Tomlinson model improved with no ad-hoc dissipation

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The origin of friction force is a very old problem in physics, which goes back to Leonardo da Vinci or even older times. Extremely important from a practical point of view, but with no satisfactory explanation yet. Many models have been used to study dry sliding friction. The model introduced in the present work consists in one atom that slide over a surface represented by a periodic arrangement of atoms, each confined by an independent harmonic potential. The novelty of our contribution resides in that we do not include an ad hoc dissipation term as all previous works have done. Despite the apparent simplicity of the model it can not be solved analytically, so the study is performed solving the Newton’s equations numerically. The results obtained so far with the present model are in accordance with the Tomlinson model, often used to represent the atomic force microscope. The atomic-scale analysis of the interaction between sliding surfaces is necessary to understand the non-conservative lateral forces and the mechanism of energy dissipation which can be thought as effective emerging friction.

INTRODUCTION

Friction is one of the most important problems and a key phenomenon in physics and engineering, whose fundamental origin has been studied for centuries and still remains controversial [1–3]. From Leonardo da Vinci, Coulomb and Rynolds, sliding friction has been a topic of great interest studies intensively by many of the brightest scientists. In the last years, theoretical models for atomic friction, mostly based on the early work of Tomlinson [4], and Frenkel-Kontorova [5–7] models, were proposed and characterized by being highly simplified and yet retaining enough complexity to exhibit interesting features [8–13]. Such models have allowed to explain essential features of atomic-scale friction such as the occurrence of the “stick-slip” phenomenon observed in the movement of the tip over a surface material in the friction force microscope (FFM) [14, 15]. Friction is the result of the transformation of sliding motion into heat or different forms of energy, i.e., is the dissipated energy per unit length [16, 17], where the frictional work it is assumed to be dissipated through plastic deformation and material damage [18]. In the Tomlinson model, the energy dissipation is attributed to the instability induced by the stick-slip motion and consequent atomic vibration. What is expected is to increase the control over the mechanisms of friction and thus reduce the loss of energy. In this contribution we aim to understand the fundamental mechanisms on these energy exchange between the tip and the surface without include any ad hoc dissipation term as previous works have done. We want to show that without the ad hoc term, the energy lost by the tip is absorbed by the substrate. Despite the apparent simplicity of the model it can not be solved analytically, so the study is performed solving the Newton’s equations numerically, demonstrate that the energy dissipation is almost all absorbed by the stiffness of the substrate.

MODEL

The proposed model in the present study aims to explore the effect of various parameters involved on the emergence of frictional force and how the energy generated during the process is dispersed when there is no ad hoc dissipation. In this sense, our model in Fig. 1 was never presented in previous works. The tip is represented by a particle of mass \( M \), connected by a spring of constant \( K \) to a driven support that moves at constant velocity \( v_c \). The substrate is represented by a series of particle-spring systems of mass \( m \) and constant \( k \), independent between them , but interacting with the tip via a short range Gaussian type potential. To avoid edge effects we modeled the chain as being infinite.

The system is described by the Hamiltonian

\[
H = \frac{P^2}{2M} + \sum_{i=1}^{N} \frac{P_i^2}{2m} + \sum_{i=1}^{N} U(X, x_i) + U(X) + \sum_{i=1}^{N} U(x_i) \tag{1}
\]

where \( X, P \) and \( x, p \) are the tip and substrate coordinates respectively; \( U(X, x_i) = U_0 e^{-\frac{(X-x_i)^2}{\sigma^2}} \) is the inter-
action between the tip and each of the particles of the substrate. We choose the value of $\sigma$ in such a way that the Gaussian potential of each particle does not overlap with that of its neighbors. So the tip can interact with each of them separately.

In this case, $\sigma = a_x/n$, where $a_x$ is the separation between the particles of the substrate and $n$ is a constant.

$U(X) = \frac{K}{2}(X - x_c)^2$ is the elastic interaction between the tip and the cantilever. The support position $x_c$ is $x_c = v_c t$. And $U(x_i) = \frac{K}{2}(x_i - x_0)^2$ is the elastic potential of each particle (independent between them).

