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Driven dynamics of simplified tribological models

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Abstract

Over the last decade, remarkable developments in nanotechnology, notably the use of atomic and friction force microscopes (AFM/FFM), the surface-force apparatus (SFA) and the quartz-crystal microbalance (QCM), have provided the possibility to build experimental devices able to perform analysis on well-characterized materials at the nano- and microscale. Simultaneously, tremendous advances in computing hardware and methodology (molecular dynamics techniques and *ab initio* calculations) have dramatically increased the ability of theoreticians to simulate tribological processes, supplying very detailed information on the atomic scale for realistic sliding systems. This acceleration in experiments and computations, leading often to very detailed yet complex data, has deeply stimulated the search, rediscovery and implementation of simpler mathematical models such as the generalized Frenkel–Kontorova and Tomlinson models, capable of describing and interpreting, in a more immediate way, the essential physics involved in nonlinear sliding phenomena.

(Some figures in this article are in colour only in the electronic version)

1. Tribological modelling at the nanoscale

Friction with its related nonlinear dynamics is a vast and interdisciplinary field. Understanding the complex processes occurring at the interface of two interacting materials in relative motion (the science of *tribology*) is central to pure and applied sciences as well as to many technological problems, including adhesion, lubrication, wear, contact formation, elastic and plastic deformation, fracture and crack propagation, nanoindentation, just to name a few. Due to continuing device miniaturization, friction imposes serious constraints and limitations on the performance and lifetime of advanced technological microdevices. Durable low-friction surfaces and suitable liquid or solid lubricants are increasingly in demand in hi-tech applications such as magnetic storage systems, micro-electro-mechanical devices, and aerospace components. It has been estimated that about 6% of the gross national product in

developed countries is 'wasted' on friction and related wear (nearly 800 billion dollars per year in the USA alone).

Interfacial phenomena involve complex physical processes over a wide range of length scales, from atoms to tectonic plates. Over the last decade, remarkable development in nanotechnology (AFM/FFM, SFA, QCM, etc) and tremendous advances in computing hardware and methodology (molecular dynamics (MD) techniques and *ab initio* calculations) have provided the possibility to study tribological processes, supplying very detailed information on the atomic scale for realistic moving interfaces [1, 2]. Thus, nowadays tribology approaches the fundamental microscopic level of investigation through the study of the contacts themselves, in terms of chemical bonding and of the elementary processes that are involved in the excitation and dissipation of energy. Together with these nanoscopic approaches, many primary questions have already been answered, but many more are overbearingly emerging. The difficulty of the problem of friction is related to its complexity, namely dealing with systems under a strict size confinement that leaves very limited access to the interface itself. Intriguing structural and dynamical features have already been observed experimentally and partially explained theoretically in nanoscale liquids confined between two solids, e.g. layering and structural ordering induced by the surfaces, oscillatory or chaotic stick–slip motion with the frequency and amplitude dependent on the driving velocity, the increase of the effective viscosity in the sliding regime relative to the bulk, the dependence of friction on the system history, etc. Although significant progress in understanding some factors that determine the response of confined systems under shear has been achieved during the last decade, a fundamental understanding of the basic mechanisms that control tribological phenomena at the atomic scale is still lacking. Studies at the molecular scale show a behaviour that is markedly different, not only quantitatively but often even qualitatively, from that observed in macroscopic devices (e.g. solids may slide over each other with less friction than fluids, a thin fluid film may behave like a solid, etc). If, macroscopically, friction seems to be unavoidable, this might not hold anymore at the nanometre scale. Actually, one of the main challenges of modern tribology is to develop an essential understanding of friction, allowing us to bridge the different length scales and properly relate the atomistic processes with the macroscopically observed properties. Due to the intrinsic interdisciplinarity of the subject, it is obvious that the fundamental and predictive understanding of tribology with all its nonlinear and complex aspects can only be achieved by a combination of experimental, theoretical and computational efforts, where different, yet complementary, skills can flow into each other.

Macroscopically, most theoretical approaches to contact mechanics are based on the continuum elasticity theory (e.g. the approaches due to Hertz, Johnson–Kendall–Roberts, Derjaguin–Muller–Toporov, Maugis–Dugdale, etc). However, continuum mechanics is poorly applicable as the characteristic dimensions of the contact between the sliding bodies are reduced down to the microscales, where the effects of the discrete nature of matter cannot be neglected anymore.

Advances in the theoretical understanding of interatomic interactions in material science and computer-based modelling of complex systems have led to MD simulations for exploring atomic-scale dynamics. Numerical simulations have revealed themselves to be extremely useful in investigating frictional processes at the microscopic scale and, in the years to come, are expected to play an expanding role in tribology. Their distinctiveness consists of allowing us to follow and analyse the dynamics of all atoms in controlled computational 'experiments' where the interface geometry, sliding conditions and interparticle interactions can be varied at will to explore their effect on friction and wear. This approach has revealed, no doubt, a great deal of information about the atomistic origins of static and kinetic friction, hysteresis, stick–slip dynamics, boundary lubrication, and the interplay between molecular geometry and

tribological properties. However, it is not yet possible to treat all the characteristic length scales that mark the dynamical processes entering the friction coefficient of engineering materials, and a number of efforts are nowadays devoted to increase cleverly the accessible timescale.

Within the standard framework of the MD approach (see, e.g., [3]), firstly the interaction potentials among the particles of the system have to be defined and the corresponding interatomic forces evaluated. Next, one defines the geometry of the sliding interface and the boundary conditions. Then, after specifying the initial coordinates and velocities of the particles, the differential equations of motion are integrated numerically. By following the whole particle dynamics, quantities of relevant physical interest such as the frictional force, mean (centre of mass) velocity, heat flow, and correlation functions are calculated as functions of time to determine possible regimes of motion and the corresponding steady-state values. Transitions between the different dynamical states are analysed and related to the detailed motion of individual particles.

To design a meaningful simulation of a complex system such as the sliding interface in tribology, first the theoretical model of its major components must be implemented, and any significant 'interacting ingredients' between the system under consideration and its operational environment have to be taken into consideration. The development of an efficient mathematical description for a given physical system is typically quite a difficult task. In cases when the system dynamics is not well understood, a series of preliminary computational experiments has to be performed to collect data that can then be processed, using various techniques, to yield a satisfactory model for the addressed physical problem. In this view, a prior good understanding of the theoretical background will help in determining which aspects of the simulations deserve particular focus and which details are less relevant.

In particular, care must be taken in the choice of the appropriate interaction potentials (starting from the simplest case of just elastic springs up to very complex long-range potentials or electronic density-functional interactions) and the statistical ensemble (e.g. the microcanonical constant energy and volume ensemble or the ensemble with constant temperature and pressure, the model with the constant driving force or the one with the fixed sliding velocity) that capture the essential physics of the problem.

Besides, in order to make reliable predictions, another common crucial issue in tribological simulations is the apporopriate implementation of the geometry and boundary conditions, avoiding as much as possible the convenience of artificial and unrealistic treatment (e.g. constant separation rather than constant load and/or identical perfectly aligned surfaces rather than incommensurate contacts).

The frictional response may also depend strongly on the method of inducing motion in the system. Imposing an external driving force or a shear constant velocity pumps energy continuously into the system, which needs to be removed somehow. Especially for systems far from equilibrium, temperature control may be a relevant aspect to be taken into due consideration, since a careless 'thermostating' procedure may certainly introduce unwanted artefacts.

A worthwhile guide for conducting atomistic MD simulations of frictional processes and focusing on fundamental technical aspects (realistic construction of the interface, appropriate ways to impose load, shear and the control of temperature) can be found in the recent review articles by Müser and Robbins [4, 5]. As far as the briefly sketched classical MD approach is concerned, we refer the reader to the excellent well-known books by Allen and Tildesley [6] and by Frenkel and Smit [3].

