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Stick-slip friction: A Monte Carlo study

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ABSTRACT

The aim of this study is to analyze the underling molecular mechanics of the stick-slip phenomenon in confined thin films, and its dependence on parameters such as sliding velocity, load, time and temperature. The study was carried out using the kinetic Monte Carlo method, where adhesion hysteresis was explicitly introduced in a one-dimensional simulation model. A dual-interaction potential model was implemented to carry out this work. The results indicate: (i) the importance of adhesion hysteresis to explain the increase in stick-slip frequency (therefore, in sliding velocity); (ii) a consistent dependence behavior of friction in the stick-slip regime with sliding velocity, load, time and temperature; and (iii) a relationship between sliding velocity and static friction of $V_{Sliding}$ $\alpha 1/F_{Static}$.

1. Introduction

Stick-slip (SS) in the boundary lubrication (BL) regime is a very important phenomenon from both technological and industrial points of view, due to that, in this regime, higher energy consumption and an increased wear of the contacting surfaces are observed [1]. With the advent of the Atomic Force Microscope (AFM) [2], the Surface Force Apparatus (SFA) [3,4] and the Quartz Crystal Microbalance (QCM) [5], it has been possible to explore the underlying physical mechanisms at the molecular level. A lot of research has been focused in the understanding of friction of systems involving confined thin films, which are of great importance in applications such as boundary lubricated engineering components, biological interfaces and microelectromechanical systems (MEMS). In particular, this type of systems have been extensively studied through SFA experiments by Israelachvilli, who, among other things, found that friction at the nano-scale could be correlated with the adhesion hysteresis phenomenon [6]. Furthermore, in order to achieve a fundamental understanding of these processes, efforts have and are still been made from both experimental [7–15] as well as theoretical and simulations points of view, such as through Molecular Dynamic Simulations (MDS) [16–28]. However, a satisfactory explanation of the friction mechanisms involved in this type of systems is still lacking, for example, with respect to the origin of phase transitions evidenced by the SS behavior and the effects of the adhesion hysteresis phenomenon.

In this contribution, the SS friction of a very thin film of simple molecules confined between two molecularly smooth surfaces, is studied by analyzing the behavior of a sample particle (SP) from the first monolayer (monolayer M) that is susceptible to sliding due to the action of an external force (see Fig. 1), by means of the kinetic Monte Carlo method.

The proposed model takes into account displacements of the confined film normal to the sliding contact, and allows to propose an explanation of the variations in thickness of the film during the development of the SS process, as well as phase transitions and oscillatory variations of the gap distance between the surfaces [21]. Also, by considering an incomplete dissipation of the energy delivered to the system by the action of an external force, an adhesion hysteresis phenomenon is introduced and its effects on the frictional behavior can be analyzed. The main objective of this work is to analyze the behavior of friction with some system parameters, and not to rigorously calculate the intrinsic friction value. The behaviors of friction with load, sliding velocity, temperature and time, previously reported by MDS and experimental results, are qualitatively reproduced by the model proposed in the present work.

2. Model and methods

Before presenting the proposed model, some interpretations of the stick-slip type of behavior experimentally observed at sliding interfaces should be mentioned: (i) static friction is related to the "stick" event while dynamic friction to the "slip" event; (ii) thus, the stick-slip behavior is a consequence of the presence of static friction that "refuses to disappear"; (iii) it is considered that the subsequent sticks have the same molecular origin as the first one; (iv) the system

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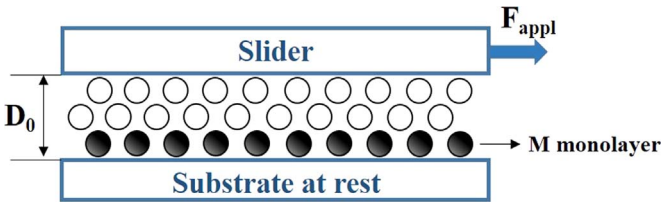

Fig. 1. Schematic representation of two surfaces with a confined thin film in between. In this case, the M monolayer is adhered to the fixed substrate and is susceptible to sliding. D_0 corresponds to the initial gap between the two surfaces.

starts to slide after the stick event and stops right at the end of the slip event; (v) static friction refers to the friction produced during the stick events.

It has been proposed that static friction has its origins in a monolayer of particles of a film that is in direct contact with the sliding interface [18–20,26,28]. The present model is based on this idea, and a basic mechanism for the study of the static friction is proposed. Furthermore, it has been shown that the friction force is linearly proportional to the number of particles that interact across the contact [29]; therefore, for a certain fixed surface density of a full monolayer, the frictional behavior has been, in the present work, analyzed by studying the average behavior of a single particle (SP). If an external force is applied to the slider (see Fig. 1), it will be transmitted to the monolayer M through the upper layers of the film, probably due to a delicate balance between particle-substrate adhesion and cohesion forces within the film in the *solidlike* state. Therefore, the particles of monolayer M will be subjected to an indirect force that performs work on each particle.

