Prandtl-Tomlinson Model: A Simple Model Which Made History

Valentin L. Popov* and J.A.T. Gray

Abstract. One of the most popular models widely used in nanotribology as the basis for many investigations of frictional mechanisms on the atomic scale is the so-called Tomlinson model, consisting of a point mass driven over a periodic potential. The name "Tomlinson model" is, however, historically incorrect: The paper by Tomlinson from the year 1929 which is often cited in this context did not, in fact, contain the model known as the "Tomlinson model" and suggests, instead, an adhesive contribution to friction. In reality, it was Ludwig Prandtl who suggested this model in 1928 to describe the plastic deformation in crystals and dry friction. Staying in line with some other researchers, we call this model the "Prandtl-Tomlinson model," although the model could simply and rightly be dubbed the "Prandtl model." The original paper by Ludwig Prandtl was written in German and was not accessible for a long time for the largest part of the international tribological community. The present paper is a historical introduction to the English translation of the classical paper by Ludwig Prandtl, which was published in 2012. It gives a short review of the model as well as its properties, applications, and extensions from a contemporary point of view.

Keywords: Prandtl-Tomlinson model, atomic scale friction, superlubricity, velocity dependence, temperature dependence, dislocations.

1 Introduction

Throughout history, there have been contributions which have forever changed science. The discoveries of Newton or Einstein, of course, are among these. However, there are also such discoveries in more specialized fields, theories or models

V.L. Popov · J.A.T. Gray
Berlin University of Technology, 10623 Berlin, Germany
e-mail: v.popov@tu-berlin.de
* Corresponding author.

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which have developed into an integral part of science. In contact mechanics and friction, these include the Herzian contact problem or the lubrication theory of Petrov-Reynolds. This chapter is dedicated to one of the contributions from Ludwig Prandtl, a model, which he suggested and investigated. This model played a prominent role in frictional physics, especially in nanotribology.

The name Prandtl is associated most often with fluid mechanics. It is easy to believe that the publication [1] was written by him. Less known, however, is that he was also responsible for several meaningful contributions to the physics and mechanics of plastic deformations, friction, and fracture mechanics (e.g., [2]). In 1928, Ludwig Prandtl suggested a simple model for describing plastic deformation in crystals [3]. He considered the process of plastic deformation and abstracted it stepwise to a model in which a stage with many elastically coupled "atoms" is moved along a periodic potential. To start with, Prandtl simplifies it even further and considers only one-dimensional movement of a point mass being dragged in a periodic potential by means of a spring with a constant velocity v_0 and being damped proportional to velocity (Fig. 1)[1]:

$$m\ddot{x} = k\left(v_0 t - x\right) - \eta\dot{x} - N\sin\left(2\pi x / a\right). \tag{1}$$

Here, x is the coordinate of the body, m its mass, k the stiffness of the pulling spring, η the damping coefficient, N the amplitude of the periodic force, and a the spatial period of the potential. In the case of a very soft spring, the motion over one or several periods does not change the spring force F, which can be considered to be constant. In this case, the model can be simplified to the form

$$m\ddot{x} = F - \eta\dot{x} - N_0\sin(2\pi x / a). \tag{2}$$

This is illustrated in Fig. 2. After analyzing the one-dimensional model (1), Prandtl generalizes it back to a system with many independent "atoms" coupled to a stage as well as to an ensemble of "atoms" with different coupling stiffnesses, and then even to an ensemble of "systems," which from a macroscopical point of view simulates a multi-contact situation.

Over many years, the basic models (1) and (2) have been referred to as the "Tomlinson model" and the paper [5] by Tomlinson from 1929 has been cited in this connection. However, the paper by Tomlinson did not contain the above model. It is now difficult to ascertain who made this historical error and also who corrected it. We believe, however, that we have Martin Müser to thank for this historical rectification. Together with two prominent figures in nanotribology, Michael Urbakh and Mark Robbins, he published a fundamental paper in 2003 [6], in which the above mentioned model was termed the "Prandtl-Tomlinson Model." Since then, this name has become ever more frequently used.

