, $u_i=u_{i+N_a}, v_i=v_{i+N_b}$ are adopted. The interatomic force F_I is obtained from the interatomic potential U_I as,

$$F_I(x)=-\frac{d}{dx}U_I(x)\ , \tag{4}$$

where the actual form of $U_I(x)$ is assumed to be

$$U_I(x)=-\frac{K_I}{2}\exp\left[-4\left[\frac{x}{c_b}\right]^2\right]\ , \tag{5}$$

in order to make the correspondence with the Frenkel-Kontorova model mentioned in Sec. I. Here K_I is the strength of the interaction. With U_I given by Eq. (5), the interatomic force acting on u_i is almost a sinusoidal function when the lower atoms are fixed. So the present model reduces essentially to the Frenkel-Kontorova model in that case.

In the calculation we modify Eq. (3a) as

$$m_a\gamma_a\dot{u}_i=K_a(u_{i+1}+u_{i-1}-2u_i)+\sum_{j\in b}F_I(u_i-v_j)+G_{\rm ex}\ , \tag{6}$$

where

$$G_{\rm ex}=m_a\gamma_a\langle\dot{u}_i\rangle_i+F_{\rm ex}\ .$$

In principle, $G_{\rm ex}$ has temporally oscillating components, whose amplitude, however, decreases with system size. Hence we neglect this oscillatory component and solve the above equation of motion by the Runge-Kutta procedure for a given constant $G_{\rm ex}$. In Eq. (6) we also neglect the inertial term, which is valid under the condi-

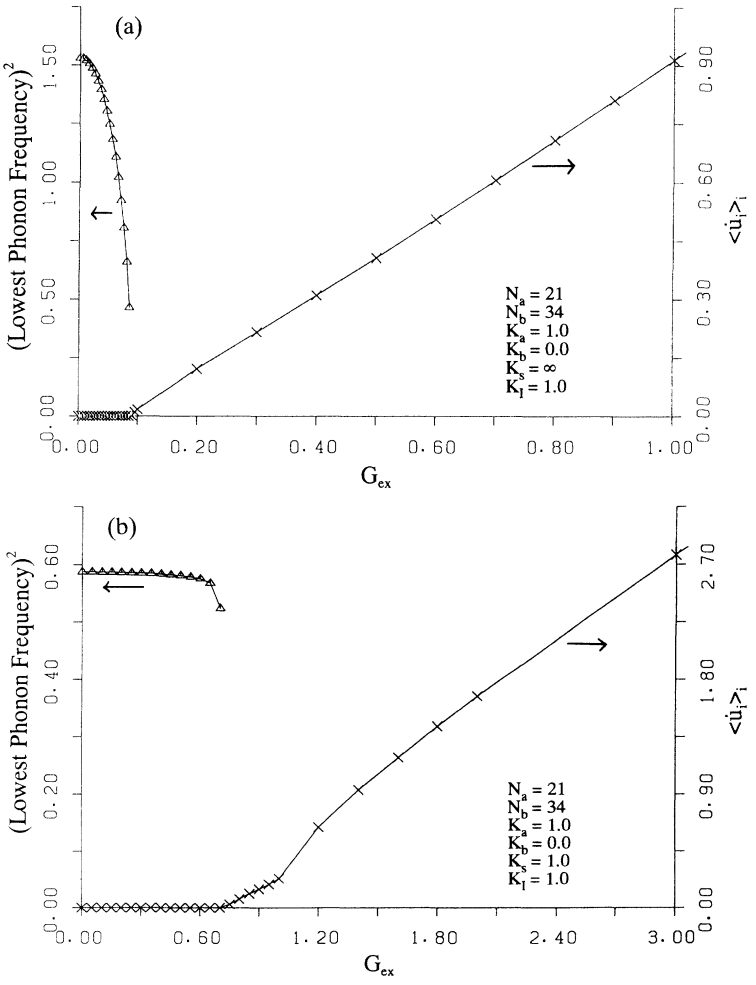

FIG. 1. $G_{\rm ex}$ dependence of the velocity and the square of the lowest phonon frequency for $K_a=1$, $K_b=0$, $K_I=1$ and $K_s=\infty$ (a) and 1 (b).

tion $\langle \dot{u}_i \rangle_i / c_a \ll \gamma$.