This results in the following equation of motion:

$$M\ddot{X} = -K(X - v_c t)$$
$$+ \frac{2U_0}{\sigma^2} \sum_{i=1}^{N} (X - x_i)e^{-\frac{(X - x_i)^2}{2\sigma^2}}$$

(2)

$$m \sum_{i=1}^{N} \ddot{x}_i = -k \sum_{i=1}^{N} (x_i - x_0)$$
$$- \frac{2U_0}{\sigma^2} \sum_{i=1}^{N} (x_i - x_0)e^{-\frac{(X - x_0)^2}{2\sigma^2}}$$

(3)

Introducing the adimensional units $Q = \frac{X}{x_i}, q = \frac{q_i}{x_0}, \tau = \sqrt{\frac{K}{M}} t, \tilde{U}_0 = \frac{2U_0}{k\sigma^2}, \tilde{v}_c = \frac{v_c}{x_0} \sqrt{\frac{M}{K}}$, the equations 2 and 3 can be reduced to:

$$\ddot{Q} = -q + \tilde{v}_c \tau + \tilde{U}_0 \sum_{i=1}^{N} (Q - q_i)e^{-(Q - q_i)^2}$$

(4)

$$\sum_{i=1}^{N} \tilde{q}_i = \epsilon_1 \sum_{i=1}^{N} (q_i - q_0)$$
$$\epsilon_1 \tilde{U}_0 \sum_{i=1}^{N} (Q - q_i)e^{-(Q - q_i)^2}$$

(5)

where $\epsilon_1 = M/m$ is the ratio of the mass of the tip and the substrate particles (assuming all have the same masses) and $\epsilon_2 = K/k$ is the ratio of the stiffness of the tip and the substrate.

METHODS

The problem was solved numerically by using classical molecular-dynamics methods [19, 20] using a set of realistic parameters [11, 17, 21], $M = m = 10^{-10}$ kg, $K = k = 10 N/m$, $a_x = 3$ Å, $U_0 = 0.085$ eV, $v_c = 1 \mu m/seg$ which are typical of an AFM experiments [22, 23].

The most evident consequence of not having dissipation is that the particles that are perturbed by the tip do not return to their initial state, remaining oscillating infinitely, as it is presented on Fig. 2 for the first five particles in dashed lines.

For the frictional force calculation we compare three different methods.

It is known that $F$ is defined as the mean value of the lateral force [11, 16, 21, 23]. Since the problem is in one dimension, from here, we will refer to the lateral force as friction force $F$.

$$F = K(X - x) = K(X - v_c t)$$

(6)

The second way to obtain $F$ is through the energy accumulated by the substrate. The power is the instantaneous product of force times velocity and the time derivative of energy.

$$F v_c = \frac{dE}{dt}$$

(7)

From this relation, it is possible to obtain the frictional force as the slope of the total substrate energy by linear regression. Another method to calculate the friction force in these mechanical problem is calculating the average of the force between the tip and the substrate generated by the gaussian interaction force. These three methods are compared in Fig. 3 with their respective error bars.

The total simulation time $\tau$ was divided into ten equal regions. For each of these intervals, the mean of the force was calculated in order to compare their values. $< F_x >$ represents the value obtained from eq. 3, $< F_{ts} >$ from the gaussian potential between the tip and the substrate; and $< F_{st} >$ is the slope of the accumulated energy of the substrate.

In Fig. 4 it is shown the accumulation of energy by the substrate and the values of the frictional force obtained
by the three methods. In this case, \( \tau \) was divided into three regions.

The comparison of the three methods shows that the smallest error in the measurements corresponds to the force obtained through the energy accumulated by the substrate. For this reason, we have chosen it to perform the rest of the simulations where all the parameters of the model will be analyzed.

A very important parameter in Molecular Dynamics simulation is the time step \( \Delta t \). If the time step chosen is very large, the MD simulation becomes unstable in the integration process, not showing behaviors existing in the mechanical problem. On the other side, if the time step is very small, the simulation will not be efficient since it takes a very long calculation time. Having this in mind, and since every mechanical problem is different from each other we decide to solve the equations for different \( \Delta t \) in order to choose the indicated in a way that not take long simulation time, but at the same time, obtain reliable results referring to the friction force.