In the framework of multiscale modelling and hybrid simulation methods have recently been introduced to bridge the molecular dynamics level of investigation and the continuum approach. These methods usually combine an atomistic treatment of the interfacial mating

region, at places where the displacement field varies on an atomic length scale, with a finite-element and continuum method description elsewhere, where strains are small and change continuously (e.g. see [7] and references therein). The main difficulty lies in the appropriate matching conditions between the atomistic and continuum regions. Since the details of lattice vibrations (the phonons), which are an intrinsic part of the atomistic model, cannot be represented at the continuum level, conditions must be met that the phonons are not reflected at the atomistic continuum interface. In addition, the matching between the atomistic-continuum interface has to be such that large-scale information is accurately transmitted in both directions [8].

This paper is meant as a short, and certainly not exhaustive, overview to illustrate some relevant applications and results obtained in the framework of *low-dimensional and simple tribological models*, compared to the more realistic three-dimensional calculations. Undoubtedly, the complexities of realistic 3D sliding systems can make it difficult to analyse and interpret the general dynamic mechanisms that underlie friction. Moreover, the amount of computational effort typically grows at least linearly with the number of particles. Thus, the recent proliferation of very detailed, yet complex, data both in experiments and in MD computations at the micro-and nanoscales, has greatly stimulated the search for, rediscovery and implementation of simpler mathematical tools, such as the generalized Frenkel–Kontorova and Tomlinson models, capable of describing and unravelling in a more immediate way the essential physics involved in nonlinear sliding phenomena. These models are able to capture and illustrate general results for the origin and trends of wearless static and kinetic friction, the importance of commensurability, the significance of metastability, and the role of interface geometry. Due to space limitations, we will not consider here the class of phenomenological rate-state models which have proved to be very efficient in accounting for, e.g., memory effects in friction measurements.

The paper is organized as follows. In section 2 the nonlinear nature of frictional processes in driven systems is briefly outlined. Then, in sections 3 and 4, we show explicitly, through a few specific examples, the ability to capture the qualitative phenomenology of the tribological microscopic mechanisms in the framework of simple low-dimensional mathematical models. Via a Langevin MD approach, section 5 introduces a more complex 3D model, mimicking the tribological behaviour of a confined lubricant film under shear. Conclusions are briefly given in section 6.

2. Nonlinear dynamics of systems under shear

Nonlinear systems driven far from equilibrium exhibit a very rich variety of complex spatial and temporal behaviours. In particular, in the emerging field of nanoscale science and technology, understanding the nonequilibrium dynamics of systems with many degrees of freedom which are pinned in some external potential, as commonly occurs in solid-state physics, is becoming a central issue more and more often. Examples are the theory of dislocations in metals, domain walls in ferroelectrics, the problem of crowdion in a metal, sub-monolayer films of atoms on crystal surfaces, surface reconstruction phenomena, the theory of Josephson junctions, the charge density waves and so on. Dry friction also belongs to this class of systems, because the microscopic asperities of the mating surfaces may interlock.

It has frequently been shown that simple phenomenological models of friction, which are typically low dimensional, give good qualitative agreement with experimental results on nanoscale tribology or with more complex simulation data, being able to capture the main features of the complicated dynamics involved. With respect to this, the application of driven Frenkel–Kontorova (FK) like models (see, e.g., [9, 10] and references therein), describing the

dissipative dynamics of a chain of interacting particles that slides over a rigid periodic substrate potential due to the application of an external driving force, has recently found increasing interest as a possible interpretative key to understanding the atomic processes occurring at the interface of two materials in relative motion.

A common feature of all these systems is a strongly nonlinear mobility. If some external field or force F is applied to the array of particles, its mobility μ, defined as the ratio of the average system velocity $\langle v \rangle$ to the imposed driving F, turns out to be zero below some usually well-defined threshold F_s and nonzero above it. In general, μ is some highly nonlinear function of the applied force F.

At this point, we would like to remind the reader of two different and fundamental tribological concepts, probably already encountered in some early stage during courses on classical mechanics or general physics: the *static friction* and the *kinetic friction*. The *static* frictional force F_s is defined as the minimal threshold force needed to initiate relative motion. Its value is mainly determined by the atomic structure and geometry of the sliding interface and by the adhesion interactions. Observation of static friction implies that the contacting solids have locked into a local energy minimum, and F_s represents the force needed to lift them out of this minimum. The *kinetic* frictional force F_k is the force required to maintain the two surfaces in relative motion at a steady velocity v. F_k has to be considered as arising from some dissipative mechanism converting the energy of translational motion into heat. Therefore, its value (equating the work done on the system by the external force divided by the distance moved) is intrinsically determined by the rate of excitation of various degrees of freedom of the system due to sliding; the energy of these excitations is eventually transformed into heat.

The transition, occurring at F_s, from a pinned state with zero mobility to a moving state with nonzero mobility is called the *pinning–depinning transition* or, simply, the depinning transition. The process, reminiscent of a sort of 'melting', is a typical nonequilibrium process. Since there is no ground state as a consequence of the presence of the applied external driving F, the locked system has to be in some metastable state. Due to finite thermal fluctuations, the system can overcome the barrier separating the nearest metastable states and move into another metastable state with a lower value of energy. This dynamics leads to creep with a very low mobility. Moreover, above the depinning transition, energy usually flows through the system at a high rate. Therefore, this behaviour cannot be deduced from the linear response theory, which operates near thermal equilibrium only. The value of the mobility of the sliding state strongly depends on the rate of energy dissipation.

In the mobility–driving force characteristics, the transitions between pinned, intermediate and sliding states, for adiabatically increasing and decreasing external forces, do not have to occur at the same value of the applied driving force (the existence of *hysteretic phenomenon*). The behaviour depends strongly on whether the system degrees of freedom have sufficient inertia or if, in contrast, the inertia forces are negligible compared to the dissipative forces.

In the presence of strong dissipation, when the viscous friction coefficient is much larger than the characteristic vibrational frequencies[3] of the system, the motion is *overdamped*; the depinning transition is in most cases expected to be of the second order, and indistinguishable from the reverse pinning transition. Interesting results were obtained by reducing the time-independent Smoluchowski equation for the steady state of the driven system to the one-particle equation with an effective on-site potential, which was then solved numerically by the transfer operator technique [11, 12]. In this strongly dissipative regime, the results show the existence of a nonlinear mobility region, but without any bistability phenomenon.

[3] Similarly to the damped oscillator with natural frequency $\omega_0 = (K/m)^{1/2}$ and viscous damping η, the motion is called *overdamped* if $\eta \gg \omega_0$ and *underdamped* when $\eta \ll \omega_0$.

If, on the other hand, the motion is *underdamped*, we expect that hysteresis is possible because the inertia can help to overcome the pinning centres. However, the bistability tends to be reduced (or even disappear, in the case of a single particle) in the presence of an external noise, because the thermal fluctuations can kick the system out of the locked state. Thus, depending on the parameter values of the model, physically different situations can take place. Unfortunately, it is not always clear how to relate the parameters in the simplified mathematical models to microscopic interactions or how to extrapolate them from one system to another.