Due to the periodic boundary conditions, the system sizes of upper and lower bodies are the same. Then the ratio of the mean lattice spacings of the two bodies is equal to the inverse of the ratio of the numbers of each type of atom, $c_a/c_b = N_b/N_a$. In this paper we have chosen $c_a/c_b = N_b/N_a = 34/21 = 1.6190\ldots$, which is the truncated value of the continued-fraction expansion of the golden mean $(\sqrt{5}/2+1)/2 = 1.6180\ldots$, at the eighth order. In a finite-size system there is a possibility of the appearance of commensurability pinning. In the present system we observe no such effect within our numerical accuracy. We set $m_a = m_b = 1$, $\gamma_a = \gamma_b = 1$, $c_b = 1$, $K_a = 1$, and $K_b = 0$.

B. Numerical results

In Fig. 1 we show the velocity and the square of the lowest phonon frequency, which is proportional to the restoring force, as a function of G_{ex} for the two cases where the atoms of the lower body are fixed (a) and are able to relax (b). The maximum G_{ex} where the velocity vanishes is the maximum static frictional force. A remarkable difference between the two cases is the magnitude of the maximum static frictional force, which is much larger in the case of mobile lower atoms than in the case of fixed ones. This is due to the fact that in the former case the system can find its stable configuration under an external force more easily than in the latter case. Another difference between them is the behavior of the lowest phonon frequency. In Fig. 1(a) the frequency and thus the restoring force decreases gradually with G_{ex} and vanish at the maximum static frictional force. But the frequency has an almost constant value up to just below the maximum static frictional force and then vanishes abruptly in (b).

Figure 2 shows the maximum static frictional force as a function of the strength of the interatomic force between the two bodies, K_I, with several choices of the rigidity of the lower body, K_s. It is shown that, in the case of fixed lower atoms, $K_s = \infty$, there is an Aubry transition[12] and the static maximum frictional force vanishes below some critical value of K_I and grows gradually above it. Such a transition really exists even in the case of mobile lower atoms within our numerical accuracy, but the critical value of K_I and the region where the maximum static frictional force vanishes decrease with decreasing K_s. Simultaneously the maximum static frictional force above the critical value grows rapidly.

As regards the kinetic frictional force, the velocity dependence is shown in Figs. 3 and 4, where Fig. 3 (4) represents the case of fixed (mobile) lower atoms. As

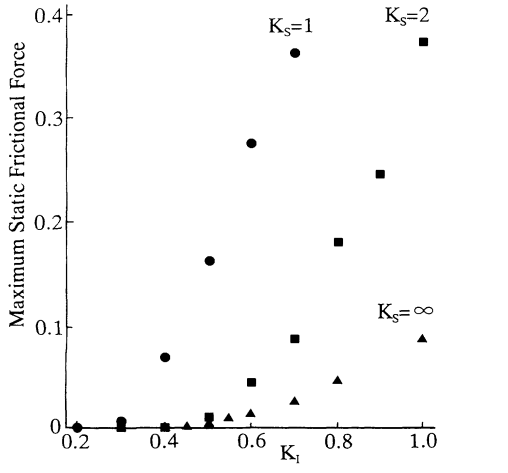

FIG. 2. Maximum static frictional force as a function of K_I for various values of K_s.