Fig. 5 shows the energy of the substrate

\[
\text{Substrate Energy} = \sum_{i=1}^{N} \left( \frac{1}{2} m \ddot{x}_i^2 + U(x_i) \right)
\]

for different \( \Delta t \), from 0.001 to 10 ns. Since we are interested in getting the value of \( F \) from the slope of the curve, it can be observed that the choice of higher or lower time steps does not affect significantly the final result, in fact, the biggest difference between their values is of the order of 0.005 nN. For the numerical simulations we choose the value of \( \Delta t = 0.1 \) ns.

RESULTS

Once the method and the time step have been chosen, we calculate \( F \) varying each of the parameters of the model. The variation of \( F \) with the velocity of the driven support it is shown in Fig. 6. For small velocities \( v_\text{c} < 1 \mu m \), \( F \) remains constant and for higher values, it drops to zero. This is expected since the model does not have a velocity-dependent damping term. The total energy of the substrate decreases as the support velocity increases because the tip does not interact enough time with the substrate particles. As a consequence, the amplitude of oscillation around the equilibrium position is not significant.

When the variable parameter is the elasticity \( k \) of the substrate particles (Fig. 7), we can identify a behavior of the shape \( F = 1/k \) in three different regions. For the first interval, \( k < 1 \) N/m, the adjustment parameter is
n = 1. This means that as k increases, F decreases. The softer the material, the higher the energy lost. When 1 N/m < k < 130 N/m there is an unpredictable region with maximums and minimums. Although there is an oscillation in the values of the friction, we assume that the average value remains constant. For that reason, the parameter \( n \approx 0.26 \). The third region, shows a more expected result. Due to the hardness of the substrate, the particles do not deviate from their equilibrium position, so the elastic potential is almost null as well as the kinetic energy. In these region, the parameter \( n = 4 \).

The variation of the friction with the amplitude of the potential \( U_0 \), reproduced in Fig. 8, follows the shape \( F = mU_0 \), where again \( m \) varies for three different regions. In this case, since the data is better visualized and interpreted in linear scale, we did not see the need to represent the results in logarithmic scale. It can be observed that \( F \) increase with the high of potential energy following the shape When \( U_0 \) is up to 0.5 eV, \( m \approx 1.81 \). The friction almost doubles its value for each increment in \( U_0 \). For the second region, the growth rate decreases to a quarter of the presented in the first interval, here \( m \approx 0.46 \). And for the third interval, the growth is already very small, taking into account that it represents the eighth part of the first region growth. This is because the tip remains in between two particles for more time (while the support advances), as the amplitude increases.

The last Figure correspond to the friction force behavior with the mass ratio between the particles of the substrate and the tip \( m/M \) (Fig. 9). We can see that when \( m < M \) the frictional force maintains its constant value, then begins to decrease until reaching a minimum, corresponding to \( m = 2M \). After this point increases again and for a small gap of values between \( m = 5M \) and \( m = 10M \) again \( F \) shows independent on the masses ratio. Finally, fall to zero for very large substrate masses. When the masses are too big, the potential energy of the substrate is very small since the mass of the tip does not manage to move them.

**CONCLUSION**

In this paper we investigated a simple model to understand the fundamental mechanisms on the energy exchange in dry friction without include any \textit{ad hoc} dissipation term as previous works have done. We compare three different methods to calculate the friction force in order to obtain the most accurate value. The work was performed solving the Newton’s equations numerically, for different \( \Delta t \) with the aim of gain computational time. We study the variations of \( F \) varying all the parameters
involved in the description of the model We could show that the energy lost by the tip is absorbed by the substrate. Our goal in the future is to study the same model by placing particles of different masses in the substrate and $T \neq 0$ to observe how evolves

ACKNOWLEDGMENTS

This work was supported by the Centro Latinoamericano de Física (CLAF) and the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq,Brazil).

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