It is worthwhile mentioning that there are mainly two different operational frameworks for evaluating friction forces. In order to calculate the static friction F_s, one can ramp up the external applied force adiabatically and identify the value at which the system depins and starts to slide. As already stated, the precise value of F_s is largely dependent on the geometrical features of the contacting interface and on the adhesion interactions. The shape of substrate potentials and the choice of anharmonic interparticle interactions are, for example, factors of significant importance, leading to the appearance of different types of nonlinear excitations (kinks), phonon branches, changes in kink–antikink collisions, and modification of breather (kink–antikink bound state) solutions. All of these characteristics may lead to a consequent drastic change in the frictional response between the two solid interfaces in relative motion. However, near the depinning threshold, the presence of finite thermal fluctuations may assist the system in overcoming the locking barrier, and small corrections to F_s will presumably apply. As far as the kinetic friction F_k is concerned, one can measure the force that the external driving apparatus exerts on the atoms of the top surface. Usually, a rather generic way to impose driving is to couple the upper wall to a spring of stiffness K that is moved at a constant velocity. This simple, yet quite effective, pulling procedure can be viewed as a way to mimic not only the experimental driving device, but to some degree also the elasticity of the slider. Alternatively, to obtain the value of F_k it is possible to sum up the forces between the top-wall atoms and all atoms at the sliding interface. Obviously, these two different methods have to provide identical results, since otherwise the upper surface would be accelerated.

There is no doubt that the dynamics of sliding systems can be very complex, highly nonlinear and dependent on many factors. Recent studies on the one-dimensional low-dissipative FK model has shown, for example, the occurrence of hysteresis in the pinning–depinning transition, even at a finite temperature [13]. The hysteresis was found to result from a distinct difference in the mechanisms of the depinning (locked-to-running) and pinning (running-to-locked) transitions. The forward transition, observed on adiabatic increase of the driving force F, is initiated by the instability of a fast moving topological local compression (kink) in the 1D chain, leading to an avalanche of kink–antikink pair production. The collision of the newly created kink and antikink initiates the growth of a domain of running atoms, finally bringing the system to the running state. This scenario is quite distinct from the reverse pinning transition for slowly decreasing force, where intermediate steady states were found to exist between the depinned and locked states.

When the static frictional force F_s is nonzero, the dynamical behaviour generally displays two different tribological regimes. At high rates or stresses (large values of the driving velocity or of the pulling force F) systems usually slide smoothly. In contrast, at low rates the motion often becomes intermittent, with the system alternately sticking and slipping forward. This mechanism is quite general and has been observed in many simulations of microscopic friction, as well as in the tip dynamics of atomic force microscopy. Energy is stored in the springs, while atoms are trapped in a metastable state (sticking), and it is converted to kinetic energy as the atoms pop to the next metastable state (slipping). The value of the spatial distance covered during the slip events can be affected by several factors: first, the intrinsic periodicity of the lattice defining the substrate potential; second, the potential energy landscape of accessible

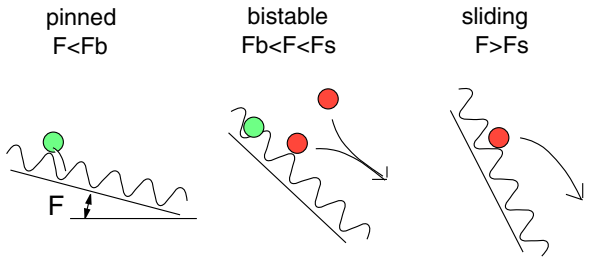

Figure 1. Bistability of a single driven atom in the periodic substrate potential. The atom is either locked in the minimum of the potential at $F < F_b$, or it is in the sliding state if $F > F_s$ when the substrate minima are suppressed due to the external F-tilting. For intermediate forces, $F_b < F < F_s$, the system is bistable, and its behaviour (pinned or running) depends on the initial state.

metastable states (occurrence of microslips); third, the specific features of imposing loading and driving. Moreover, the temporal alternation between stick and slip may possess regular periodic or intermittent chaotic feature.

3. Simple models: from non-interacting to interacting atoms

In the simplified tribological models, the studies are restricted to describe microscopic dynamics in one (1D) or two (2D) spatial dimensions. The substrates defining the sliding interface are modelled in a naive, although often effective, way as purely rigid surfaces or as one- or two-dimensional arrays of particles interacting through simple (typically harmonic) potentials. As mentioned in the previous section, two different algorithms are commonly used to induce motion: the constant-force algorithm, when the driving force is applied to the top substrate (or even directly to the lubricant layer) and is changed adiabatically, and the constant-velocity algorithm, when one of the surfaces is driven through an attached spring moving at constant speed. Both operational procedures are useful in different situations.

The best known among simple models in microscopic tribology are certainly the Tomlinson model [14] and the Frenkel–Kontorova model [15, 16], whose main features we will outlined briefly later. However, even the simplest, minimalistic description of a single atom driven by an external force over a periodic substrate potential (see figure 1) can capture the essential phenomenology of friction in terms of the Langevin motion equation in the *underdamped* limit. This model allows a rigorous treatment, as summarized in the monograph by Risken [17].

Namely, let us consider a particle of mass M placed into the external sinusoidal potential $V(x)$, with height $\mathcal{E}$ and spatial period a, and let us drive it by the dc force F. In the framework of Langevin dynamics, thermal effects can be incorporated into the model by adding a thermal random force $\Gamma(t)$ and a damping viscous term $M\eta\dot{x}$ to the equation of motion,

$$M\ddot{x} + M\eta\dot{x} + \frac{\mathrm{d}V(x)}{\mathrm{d}x} = F + \Gamma(t), \tag{1}$$

where $\Gamma(t)$ and η are linked by the fluctuation–dissipation relation

$$\left\langle \Gamma(t)\Gamma(t') \right\rangle = 2M\eta K_B T \delta(t - t') \tag{2}$$

with K_B and T denoting the Boltzmann constant and the temperature, respectively. These two added terms can be thought of as representing degrees of freedom inherent in a real

physical system which are not explicitly included in the simplified mathematical description (e.g. vibrational or electronic excitations in the substrate).

At zero system temperature, $T = 0$, the average velocity $\langle v \rangle$ of the particle as a function of the driving F exhibits hysteresis. The forward depinning transition takes place at the force $F_s = \pi \mathcal{E}/a$, while the backward pinning transition, as is shown briefly, occurs at the threshold force $F_b = (2\sqrt{2}/\pi)\eta\sqrt{M\mathcal{E}}$. Thus, in the *underdamped* case, where $\eta < \eta_c = (\pi/4)\,\omega_s$, we have $F_b < F_s$, and the system has to exhibit hysteresis due to inertial effects of the particle (here $\omega_s = (2\pi/a)\sqrt{\mathcal{E}/2M}$ is the frequency of small-amplitude oscillations of the atom at the bottom of an external potential well). In the simplest model of friction, the force F_s corresponds to the static frictional force, while the backward threshold force F_b defines the kinetic frictional force. The inequality $F_b < F_s$ is just the necessary condition for the existence of stick–slip motion.

The threshold force F_b can be found from the calculation of energy gain and loss. When the particle moves over a distance a (i.e. for one period of the external potential), it gains the energy $E_{gain} = Fa$ and loses an energy E_{loss} because of the external damping. In the regime of steady motion, these energies must balance, $E_{gain} = E_{loss}$. Thus, the backward force for the transition from sliding motion to the locked state is determined by $F_b = \min(E_{loss})/a$. The energy losses are caused by the external frictional force $F_{fric} = M\eta v$,

$$E_{loss} = \int_0^\tau \mathrm{d}t\, F_{fric}(t)\, v(t) = \int_0^\tau \mathrm{d}t\, M\eta v^2(t) = M\eta \int_0^a \mathrm{d}x\, v(x), \tag{3}$$

where $\tau = a\,/\langle v \rangle$ is the 'washboard period' (the time of motion for covering the distance a). The minimal losses are achieved when the particle has zero velocity on top of the total external potential $V_{tot}(x) = V(x) - Fx$.