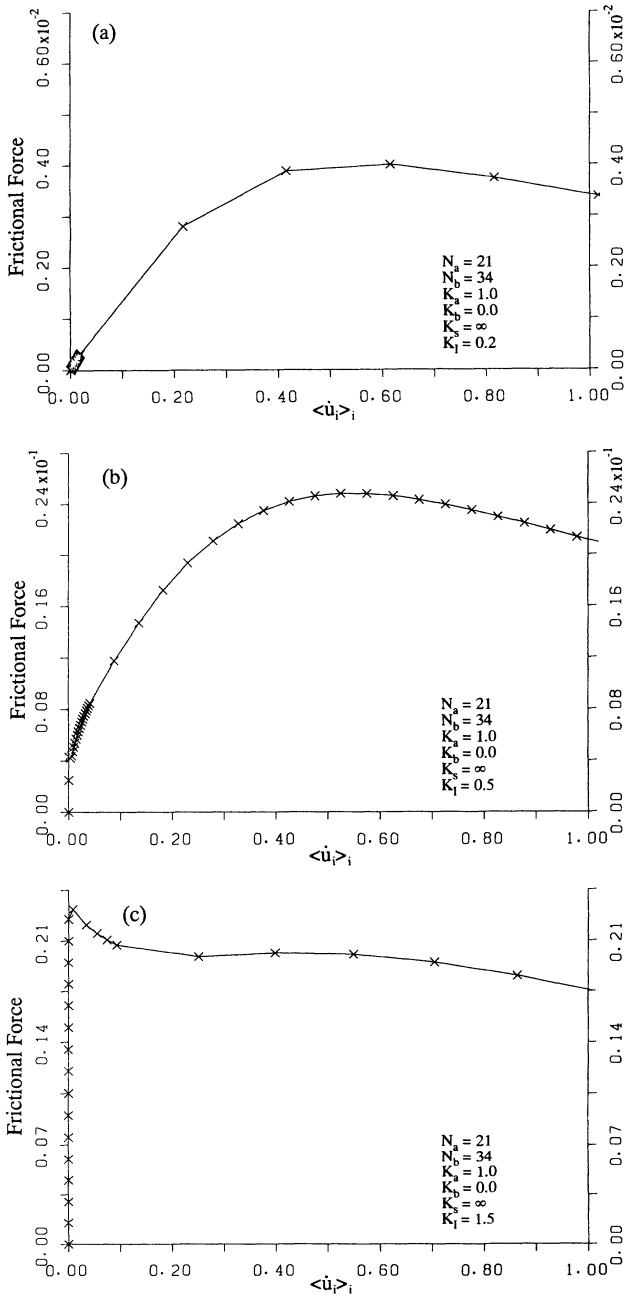

FIG. 3. Velocity dependence of the frictional force for $K_a = 1$, $K_b = 0$, $K_s = \infty$, and $K_I = 0.2$ (a), 0.5 (b), and 1.5 (c).

shown by (a), where the value of K_I corresponds to that just below the critical value of Aubry's transition, the kinetic frictional force is always finite even if the maximum static force vanishes. In (b) we show the case where the value of K_I corresponds to that just above the critical value. In this case the kinetic frictional force increases gradually with velocity from the maximum static frictional force, takes its maximum, and then decreases, that is, the kinetic frictional force can be larger than the maximum static frictional force. As the maximum static frictional force increases with K_I the velocity dependence of the kinetic frictional force becomes weaker, as seen in Fig. 3(c) and 4(c) for two choices of K_s. In that case the kinetic friction shows similar behavior to that described by one of the laws of friction, (iii) in the Introduction. Temporally sequential snapshots of the configurations of the atomic positions are shown in Fig. 5 for the case of low velocity. It is clearly seen that the lower atoms jump from one metastable position to the next one as time goes on. This corresponds to stick-slip motion. As the velocity of the system increases, such motion diminishes as shown in Fig. 6.