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[1] Prandtl visualized this system with a mechanical model consisting of a wave-like surface upon which a heavy roller rolls back and forth. The elastic force is realized by the springs whose ends are fastened to a gliding stage.

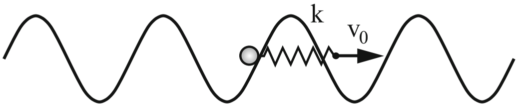


Fig. 1 The Prandtl model: A point mass dragged in a periodic potential

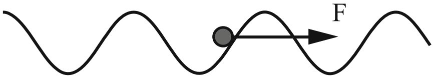


Fig. 2 Simplified Prandtl model in the case of a very soft spring (modeled here by a constant force)

The model from Prandtl describes many fundamental properties of dry friction. Actually, we must apply a minimum force to the body so that a macroscopic movement can even begin. This minimum force is none other than the macroscopic force of static friction. If the body is in motion and the force reduced, then the body will generally continue to move, even with a smaller force than the force of static friction, because it already possesses a part of the necessary energy due to its inertia. Macroscopically, this means that the kinetic friction can be smaller than that of the static friction, which is a frequently recurring characteristic of dry friction. The force of static friction in the model described by Eq. (1) is equal to N .

The success of the model, variations and generalizations of which are investigated in innumerable publications and are drawn on to interpret many tribological processes, is due to the fact that it is a simplistic model that accounts for two of the most important fundamental properties of an arbitrary frictional system. It describes a body being acted upon by a periodic conservative force with an average value of zero in combination with a dissipating force which is proportional to velocity. Without the conservative force, no static friction can exist. Without damping, no macroscopic sliding frictional force can exist. These two essential properties are present in the PT-model. In this sense, the PT-model is the simplest usable model of a tribological system. It is interesting to note that the PT-model is a restatement and further simplification of the view of Coulomb about the "interlocking" of surfaces as the origin of friction.

The PT-model was designed for understanding plasticity [3], but its extensions and variations are widely used for understanding processes of various physical natures, including dislocations in crystals (Frenkel-Kontorova model [7],[8]), atomic force microscopy [9], solid-state friction [6], control of friction by chemical and mechanical means as well as in the design of nano-drives [10],[11], and handling of single molecules [12].

In his original paper, Ludwig Prandtl considered not only the simplest deterministic form of the model, but also the influence of thermal fluctuations. He was the first "tribologist" who came to the conclusion that thermal fluctuations should lead to a logarithmic dependency of the frictional force on velocity.

The rest of this paper is organized as follows: In Sect. 2 we describe the main findings of the paper by Prandtl, in Sect. 3 we discuss further well known extensions and applications of the Prandtl model. We would like to stress that this paper is not based on a deep historical review and all following discussions make no claims of being complete.

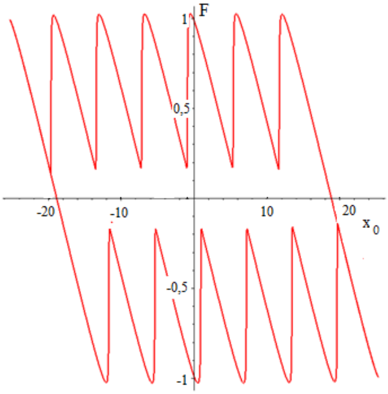
2 Results of Prandtl

Prandtl notes, first, that the movement of the mass point does not follow the movement of stage continuously, provided that the pulling spring is soft enough. For small pulling velocities, this condition of *elastic instability* reads