In the limit $\eta \to 0$ and $F \to 0$, the minimal energy losses can easily be found analytically. From the energy conservation law, $\frac{1}{2}Mv^2 + \frac{1}{2}\mathcal{E}[1 - \cos(2\pi x/a)] = \mathcal{E}$, we can find the particle velocity $v(x)$. Substituting it into equation (3), we obtain $F_b = C\eta(\mathcal{E}M)^{1/2}$, where the numerical constant $C = 2\sqrt{2}/\pi \approx 0.9$ depends just on the shape of the external potential. This equation can be rewritten as $F_b = M\eta\bar{v} = (2/\pi)M\eta v_m$, where $\bar{v} = a^{-1}\int_0^a \mathrm{d}x\, v(x)$, and $v_m = (2\mathcal{E}/M)^{1/2} = \pi\bar{v}/2$ is the maximum velocity achieved by the particle when it moves at the bottom of the external potential. Note that the average particle velocity, $\langle v \rangle = \tau^{-1}\int_0^\tau \mathrm{d}t\, v(t) = a/\tau$, tends continuously to zero when $F \to F_b$, because $\tau \to \infty$ in this limit.

When the external applied force changes *adiabatically*, the hysteresis of the function $v(F)$ exists at $T = 0$ only. At any small but non-zero temperature, there is no hysteresis for the single-particle system. The forward and backward transitions from the pinned (thermally activated) state to the sliding state, and vice versa, both take place at the same value of the force $F = C'\eta(\mathcal{E}M)^{1/2}$, where $C' \approx 2.3742$ [18, 19]. Now, if we attach a spring to the atom instead of driving it directly, we observe, depending on the external driving velocity, either the stick–slip dynamics or the smooth sliding regime, as well as the transition between these two regimes (see, e.g., [20]). In fact, in this way we just come to the famous *Prandtl and Tomlinson model* [14, 21] shown in figure 2 (left panel).

This model is, probably, the most widely used in the interpretation of tribological experiments due to its simplicity and ability of accounting for the main physical features of atomic-scale friction. It clearly shows that a finite static friction emerges due to multistability of the system. In this mathematical description, a surface particle of mass M is coupled, via a harmonic spring of stiffness K, to a moving stage which slides at constant velocity V_{ext}. Moreover, the particle experiences a periodic (sinusoidal) coupling $V(x) = \frac{1}{2}\mathcal{E}[1 - \cos(2\pi x/a)]$ to the substrate, where x is the current position of the surface atom. Introducing the viscous damping η (proportional to the atom–substrate relative velocity $\dot{x}$) and the Langevin

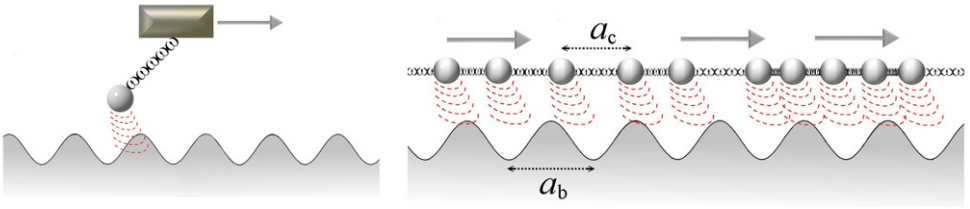

Figure 2. The Tomlinson model (left panel) and the Frenkel–Kontorova model (right panel).

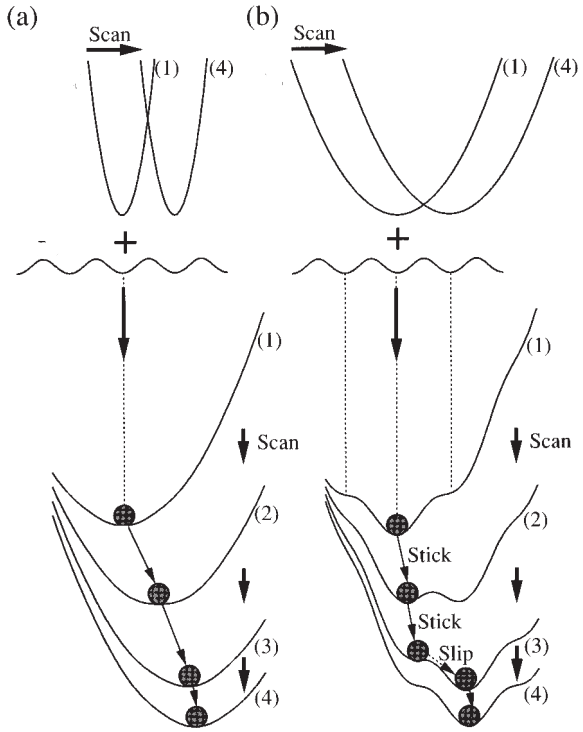

Figure 3. Sketch of the energy landscape in the Tomlinson model for (a) a stiff spring (large K) and (b) a soft spring (low K). In (a) the total potential (harmonic spring + sinusoidal substrate) has only one minimum and the atom slides continuously over the surface, while in (b) the total potential possesses different metastable minima, giving rise to the stick–slip behaviour (from [22]).

stochastic force $\Gamma(t)$, the equation of motion for the atom, accounting also for thermal effects, becomes

$$M\ddot{x} + M\eta\dot{x} = -\frac{\mathrm{d}V(x)}{\mathrm{d}x} - K(x - V_{\mathrm{ext}}t) + \Gamma(t). \tag{4}$$

As shown in the left-hand panel (a) of figure 3, if the spring is stiff enough (i.e. if K is larger than the maximum value of the second derivative of the substrate potential), then there is always a unique equilibrium position $x_{\mathrm{eq}} \approx V_{\mathrm{ext}}t$ for the atom. Consequently, at small driving velocity, the friction will be linear in V_{ext}. Things become more interesting once the maximum of $V''(x)$ exceeds K. In this situation, as sketched in the right-hand panel (b) of figure 3, the potential energy landscape is characterized, at certain instances of time, by more than one stable position. The time dependence of the combined spring and substrate potential reveals that mechanically

stable positions disappear at certain instances in time due to motion of the spring. The system is locked in one of the minima of the potential energy landscape until the increasing elastic stress of the spring allows the barrier to be overcome. After that, the slider is accelerated. The potential energy of the elastic stress is converted into the kinetic energy of the slip event and, eventually, dissipated into heat via the damping η-term. Then, the atom rapidly drops to the next-nearest metastable minimum, where it locks again. As a consequence, for a sufficiently small driving velocity, the dissipated energy per sliding distance is rather independent of $V_{\rm ext}$, in agreement with many experimental results. Obviously, this simple mechanical description can provide only qualitative interpretations of the underlying tribological processes. The Tomlinson model is described in detail in many surveys, e.g. in [23, 24], with a long list of applications to concrete physical systems (in particular to those concerning tip-based devices).

Another model that is widely used in tribology is the *Frenkel–Kontorova* (FK) *model* [15, 16] (see also Braun and Kivshar [9, 10] and references therein). In one dimension, the FK model describes a chain of interacting atoms placed into a periodic substrate potential (figure 2, right-hand panel). First analytically treated by Dehlinger [25] and then introduced to describe dislocations in solids [15, 16, 26, 27], the FK model subsequently found a wide area of applications, in particular in surface physics, where it is often used to describe the physical behaviour of an adsorbed monolayer. The interface atomic layer can be treated as a one-dimensional (1D) chain or a two-dimensional (2D) array of particles subjected to the external potential produced by the surrounding atoms of the substrate lattice below. The interaction with these other atoms can be modelled by an effective periodic on-site potential. Importantly, it has been shown that the effective periodic potential can be justified via a self-consistent microscopic model where only interparticle interactions are taken into account [28].