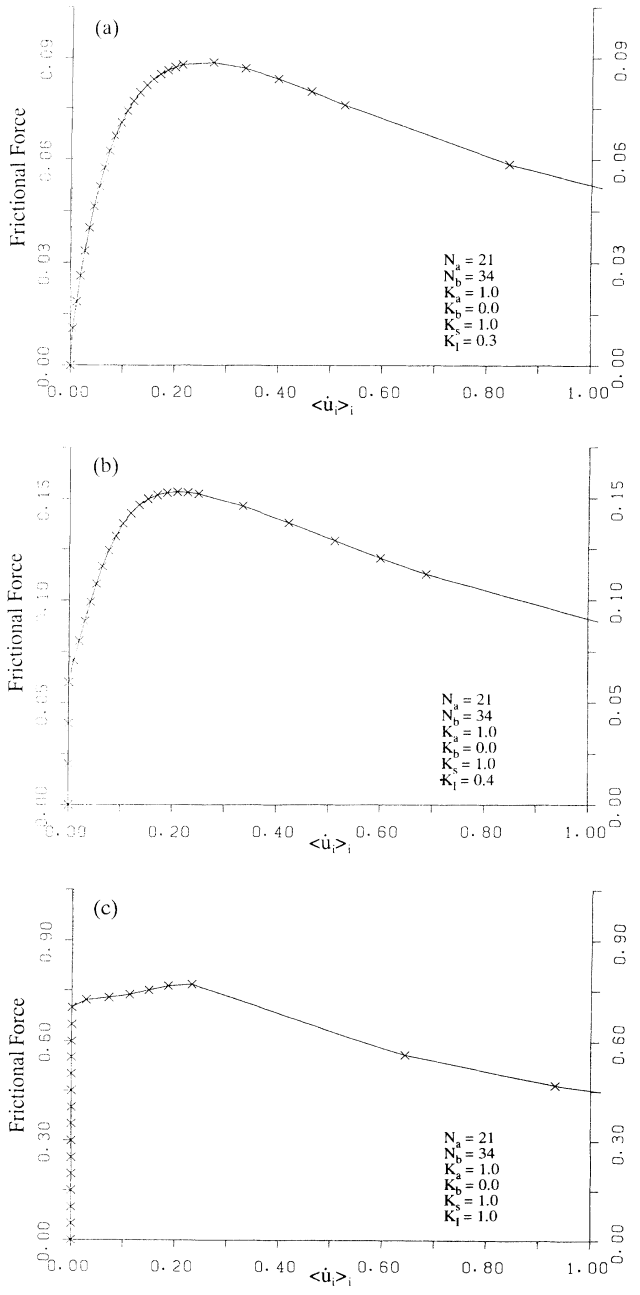

FIG. 4. Velocity dependence of the frictional force for $K_a=1$, $K_b=0$, $K_s=1$, and $K_I=0.3$ (a), 0.4 (b), and 1.0 (c).

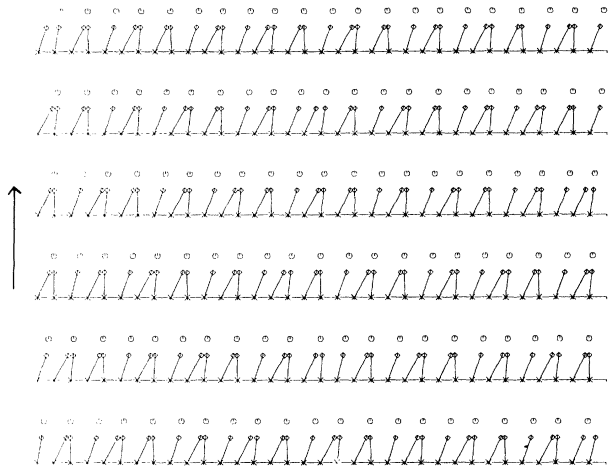

FIG. 5. Sequential snapshots of the configurations for $K_a=1$, $K_b=0$, $K_I=1$, $K_s=1$, and $G_{ex}=0.75$. The circles (squares) represent the upper (lower) atoms and the lines connecting the squares and crosses represent the springs between lower atoms and the substrate. The average velocity is 2.75×10^{-2} and the mean displacement from the bottom to the top is about one lattice spacing of the lower body.