$$k < N\frac{2\pi}{a}. \tag{3}$$

In this case, a hysteresis is observed when the stage is moved over large distances back and forth (Fig. 3a). This is, according to Prandtl, the physical reason for plastic hysteresis. Since the 1980s, it has been known in the nanotribological community that the existence of elastic instabilities is indeed the necessary condition for a finite static frictional force in atomic scale friction [9],[13]. An example of the atomic stick-slip motion and the hysteresis is shown in Fig. 4. If the stiffness k is larger than the critical value, the average spring force (interpreted as a macroscopic force of friction) becomes identically zero (Fig. 3b). This property has been proven exactly for an arbitrary periodic potential [14]. This model has been frequently used in nanotribolgy, above all to describe the movement of the tip of an atomic force microscope along a smooth surface. This is really almost the Prandtl model to the letter, and everything that one may predict with the model can be measured. Elastic instability occurs at either sufficiently small stiffness or at sufficiently large amplitudes of the potential. The latter may be varied by adjusting the pressure that the tip of the atomic force microscope exerts on the substrate (Fig. 5), which Prandtl already realized at the end of his paper. Thereby, one can clearly see that there are actually certain conditions for which the average friction force practically disappears completely. This can be clearly seen in the hysteresis curves, which can be described very well with the simplest Prandtl model for all but small fluctuations and confirmed experimentally (Fig. 4).

In recent years, a mysterious effect has been discovered in that the movement of the tip exhibits a defined stick-slip characteristic although the average friction is very small. Even this possibility is fundamentally contained in the Prandtl model, as shown in the graphics below. The physical reason is that the mass loses stability at one position, is accelerated by the spring, and then becomes stuck once again in state in which the spring is compressed (Fig. 6b). In this case, there exists nearly no dissipation, and thereby, only little associated friction.



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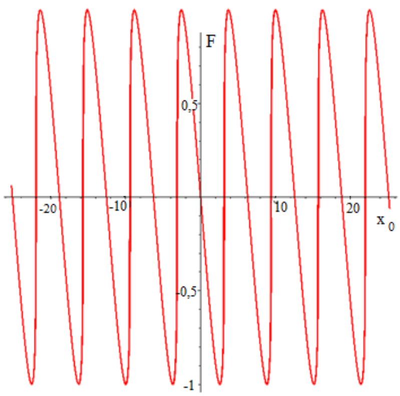

b

Fig. 3 Dependence of the force on the position x_0 of the slider: (a) $k = 0.2 \cdot k_c$. In this case, a pronounced atomic "stick-slip" and hysteresis are seen, the average "friction force" is non-zero; (b) $k = k_c$. In this case, the tangential force depends continually on the coordinate and the average frictional force is zero, there is no hysteresis.

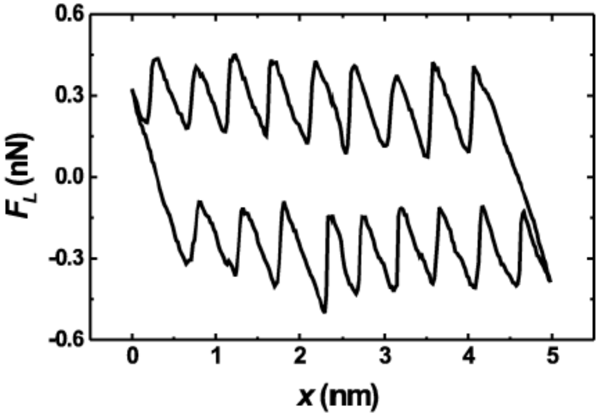

Fig. 4 Friction loop formed by two scan lines measured on a NaCl(100) surface forward and backward, respectively at $F_N = 0.65\ nN$ and $v = 25\ nm/s$. Source: [17]