Mathematically, the standard FK model, whose systematic study was due to the pioneering work by Aubry [29], is characterized by the Hamiltonian

$$H = \frac{m}{2}\sum_i \dot{x}_i^2 + \sum_i \left[\frac{K}{2}(x_{i+1} - x_i - a_{\rm c})^2 + \frac{\mathcal{E}}{2}\left(1 - \cos\frac{2\pi}{a_{\rm b}}x_i\right)\right], \tag{5}$$

describing the physics of the 1D chain of N harmonically coupled atoms subjected to the sinusoidal substrate potential. The first term in equation (5) identifies the kinetic energy of the chain, the second term describes the harmonic interaction of the nearest neighbours in the chain with elastic constant K and equilibrium distance $a_{\rm c}$, and the last term takes into account the interaction of the chain with the external sinusoidal potential with height $\mathcal{E}$ and spatial period $a_{\rm b}$.

The essential feature of the static and dynamic properties of the FK model consists of the competition between the interparticle interaction and the substrate periodic potential. Indeed, if the former favors a uniform separation $a_{\rm c}$ between particles, the latter tends to pin the atom positions to the bottom of the wells, evenly spaced by the period $a_{\rm b}$. This competition, often referred to as frustration or, more specifically, *length-scale competition*, results in a fascinating complexity of spatially modulated structures.

Besides its 'apparent' simplicity, one important distinctiveness which can explain why the FK model has attracted much attention in different branches of solid-state physics and nonlinear physics is the fact that, in the continuum-limit approximation, the model reduces to the exactly integrable *sine–Gordon equation*, which allows exact solutions describing different types of nonlinear waves and their interactions. In particular, the sine–Gordon system represents an example of a fundamental mathematical model for which almost everything is known about the dynamics of nonlinear excitations. This equation describes three different types of elementary excitations, namely phonons (continuous waves in the linear limit), kinks (topological solitons) and breathers (dynamical solitons), whose dynamics determines the general behaviour of the

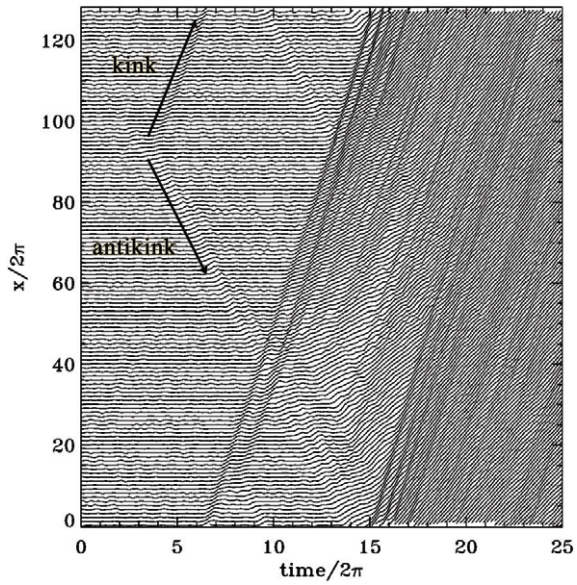

Figure 4. Detailed behaviour (atomic trajectories versus time) at the depinning transition at a small non-zero temperature for the FK chain with $\theta = 1$. As shown, the scenario starts with the creation of one kink–antikink pair. The kink and antikink move in opposite directions, quasi-elastically collide (because of the periodic boundary conditions), and soon a new kink–antikink pair is created in the tail of the primary kink. This process repeats with an exponential (avalanche-like) growth of the kink–antikink concentration, leading to the totally sliding state (from [13]).

system as a whole. Although the nature of the FK model is inherently discrete (and this manifests itself in the presence of the so-called Peierls–Nabarro (PN) barrier (see, e.g., [10, 30]) affecting the excitation motion), it is possible to get a deep physical insight and to simplify the understanding of its nonlinear dynamics using the language of the sine–Gordon quasi-particles as weakly interacting nonlinear excitations.

In the context of tribological processes, the most important 'object' in the FK model is the kink excitation. Let us consider the simplest case of the trivial ground state (GS) when the number of atoms, N, coincides with the number of minima of the substrate potential, M (or, equivalently, $a_c = a_b$), so that the dimensionless concentration $\theta = N/M$ is 1. Then the kink (or antikink) describes a configuration with one extra atom (or vacancy) inserted into the chain, $N = M \pm 1$. After relaxation, the minimum-energy configuration corresponds to a local compression of the chain (or an extension, in the antikink case). The reason why kinks are so important is that they can move along the chain much easily than the atoms themselves. The activation energy for kink motion (the PN barrier) is always smaller or much smaller than the amplitude of the substrate potential. Because the kinks (antikinks) correspond to extra atoms (vacancies), their motion provides a mechanism for mass transport along the chain. Therefore, namely kinks are responsible for mobility, conductivity, diffusivity, etc in such nonlinear systems. The higher the concentration of kinks is, the higher will be the system mobility. In the case when the GS is trivial (i.e. $\theta = 1$), the first step in system motion is the creation of a kink–antikink pair (see figure 4).

When the system is finite, kinks are generated at one end of the chain and then propagate along the chain until disappearing at the other free end. Each run of the kink (antikink) through the chain results in the shift of the whole chain by a distance of one lattice constant. In the case of a finite film confined between two solids, one may expect that the onset of sliding is initiated

by the creation of a local compression (kink, misfit dislocation) at the boundary of the contact, while a kink's motion is just the mechanism of sliding.

The most relevant concept of the FK model is the so-called *incommensurability*, as well as the *Aubry transition* [29] connected with it. Namely, let N and M be 'incommensurate' (more rigorously, let the substrate period $a_b = L/M$ and the natural period of the chain $a_c = L/N$ be such that, in the limit of infinite system length $L \to \infty$, their ratio a_b/a_c is equal to an irrational number). For a fixed amplitude of the substrate potential $\mathcal{E}$, the FK ground state undergoes a transition (usually named *the transition by breaking of analyticity* or, simply, the Aubry transition) at a critical value K_c of the interatomic interaction strength (i.e., the chain stiffness). This critical value K_c depends crucially on the incommensurability a_b/a_c defining the interface. In particular, it has been proved that for the standard FK model K_c takes the minimal possible value for the ratio a_b/a_c equal to the irrational golden mean $(1 + \sqrt{5})/2$. From a physical point of view, this means that for $K > K_c$ there exists a continuum of ground states that can be reached by the chain through non-rigid displacements of its atoms with no energy cost (*sliding mode*); on the other hand, for $K < K_c$ the atoms are trapped close to the minima of the substrate potential and thus require a finite energy (equal to the PN barrier) to be moved. Thus, for incommensurate contacts and above the Aubry transition ($K > K_c$), the sliding of the chain is initiated by even the smallest driving force and, accordingly, the static friction force is zero, $F_s = 0$. On the other hand, below K_c the two incommensurate 1D surfaces are locked together due to the creation of local regions of common periodicity. Even if $F_s = 0$ above the Aubry transition, the motion is however still not absolutely free: the kinetic frictional force is non-zero, because the dynamics results in the creation of phonons in the chain, although with a quite subtle mechanism. Note also that a *finite* FK model is always pinned, even in the truly incommensurate case of $K > K_c$, because of locking of the free ends of the chain. The pinning force in this case, however, does not depend on the chain length, $F_s \propto N^0$.

Many relevant generalizations of the FK model have been proposed so far in the literature to cover a large class of physically interesting phenomena (e.g. see [9]); they mainly account for modifications of the model interactions (substrate and/or interparticle potentials) or of the dimensionality of the system. For describing realistic physical systems (such as, for example, atoms adsorbed on a crystal surface), different types of anharmonicity can be introduced suitably in the interatomic potential of the chain (see, e.g., [31]). Such generalized FK models describe qualitatively new physical effects such as the breaking of the kink–antikink symmetry, new types of dynamical solitons (supersonic waves), a break-up of the antikink soliton followed by a rupture of the chain, a change in the interaction between the kinks, etc.