The "phase" in which the maximum static frictional force vanishes is a kind of "ordered phase."[12] Such an ordered phase is realized more easily in higher spatial dimensions of the system but is more difficult as the dimension of the degrees of freedom gets large. For example,

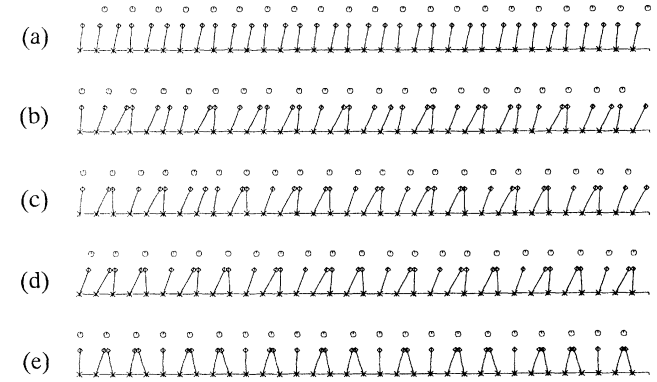

FIG. 6. Snapshots of the configurations for the same system as Fig. 5. The values of G_{ex} and the velocity are (a) $G_{ex}=2.0$, $\langle \dot{u}_i \rangle_i=1.67$, (b) $G_{ex}=1.0$, $\langle \dot{u}_i \rangle_i=2.32\times10^{-1}$, (c) $G_{ex}=0.75$, $\langle \dot{u}_i \rangle_i=2.75\times10^{-2}$, (d) $G_{ex}=0.7$, $\langle \dot{u}_i \rangle_i=0$, and (e) $G_{ex}=0$, $\langle \dot{u}_i \rangle_i=0$.

the 1D Ising model does not have an ordered phase at finite temperature but the 2D Ising model does, while the 2D XY model does not. So it is interesting to study whether Aubry's transition[12] exists or not in a model with higher dimension of the degrees of freedom. We studied the model in which each atom has two degrees of freedom, i.e., can move up and down and forward and backward. The interatomic potential between upper and lower atoms is taken as

$$U_I(\mathbf{r}) = -\frac{K_I}{2}\exp\left[-4\left[\frac{|\mathbf{r}|}{c_b}-1\right]^2\right].$$

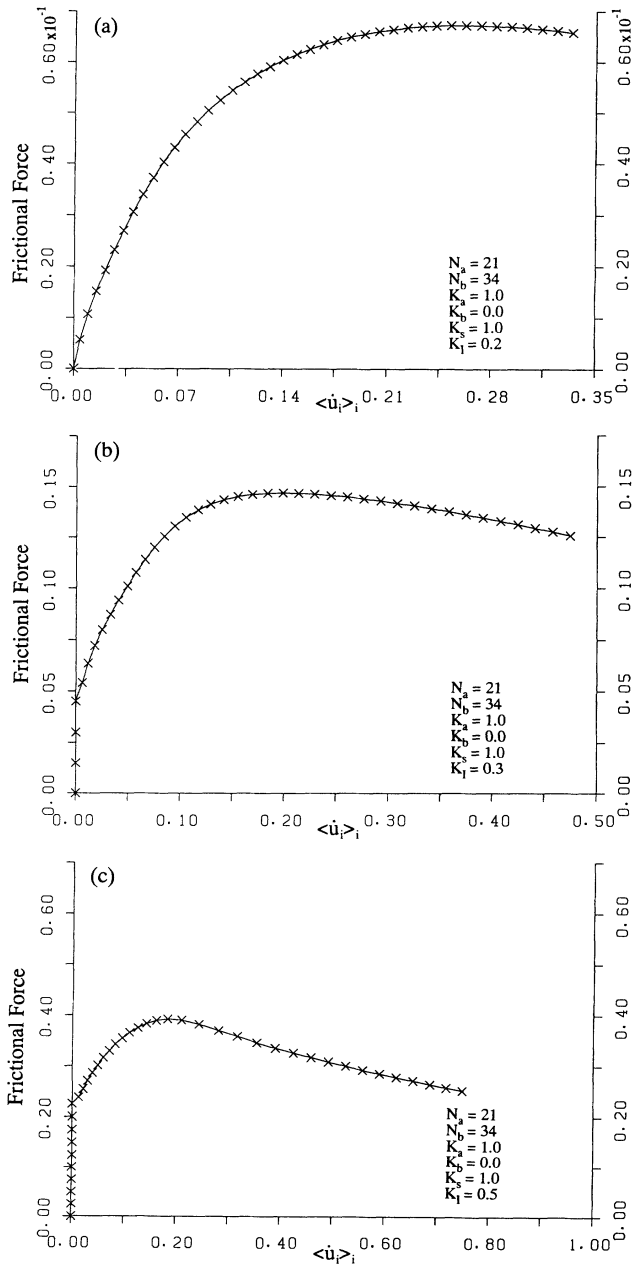

FIG. 7. Velocity dependence of the frictional force of the model with two degrees of freedom for $K_a=1$, $K_b=0$, $K_s=1$, and $K_I=0.2$ (a), 0.3 (b), and 0.5 (c).