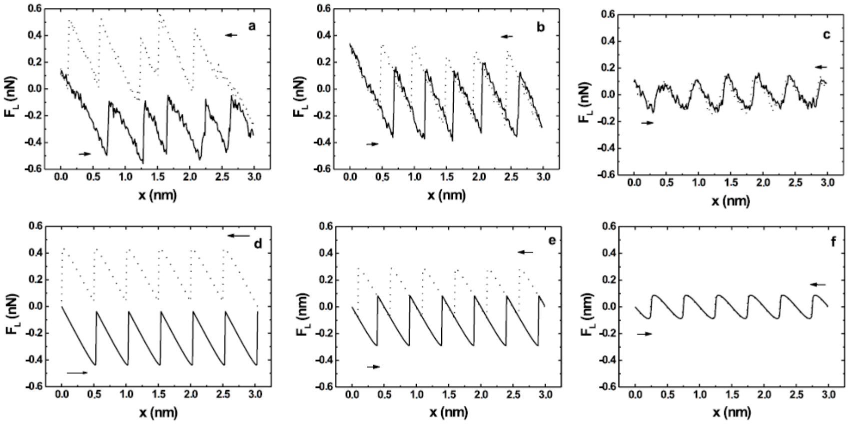

Fig. 5 Experimental data from [19] (a) –(c) Measurements of the lateral force acting on the tip sliding forward and backward in (100) direction over the NaCl(001) surface with decreasing normal force. (d) –(f) Corresponding numerical results from the Tomlinson model with suitable parameters. For small values of the normal force, the hysteresis loop enclosed between the forward and the backward scan vanishes; i.e., there is no more dissipation within this model.

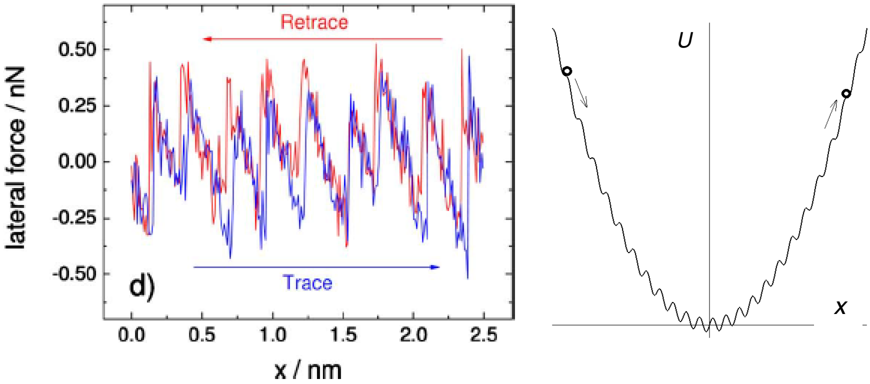

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Fig. 6 Stick-Slip without hysteresis: (a) experimental data for a scan on a graphite surface (Source: [20]) an (b) theoretical explanation

One of the surprising discoveries of nanotriblogy was the effect of super lubrication. This effect is a direct result of the fundamental properties of the Prandtl model. If the transversal stiffness is above a critical value and if several “atoms” are arranged in such a way that they have a non-compatible period relative to the opposite periodic potential (Fig. 7), then the spatial average is the same as the temporal average. Therefore, the tangential force at *every* point in time is zero. Moving the stage leads to a redistribution of the atomic structure but not to a change in the total energy. The macroscopic friction force disappears.

In literature on nanotribology, this effect is known as "superlubricity" [15]. Superlubricity can be observed either if the crystal lattices of two contacting bodies are incommensurate or if the lattices are rotated with respect to one another. In all situations, with the exception of discrete compatible orientation, the frictional force is extremely low. This is commonly illustrated by the "egg-carton model" (Fig. 8) and is also seen in experiment (Fig. 9 and Ref. [13]). Note that the similarity of the term superlubricity to the terms superconductivity and superfluidity is misleading, because it refers only to the *static* friction force. The interaction with electrons and phonons will generally lead to a final, velocity dependent frictional force. However, in dielectric materials at very low temperatures, an effect similar to true superfluidity may take place, which in [16] was called *superslipperiness*.