In a similar way, it is sometimes helpful to consider substrate potentials, which may vary substantially from the simple sinusoidal shape assumed in the standard FK model, with a possible consequent drastic change in the statics and dynamics occurring between the surfaces. The deviation of the substrate potential from the sinusoidal shape changes the parameters of both linear and nonlinear excitations. This may lead to qualitatively different features such as the appearance of different types of kinks, phonon branches, changes in kink–antikink collisions, and modification of breather solutions. For example, for atoms adsorbed on metal surfaces the on-site potential is usually characterized by sharp bottoms and flat barriers [32, 33]. Moreover, if the substrate is characterized by a complex unit cell, the substrate potential has a more complicated shape with several minima and/or maxima [34–36]. In this situation, from a tribological point of view, different types of sliding behaviour may be expected at low driving fields, when the dynamics is mainly governed by a mechanism that can be identified as the motion of kink-like structures. Another possibility is the inclusion of quasi-periodicity [37] or disorder [38–40] in the substrate.

An important and more realistic generalization of the standard FK chain with relevant consequences for the resulting tribological properties (critical exponents, scaling of friction force with system size, mechanisms of depinning, etc) is to increase the dimensionality of the model.

The FK model, and especially its generalized versions, are naturally applicable to the description of contact of two solid surfaces (i.e. the case of 'dry' friction), and especially to QCM experiments, where a 1D or 2D system of interacting atoms slides over a periodic substrate potential. Another important point is that the FK model allows a rather accurate investigation of the transient behaviour at the onset (or stopping) of sliding, which is quite difficult to study in more realistic 3D models.

There are also several combined models used in tribology, such as:

- The model with two periodic substrates with an atom confined in between, when the top substrate is driven through an attached spring [41–44].
- The 'train' FK model, where the driving force acts on the end atom of the chain only [45]. This model demonstrates an avalanche-like behaviour at the onset of sliding.
- The combined FK–Tomlinson model [46, 47].
- The model consisting of two coupled FK chains [48].
- The model describing the FK chain between two sinusoidal potentials [49–52].
- The two-dimensional Tomlinson model [53–55].
- The two-dimensional 'springs and balls' FK model describing a 2D layer of harmonically interacting atoms in the 2D periodic substrate (see [9, 10] and references therein).
- The *scalar anisotropic* 2D FK model treating a system of coupled 1D FK chains (see [9] and references therein).
- The *vector anisotropic* 2D FK model (e.g. the zigzag FK model; see [9] and references therein).
- The *vector isotropic* 2D FK model (see [56–59], and also [9] and references therein).
- The two-dimensional tribology model [60, 61].

4. Driven confined systems

One of the pervasive concepts of modern tribology with a wide area of relevant practical applications as well as fundamental theoretical issues is the idea of free sliding connected with *incommensurability*. When two crystalline workpieces with incommensurate lattices (or commensurate but not perfectly aligned lattices) are brought into contact, then the minimal force required to achieve sliding (i.e. F_s) vanishes, provided that the two substrates are stiff enough. In such a geometrical configuration, the lattice mismatch can prevent collective stick–slip motion of the interface atoms, with a consequent vanishingly small frictional force (*superlubric regime*). As we have just seen in previous section, this remarkable conclusion can be drawn, in particular, in the context of the FK model.

In real situations, however, such a case of 'dry' friction is exceptional. One of the many complications in developing a reliable theoretical approach to tribology on the microscopic scale is the complexity due to ambient conditions. Real surfaces are always 'wetted' by airborne molecules such as adsorbed nitrogen, water, or adsorbed hydrocarbon molecules—not to mention oxygen between two metal surfaces. These components including various forms of friction, indentation, or otherwise produced wear and debris particles are usually denoted as '*third bodies*'. The influence of such third bodies on mediating the real physical contact between two solids is not just anecdotical. Even a tiny amount of small adsorbed molecules

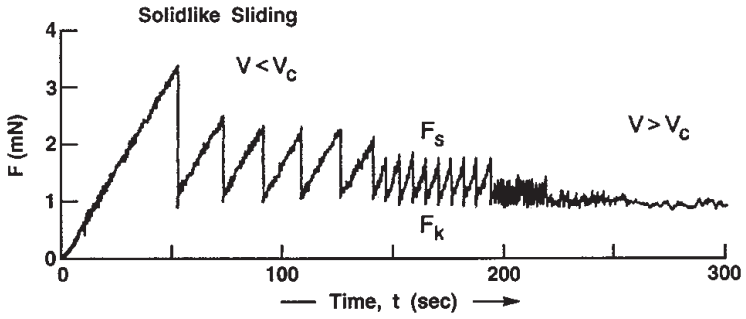

Figure 5. Time dependence of friction force for two close-packed DMPE monolayers (from [65]). With solid-like monolayers, stick–slip motion often occurs at low sliding velocities but reverts to smooth sliding above some critical velocity.

might in fact automatically lead to non-vanishing friction forces—even if the bare surfaces are perfectly superlubric.

Novel experimental techniques have been developed allowing for detailed investigations of confined molecules and macromolecules down to nanometre length scales. In tribological experiments, in particular using the surface forces apparatus (SFA) [62–64], with a constant velocity drive, one distinguishes between two possible regimes: low velocities, where the system exhibits solid-like behaviour, and high velocities, which correspond to a more liquid-like behaviour.

From an experimental point of view, the typical frictional forces observed in the different dynamical regimes are shown in figure 5. The low driving behaviour is characterized by a stick–slip motion which is basically determined by the static and kinetic friction forces and whose details also depend sensitively on the mechanical properties of the device that imposes the stress. For high velocities, the system exhibits a smooth sliding motion. Typical of the intermediate range between low and high driving velocities is a chaotic dynamical regime.

Also in this case the theoretical investigation of tribological properties in confined systems relies mainly on the two different computational approaches based on large-scale MD simulations on one side, and simplified, phenomenological models on the other. Each approach has its advantages and disadvantages and emphasizes different aspects. While in the next section we will outline the main features of a more realistic three-dimensional calculation, here we focus briefly on the ability of reproducing qualitatively, in the framework of 'minimal' models, most of the observed phenomenology of confined thin films under shear.

Rozman *et al* [41, 42] have taken an interesting approach to unravelling this problem. They have performed detailed studies of stick–slip in a rather simplified model capable of reproducing much of the complex dynamics seen in experiments of embedded lubricant layers subjected to external driving. In their simplest approach (as sketched in the left-hand panel of figure 6), they consider a one-dimensional model of two rigid plates and a single particle of mass m confined in between. The two rigid surfaces, which do not interact directly, are modelled as simple sinusoidal potentials. The top plate of mass M is driven by an elastic spring which moves at constant speed. The dynamics of the top wall and of the embedded particle is described by the coupled differential equations:

$$M\ddot{X} + \eta(\dot{X} - \dot{x}) = -\frac{\partial U(X-x)}{\partial X} - K(X - Vt), \tag{6}$$

$$m\ddot{x} + \eta\dot{x} + \eta(\dot{x} - \dot{X}) = -\frac{\partial U(x)}{\partial x} - \frac{\partial U(x-X)}{\partial X}, \tag{7}$$

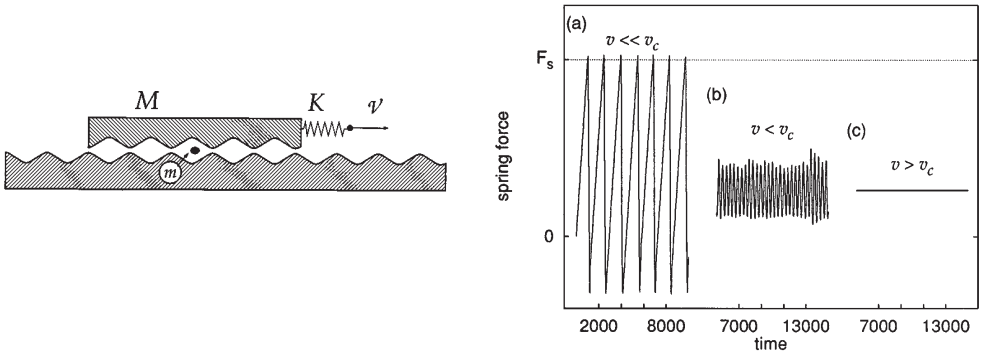

Figure 6. Schematic sketch of the model geometry (left panel). Time dependence of the spring force $-K(X - Vt)$ for the observed three dynamical regimes of motion (right panel). From [41].

where X and x denote the coordinates of the top plate and the particle, respectively. The η-terms, proportional to the relative velocities, describe the dissipative forces between the particle and the plates. The last term in equation (6) represents the driving force imposed through the spring K moving with the velocity V. The remaining terms in equations (6) and (7) stand for the effective periodic potentials $U(x)$ felt by the particle due to the presence of the two substrates.