Other potentials are similar to those of the previous model, Eqs. (3)–(5). As shown in Fig. 7 even in this model we have observed Aubry's transition and similar behaviors of the frictional force to those of the previous model.

IV. SUMMARY AND DISCUSSION

In this paper we first proposed a method of calculating the static and kinetic frictional force in a stationary state, which is given as the total sum of the interatomic forces between two bodies. We have applied this method to the 1D model of clean surfaces and calculated the frictional force. A kind of phase transition, Aubry's transition, is found to exist; there is a critical strength of the interatomic force between the two bodies and below the critical strength the maximum static frictional force vanishes. As the rigidity of the lower body decreases, the critical strength decreases, and the maximum static frictional force grows rapidly above it. On the other hand the kinetic frictional force is always finite and has a velocity dependence in general. But the dependence becomes weaker as the interatomic force between two bodies and thus the maximum static frictional force increases, and finally the kinetic friction shows similar behavior to that described by one of the laws of friction, "the kinetic frictional force does not depend on the velocity." These behaviors are also seen in the model in which each atom has two degrees of freedom.

An important problem associated with the vanishing static frictional force is the randomness, which certainly exists in real systems. It has been shown recently that the state of vanishing static frictional force is unstable against randomness.[13] Hence we consider that the vanishing static frictional force is an artifact of the model and that there is no frictional transition and the maximum static frictional force is always finite for every real system. It should be noted that even in that case the magnitude of the maximum static frictional force will be small for the system with weak randomness and there is a kind of crossover behavior instead of the phase transition. Hence we expect similar behaviors to those obtained here in that case.

In the usual situation the kinetic frictional force decreases with the velocity in the low-velocity region.[1] As a result, the constant-velocity motion becomes unstable under the condition of constant external force and shows stick-slip motion. However, the present calculation corresponds to the condition of constant velocity. Therefore we obtain decreasing kinetic frictional force with the velocity in a stationary state as shown in the figures. On the other hand, when the maximum static frictional force is small, the kinetic frictional force increases with the velocity in the low-velocity region. In that case the constant-velocity motion is stable even in the constant-external-force condition. We expect that such a velocity dependence can be observed experimentally in the case of small maximum static frictional force. We would like to emphasize that the velocity dependence of the kinetic frictional force varies from case to case.

The problem of friction has a close relationship to the

problem of pinning of sliding charge-density waves (CDW), spin-density waves, and moving vortices of the mixed state of type-II superconductors. For example, a CDW which is pinned by impurities and cannot move under small electric field starts to move above a threshold field and then the electric conductivity increases.[14–16] The I-V characteristics of sliding CDW systems are determined by the velocity dependence of the force due to impurities.[17,18] It is clear that the threshold field corresponds to the maximum static frictional force and the force acting on the sliding CDW corresponds to the kinetic frictional force. The velocity dependence of the kinetic frictional force obtained here becomes weaker as the maximum static frictional force increases, and the kinetic friction starts to show similar behavior to that described by one of the laws of friction. We notice just the same behavior for the sliding CDW.[17,18] Actually both the systems have frustration, which is caused by the random distribution of impurities for the CDW and by the incommensurate nature for the present model. We cannot expect such behavior in the commensurate model, where no frustration exists.[19] The usual situation resulting in finite friction has frustration, which comes from the surface roughness.[1] We stress that there exists a strong velocity dependence of kinetic friction when the maximum static frictional force is small. Therefore we expect the possibility that the velocity-independent kinetic frictional force is a kind of universal nature of systems with frustration and large maximum static frictional force. We plan to proceed with our study to make clear this possibility.

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