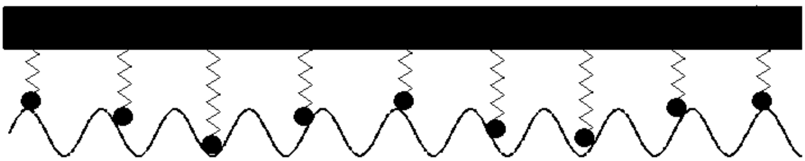

Fig. 7 In the case of a supercritical stiffness, the frictional force between incommensurate bodies vanishes

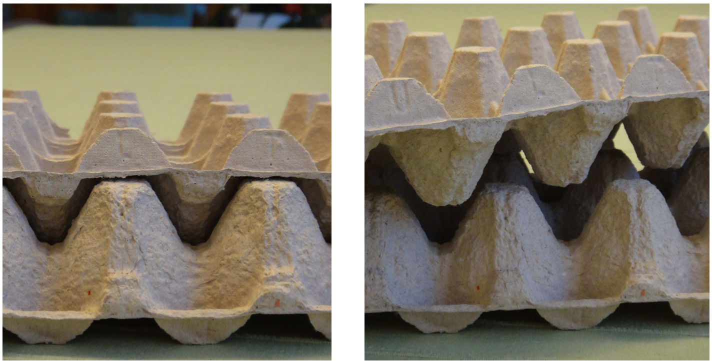

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Fig. 8 (a) The surfaces are commensurate – high friction (b) the surfaces are incommensurate – low friction

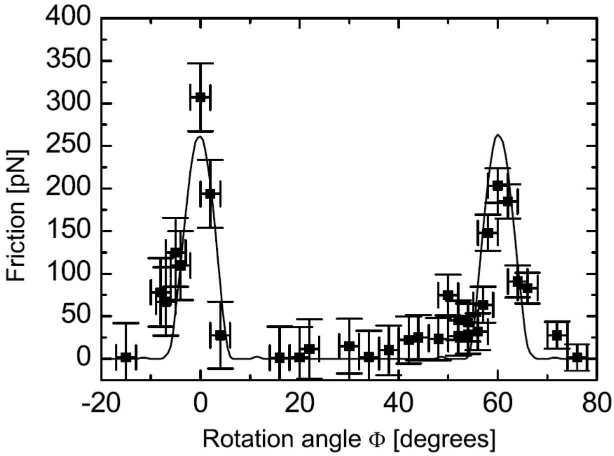

Fig. 9 Experimental data from [13]: Average friction force versus rotation angle of the graphite sample around an axis normal to the sample surface. Two narrow peaks of high friction were observed at 0 and 60°, respectively. Between these peaks a wide angular range with ultralow friction close to the detection limit of the instrument was found.

If the loading is non-monotonous, then the exact state of the system at any moment of time depends on its prehistory. In the case of an ensemble of particular systems with different parameters, this state can be very complicated. Prandtl poses the question of whether it is possible to restore the *virgin state* in which all the "atoms" are again in their initial non-stressed positions. With very simple arguments, he shows that if the stage starts to oscillate with large amplitude and the amplitude then decreases *slowly*, then each "atom" in the ensemble finally comes to the neutral, non-stressed position and the system returns to the virgin state. He compares this result with demagnetization through slowly decreasing oscillating magnetic fields, first studied by E. Madelung [18].