The dynamical behaviour of the top plate and the particle is monitored as a function of different driving velocities V. In qualitative agreement with experimental observations and more complex MD simulations, the system generally displays three distinct dynamical regimes, as shown in the right-hand panel of figure 6. At low velocities, (a) a regular stick–slip motion of the plate is observed. As the driving velocity increases (b), the top wall ceases to stop (time intervals between rare stop events increase rapidly with V), and stick–slip motion becomes more erratic and intermittent. Finally, smooth sliding (c) is achieved above a critical velocity V_c. Besides, in the framework of this minimal model, the results suggest that the information obtained following the measured macroscopic dynamics (the plate motion) does not allow one to draw an unambiguous conclusion on the nature of structural changes within the contact itself (the embedded molecular system).

Always restricting to 1D modelling of confined systems under shear, the one-particle system has been generalized [49–52] to the case of a chain of interacting atoms embedded between the confining periodic potentials. This extension takes into account two additional relevant ingredients in tribological processes: the relative strengths of the interparticle interaction and the substrate on-site potentials, and the length-scale competition occurring for the simultaneous presence, at the sliding interface, of different spatial periodicities. In physical situations of confined lubricant films, one may consider the moving contact as characterized schematically by three inherent length scales: the periods of the bottom and top substrates, and the period of the embedded lubricant structure. Interesting dynamical behaviours, with possible tribologically important implications of an irregular distribution of the lubricant velocity on the wear of the sliding surfaces, have recently been observed [66, 67] depending on the 'degree' of incommensurability defining the moving interface. An unexpected feature is an asymmetry in the relative sliding velocity of the intermediate lubricating sheet relative to the two substrates. Strikingly, this velocity asymmetry takes an exactly quantized value which is uniquely determined by the incommensurability ratios and is insensitive to all other parameters of the model (such as sliders corrugation amplitudes, external velocity, chain stiffness and

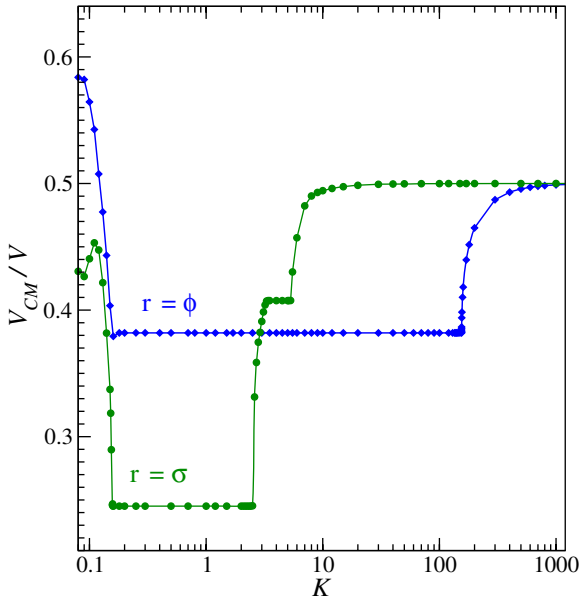

Figure 7. V_{CM}/V as a function of K for a sliding interface characterized by the golden mean ratio $r = \phi$ and the spiral mean ratio $r = \sigma$.

dissipation) for wide ranges of values. Figure 7 shows, for example, this striking behaviour of the normalized time-averaged CM velocity of the sandwiched lubricant chain, V_{CM}/V, as a function of the chain stiffness K, for the two incommensurate cases of golden mean ϕ and spiral mean σ.[4] The occurrence of these perfectly flat plateaus in the CM velocity was ascribed [66] to the intrinsic topological nature of this quantized dynamics. The phenomenon is explained by one confining substrate rigidly dragging the topological solitons (kinks) that the embedded chain forms with the other substrate. The finding of exact plateaus implies a kind of 'dynamical incompressibility', namely an identically null response to perturbations or fluctuations trying to deflect the CM velocity away from its quantized value (*dynamical pinning*). Indeed, starting now from this quantized sliding state, in the underdamped regime of motion and in analogy to what ordinarily happens for static friction, the dynamics exhibits a large *hysteresis* under the action of an additional external driving force, F_{ext} [68].

To end up with this short, and certainly not exhaustive, roundup of simple mathematical models used in mimicking the tribological behaviour of driven confined systems, we would like to draw the reader's attention to a recently investigated 2D model of rolling friction at the microscopic scale [69] (see figure 8). In this work, molecular dynamics simulations show that the rolling of spherical lubricant molecules exists only for concentrations lower than the concentration of a close-packed layer. At concentrations higher than a critical value, the rolling dynamics of nearest-neighbour molecules is hindered due to jamming of the lubricant. An optimal concentration exists which provides the minimum of kinetic friction. Besides, an increase in temperature or the introduction of additional repulsive interaction between the lubricant molecules may strongly improve the tribological properties of fullerene-like 'molecular bearings'.

[4] The golden mean, $\phi \equiv (\sqrt{5}+1)/2 \approx 1.618$, is the solution of the quadratic equation $\phi^2 - \phi - 1 = 0$; the spiral mean, $\sigma \approx 1.3247$, satisfying the equation $\sigma^3 - \sigma - 1 = 0$, belongs to the class of cubic irrationals.

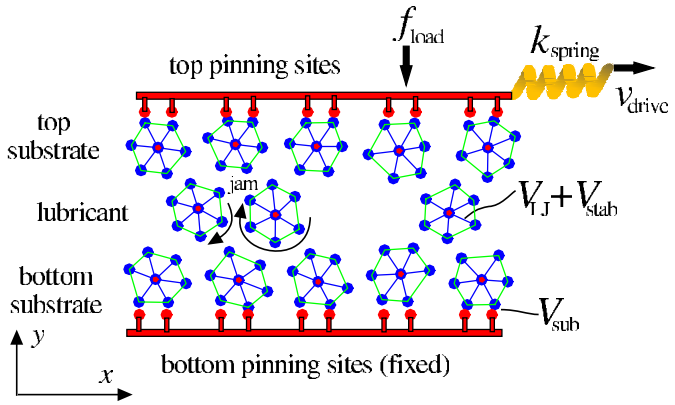

Figure 8. Schematic drawing of the 2D model (from [69]).

5. An example of realistic 3D frictional model

The simple low-dimensional models that are introduced, being very useful in understanding many physical aspects of friction, may claim mainly qualitative explanations. As already stated, the value of the static friction is sensitively dependent on the atomic structure of the mating interface. Sometimes, in order to reproduce this feature more adequately and to include subtler details in the description, this simplified approach needs to be generalized. An even more delicate situation concerns the correct evaluation of the factors that lead to the conversion of kinetic energy into heat during sliding (i.e. the determination of the kinetic friction). This process must pass through the stage of excitation of phonons at the interface. However, the rate of this process is first of all determined by the density of phonon states, which can be properly taken into account in a three-dimensional model only.