The friction phenomenon under BL conditions has been analyzed through processes occurring at the lubricant-substrate interface of a confined film, and has been related to the surface physicochemistry [30]. In the present model, the stick events have been interpreted as molecular desorption processes from an initial absorbed state involving a displacement of the SP normal to the sliding contact, and the slip event as molecular migrations-adsorption processes. The desorption processes occur due to that the particle absorbs energy from an external source, which in this work is considered as a fundamental condition for the stick event to take place. The slips take place when the particle "sees" a free adsorptive neighboring site, which is a convenient place to move to and reduce its energy. In this case, the particle migrates and bounds to the new site dissipating energy. This is consistent with reports that suggest that the energy dissipation of the system mainly occurs in the slip event [27]. Consequently, migration and adsorption events of the particle are known to be much faster than the stick events, which is in accordance with experimental results [6]; therefore, the slip events are considered to take place instantaneously right after the stick events.

There are experiments that show a dependence of the friction force with adhesion hysteresis, and that adhesion hysteresis is present regardless of the normal load values [10]; however, the effect of the presence of adhesion hysteresis during SS friction has not been tested. In addition, it is admitted that memory effects associated with the surface-film interaction are present [6]. For the simulations performed in this work, it is considered that the interactions at the substrate-film interface take place under solid-*solidlike* conditions during the stick event. A dual interaction potential that follows the principles of energy absorption/dissipation present in a Prandtl/Tomlinson-type model [31,32], has been developed in order to be applicable to this case, where the force experienced by the SP has different characteristics than the typical elastic driving force taken into account in the classical Prandtl/Tomlinson model, as it will be describe below. The SP is initially in a bound state under a "periodic" potential and

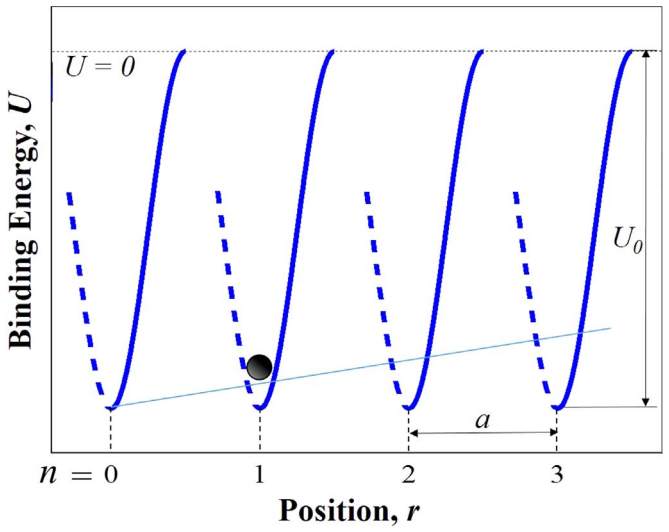

Fig. 2. Schematic representation of the particle-substrate interaction potential. The solid curves represent the binding potential (Eq. 10) at the discrete positions r. The straight solid line represents the increase of the particle potential energy, due to the undissipated energy, as sliding occurs.

subjected to a constant indirect applied external force, where the next nearest neighbors interactions within the monolayer M have been neglected. Due to the anisotropy of the medium, it is reasonable to consider that the external force on the SP can be decomposed into two mutually orthogonal components, one parallel and one perpendicular to the sliding plane. This perpendicular component is the one pulls the SP away from the sliding contact, and is calculated in this work to obtain the static friction.

In order to calculate this static friction, it is necessary to evaluate the changes in binding energy experienced by the particle during SS. Initially, the SP is at position r_0, which is at the bottom of the binding potential, U, in its initial attractive base state, where $U(r_0, t_0) = U_0$ (see Fig. 2) and is always negative (note that at an initial time t_0 , $U(r_0) = U(r_1) = U(r_n)$; then, the SP starts absorbing energy as the stick event takes place; this energy is partially dissipated during the subsequent slip event, so that the binding energy of the SP at position $r_1 = r_0 + a$ and time t_1 is given by

$$U(r_1, t_1) = U(r_0, t_0) + \varepsilon U_{abs}(r_0, t_0') \tag{1}$$

where a represents the jump length of a stick-slip event, reflecting the periodic nature of the SP interaction potential;$U_{abs}(r_0, t_0')$ is the total energy absorbed by the particle to overcome the corresponding binding energy at time t_0' (with $t_1 > t_0' > t_0$), and ε is a random dimensionless parameter that represents the fraction of energy accumulated during the stick event that is not dissipated during the slip event $(\varepsilon U_{abs}(r_0, t_0'))$; this variation in the binding potential is considered as an adhesion hysteresis effect, due to that the binding energy of a certain absorbed state is higher than the corresponding subsequent state. Fig. 2 shows a schematic representation of the model, showing the variations in binding potential at each position r_n, where the straight line under the particle is just a guide to show the variation of the SP base states during sliding, due to the undissipated energy. Note that r is a discrete position variable.

The general expression for the energy when the particle is at site n $(n > 0)$ at time t_n, with $r_n = r_{n-1} + a$, is given by

$$U(r_n, t_n) = U(r_{n-1}, t_{n-1}) + \varepsilon U_{abs}(r_{n-1}, t_{n-1}') \tag{2}$$

Here, the increase in energy experienced by the SP due to the work of the external force is linear with t (Eq. 3). Therefore, the total energy absorbed by the SP during the stick event in the