Prandtl further considers the properties of the model at finite temperatures. The principle idea exploited by Prandtl is to calculate back and forth mass currents due to thermal fluctuations. If the height of the periodic potential in (1) is U_0 and the spatial period a, then in a first approximation, a spring force F will change the heights of the "left" and "right" potential barriers and they will become $U_1 = U_0 + Fa/2$, $U_2 = U_0 - Fa/2$, thus, leading to a total sliding velocity $\dot{v}$ of

$$\dot{v} = C\left(e^{-(U_0 - Fa/2)/k_B T} - e^{-(U_0 + Fa/2)/k_B T}\right), \tag{4}$$

where k_B is the Boltzmann constant and T the absolute temperature. For *medium* forces satisfying the condition

$$kT << Fa/2 << U_0, \tag{5}$$

the back transitions in (4) can be neglected and we have $\dot{v} = Ce^{-(U_0 - Fa/2)/k_BT}$. Solving this equation for F

$$F = 2U_0/a + (2k_BT/a)\ln(\dot{v}/C) \tag{6}$$

gives the famous logarithmic dependency of the frictional force on velocity [6], which is found both at the atomic scale [17] and at the macro scale [21]. Note that the coefficient of the logarithmic term is proportional to the absolute temperature. For extremely small forces

$$Fa/2 << kT, \tag{7}$$

the velocity is a linear function of the force

$$v = Ce^{-U_0/k_BT}\left(e^{Fa/2k_BT} - e^{-Fa/2k_BT}\right) \approx Ce^{-U_0/k_BT}\frac{Fa}{k_BT}, \tag{8}$$

as it should be from general thermodynamic principles. The exact solution of (4) with respect to F has the form

$$F = a(T)\cdot \operatorname{asinh}(v/v_c), \tag{9}$$

which has been confirmed recently by direct molecular dynamic simulations [22]. Particularly, for very small velocities, Prandtl comes to the "noteworthy result" that the force is proportional to the deformation rate. Thus, a resistance of the same type as the drag in a fluid exists. In this viscous region he comes to the conclusion that the viscosity is an exponential function of temperature and pressure (as shown in experiments by Bridgeman [23]).

For larger forces in the region $Fa/2 \approx U_0$, a more detailed analysis is needed. In this case, the back transitions can be neglected. If the initial potential is approximated as

$$U = U_0\left[\frac{3}{2}\left(\frac{2x}{a}\right) - 2\left(\frac{2x}{a}\right)^3\right] \tag{10}$$

(preserving the distance $a/2$ between the minimum and the adjacent maximum and the height U_0 of the potential barrier), then in the presence of a constant force, the potential energy will be

$$U = U_0\left[\frac{3}{2}\left(\frac{2x}{a}\right) - 2\left(\frac{2x}{a}\right)^3\right] - Fx. \tag{11}$$

The distance between the minimum and the maximum is equal to

$$\tilde{a} = \frac{a}{2}\left(1 - \frac{1}{3}\frac{Fa}{U_0}\right)^{1/2} \tag{12}$$

and the energy difference is

$$\Delta U = U_0\left(1 - \frac{1}{3}\frac{Fa}{U_0}\right)^{3/2}. \tag{13}$$

Therefore, for the macroscopic sliding velocity, we obtain

$$v \approx Ce^{-\Delta U/T} = C\exp\left(-U_0\left(1 - \frac{1}{3}\frac{Fa}{U_0}\right)^{3/2} \Big/ k_B T\right). \tag{14}$$

Solving for F under the condition $\ln(v/C) < 0$ gives

$$F = \frac{3U_0}{a}\left[1 - \left(\frac{k_B T}{U_0}\right)^{2/3}\left|\ln\frac{v}{C}\right|^{2/3}\right]. \tag{15}$$

Thus, the Prandtl model predicts the following temperature dependence of the force of friction

$$F = C_1 - C_2 T^{2/3}. \tag{16}$$

This dependency, first found by Prandtl, has been rediscovered in the context of atomic force microscopy [24] and has been observed experimentally [25],[26]. It is interesting to note that the determination of the thermally activated sliding velocity formally coincides with many problems in chemical kinetics. The results of Prandtl, therefore, also find a place in these areas of application [12].