Thus, let us describe briefly the technique used in more realistic MD simulations of 3D tribological models. First of all let us explain why we have to use the Langevin motion equations in the study of far-from-equilibrium states in the driven system. In order to achieve the thermal equilibrium state in a 3D model using Newtonian equations, one has to consider $\gg 10^3$ atoms (at present, computer simulation allows one to model a maximum of $\sim 10^6$ atoms). Therefore, realistic simulation times would be of the order of $\sim 10^{-12}$ s. These timescales are too short even for reaching the steady state, and are certainly very far from typical experimental times. Besides, the approach with solely Newtonian equations cannot incorporate electron–hole damping as well as other neglected degrees of freedom.

The kinetic friction is due to energy losses which are generated at the sliding interface. Then, energy must flow away from this interface into the bulk, and be converted into the internal degrees of freedom of the substrates (phonons, electron–hole pairs). Finally, the heat produced has to be removed from the system. Thus, we cannot use solely Newtonian dynamics, since the imposed external driving would increase the energy of the system up to infinity. A standard approach in such situations is to model the substrates as being made of many atomic layers, then using the Langevin equations for a few layers far away from the interface. However, in simulation there always exists the competition 'large system $\longleftrightarrow$ long times'. Because the most important task is a detailed modelling of the interface itself, there are no essential reasons to include too many substrate layers. Therefore, it is reasonable to use the Langevin description for the lubricant atoms and for the atoms of one or just a few substrate layers; all other neglected degrees of freedom can be treated implicitly through an external damping coefficient in the Langevin equations.

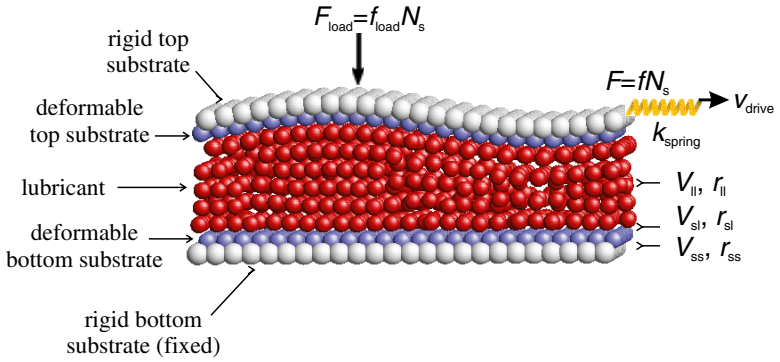

Figure 9. The model used in MD simulation of friction. Each substrate consists of two layers, the rigid layer and the deformable substrate layer, which is in contact with the lubricant. The lubricant atoms fill the space between the substrates. The atoms of the rigid layer of the bottom substrate are fixed, while the rigid layer of the top substrate can move due to applied forces.

However, a crucial issue is how to define the external damping coefficient η_{ext} in the Langevin dynamics, since it is just its value that determines the rate of energy flow out of the friction zone and, finally, governs the kinetic friction. If thermal equilibrium is of interest, an actual value of η_{ext} is irrelevant (although the rate of approaching equilibrium depends on damping and reaches a maximum at $\eta_{ext} \sim \omega_0$). In their numerous simulations [70–82], Robbins and coauthors used the following trick: the Langevin damping is applied only to the degrees of freedom that are perpendicular to the sliding direction, claiming that the actual value of the coefficient does not affect the results. This could be so at high temperatures, e.g. close to or above the bulk melting temperature of the lubricant, as was simulated in those studies, because the atomic interaction is highly anharmonic under such circumstances. In a general case, however, more reliable results should be expected when one uses a realistic damping that depends both on the coordinate z of a given atom (i.e. on its distance from the substrates) and on its velocity v with respect to the substrates, since the probability of excitation of phonons in the substrates depends on the relative velocity of the lubricant atom compared with the phononic (sound) speed in the substrate. Such an approach has recently been proposed by Braun and Peyrard [83].

The MD technique based on Langevin equations for tribological studies was first developed by Robbins *et al* and used in a series of works [70–73, 75, 74, 76–82] (see also the review papers [4, 23]). A typical three-dimensional system for simulating a lubricated contact comprises a few atomic layers of a lubricant film embedded between two (top and bottom) substrates, as sketched in figure 9. For example, in the approach proposed in [83], each substrate consists of two layers. The rigid layers form the boundaries of the system, while deformable substrate layers are in contact with the lubricant. Each rigid substrate part has N_s atoms, henceforth called s-atoms, organized into, for example, a square lattice with lattice constant a_s. The atoms of the bottom rigid substrate part are fixed, while the corresponding atoms of the top substrate part move rigidly, due to the application of an external driving. Between the rigid substrate parts we insert atoms of two different kinds: the s-atoms, which model the deformable layers of the substrates, and the l-atoms ('lubricant' atoms), forming the lubricant film. Periodic boundary conditions are used in the x and y directions. To each atom of the rigid layer of the top substrate we apply both a driving force f along the x axis and a loading force f_{load} along the z direction. The driving force f may either correspond to the dc force applied directly to the atoms (in the constant-force algorithm) or correspond

to a spring force, when sliding is imposed through a spring of elastic constant k_{spring} moving at constant velocity v_s (the algorithm with the attached spring). Then, according to Langevin motion equations (e.g. see details in [83]), the system dynamics is monitored.

For the results of 3D MD simulations of tribological processes, we may refer to the recent review by Braun and Naumovets [84] and references therein. Here, we would just mention that, in this sliding system, the ratio between the amplitudes of V_{sl} and V_{ll} (defining the substrate–lubricant interaction and the lubricant–lubricant interaction, respectively) determines the tribological behaviour of the confined lubricant film. In the case of a 'soft' lubricant, $V_{\text{ll}} \ll V_{\text{sl}}$, two lubricant layers are strongly coupled to the substrate surfaces, and the sliding occurs somewhere in the middle of the film. As a result, the lubricant is melted at sliding, and the observed stick–slip motion corresponds to the melting–freezing mechanism. Qualitatively different behaviour exhibits the 'hard' lubricant, when $V_{\text{ll}} > V_{\text{sl}}$. In this case the lubricant remains in the solid state and the sliding takes place at the lubricant–substrate interface; the stick–slip regime is due to the inertia mechanism. The latter case of a hard lubricant can provide the best lubricating conditions when two ideal crystalline surfaces are incommensurate, resulting in a vanishing static friction and an extremely low kinetic friction.

6. Conclusions

Numerical simulations have revealed themselves to be extremely useful in investigating frictional processes at the atomic scale and are expected to play an expanding role in future tribological studies. However, there are still a large number of open questions in the problem of friction and much work remains to be done. In this paper we have mainly outlined a theoretical approach to nanotribology based on simple (low-dimensional) tribological models. More than once, these models have proved to be able to describe and unravel in a quite immediate (and effective) way the general microscopic mechanisms that underlie static and kinetic friction, the importance of commensurability, the significance of metastability, the role of interface geometry, etc. Obviously, we note that in this framework the real nature of the complex processes occurring at the interface of two interacting materials in relative motion is strongly oversimplified. On the other hand, large MD simulations allow a much more direct and quantitative correlation between microscopic interactions and sliding behaviour to be established, but they are still unable to access the large length scales and long timescales of macroscopic experiments. Moreover the complexities of realistic 3D sliding systems can make it undoubtedly difficult to analyse and interpret the details of a full numerical simulation. In conclusion, each approach has limitations and strengths, and emphasizes different aspects of the problem. Therefore, a good understanding of the theoretical background is always an essential means in determining which aspects of the modelling deserve particular focus and which details are essentially irrelevant, and in choosing, subsequently, the most suitable methodological approach of investigation.

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