All of the above mentioned results of the paper have been obtained by Prandtl in a much more rigorous way as briefly summarized above. As already mentioned, Ludwig Prandtl considered an ensemble of systems and solved a kinetic equation for them in a very similar way to how it is done by contemporary researchers [24]. Eq. (1) in his paper, which in contemporary notations would read

$$\frac{dP(x,t)}{dt} = \frac{1}{\tau}\left((1 - P(x,t))e^{-\frac{U_2(x)}{k_B T}} - P(x,t)e^{-\frac{U_1(x)}{k_B T}}\right) \tag{17}$$

(with $P(x,t)$ being the probability for the atoms to take the position x in the potential relief), is nothing other than the kinetic equation for the ensemble of

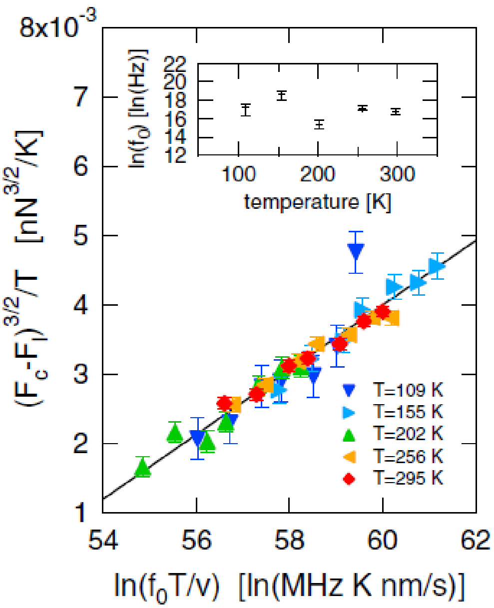

Fig. 10 Source: [26]: Force by scanning the highly oriented pyrolytic graphite (HOPG) as a function of velocity shows the dependence predicted by (15)

systems and the following treatment is essentially equivalent to solving the Fokker-Planck equation. The derivations around Eq. (20) of Prandtl's paper give, in the end, essentially the same results as were found by Kramers in his classical paper on the kinetics of chemical reactions [32]. However, one must admit that the calculations by Prandtl and his terminology are very difficult to follow. This may be one of the reasons why his paper has not had the impact to the development of science that it deserves. Now, it is of course possible to directly solve Eq. (1) with additional stochastic forces modeling thermal fluctuations. A very good review of such "molecular dynamic" investigations of the PT-model can be found in an excellent recent paper by Martin Müser [22]. Prandtl was concentrated on the study of quasi-static movements and creep, so he did not investigate the dynamic properties of the model. An overview of basic dynamic properties is given in [14].

It is interesting to note that the entire paper by Prandtl is devoted to a discussion of plasticity. Only at the end of his paper, does he come to a discussion of friction and notes that "...our conceptual model is also suitable for the treatment of kinetic friction between solid bodies." In this connection, he cites experimental results on the logarithmic dependence of the frictional force on the sliding velocity and states that "the law that frictional force increases with the logarithm of velocity is confirmed very well in a large range of velocities." He finally speculates on the reasons for the approximate proportionality of the frictional force to the normal force and suggests two physical reasons for this: On the one hand, the effective contact area of both bodies increases with the normal force; and on the other hand, through the increase in surface pressure, the molecules of both bodies are brought into closer proximity, thus, a force field with a larger wave amplitude is present. These dependencies of the local potential amplitude on the normal force have in the meantime been investigated experimentally [27] and theoretically and are indeed considered to be one of the reasons for the validity of Coulomb's law of friction [28].

3 Applications and Extensions of the Prandtl-Tomlinson Model

1. The initial application of the model was the understanding of plastic deformation and deformation creep at finite temperatures.

2. Historically, the main application of the Prandtl model has been found in nanotribology, especially for the understanding of experiments with atomic force microscopes (for review see [9]).

3. The equation of type (2) – rewritten in another notation –

$$\left(\frac{\hbar C}{2e}\right)\ddot{\phi} = j - \left(\frac{\hbar}{2eR}\right)\dot{\phi} - j_0 \sin\phi\,, \tag{18}$$

describes the dynamics of a single Josephsohn contact [29],[33]. In Eq. (18), $\hbar$ is Planck's constant, ϕ is the phase difference between contacting superconductors, C and R are the respective contact capacity and Ohmic resistance, e is the elementary charge, and j_0 is the maximum contact current. The mathematical equivalence of the two problems means that the effects seen in Josephsohn's contacts must be observed in tribological systems whose microscopic model is described by Eq. (2). One of the effects is in the modification of the current-voltage characteristic of a Josephsohn's contact undergoing an external periodic perturbation. The modification is in the appearance of plateaus where the voltage is rigorously constant (modern quantum voltage standard is based on this effect). An analogy to this effect in terms of tribology is the appearance of a plateau of a constant average velocity of a body in the presence of a periodic oscillating force. These plateaus play a key role in the further discussion of nanomachines.

4. One further extension of the simple PT-model is to consider a number of "atoms" which are elastically coupled with both the moving stage and with each other (Fig. 11). This model has been proposed by Frenkel and Kontorova [7],[8] to describe dislocation-based plastic deformation in crystals.

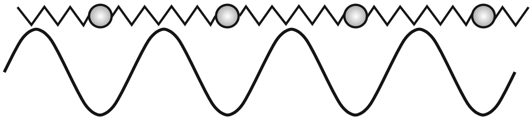

Fig. 11 Kontorova-Frenkel model

Considering the series of elastically coupled atoms as an elastic continuum, one gets the following equation of motion of the system

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} - \alpha \frac{\partial u}{\partial t} - R \sin\left(\frac{2\pi u}{a}\right) + f \ , \tag{19}$$

where u is the tangential displacement of a mass point with the initial coordinate x. α is a damping constant, f is the force density acting homogeneously on all mass points (not shown in Fig. 3), c is the sound velocity in the elastically coupled chain (without interactions with the periodic potential and the stage) and R is a constant characterizing the amplitude of the periodic potential. Eq. (19) is also known as the Sine-Gordon equation. Its static solutions correspond to dislocations in a crystal. Moving solutions of the form $u = u(x - vt)$ lead to the equation

$$\left(c^2 - v^2\right) \frac{\partial^2 u}{\partial x^2} + \alpha v \frac{\partial u}{\partial x} = R \sin \frac{2\pi u}{a} - f \ , \tag{20}$$

which is an equation precisely of the same form as the simplified PT-equation (2) (only the time should be replaced by x and the coordinate by u).

5. We consider an automobile that is power by a single-cylinder internal combustion engine and drives downhill at an angle of α to the horizontal plane. Due to the fact that the fuel injection and combustion is coupled to a distinct phase angle of the piston and, therefore, to the angle of the crank shaft, one can consider the moment that the motor exerts on the axle before the gearbox as a function of the angle θ: $M^* = M^*(\theta)$. We can write this function as

$$M^*(\theta) = M_1 + M_2 \sin\theta . \tag{21}$$

If a gearbox with a gear ratio of n is connected between the motor and the wheel axle, then the moment exerted on the axle is equal to $M = nM^*(\varphi / n)$. Neglecting the moment of inertia of the wheels, one obtains the following equation of motion for the automobile:

$$\ddot{\varphi} + \frac{\gamma}{m}\dot{\varphi} = \left(\frac{g}{r}\sin\alpha + \frac{nM_1}{mr^2}\right) + \frac{nM_2}{mr^2}\sin\left(\varphi / n\right), \tag{22}$$

where φ is the angle of rotation of the wheel, r the radius of the wheels, m the mass of the automobile, and g the gravitational acceleration. Thus, the simplest case of engine braking is also described by the PT-model!

6. Most of the ways of generating directed motion of molecular objects discussed in literature are based on the interaction between a driven object and an inhomogeneous, commonly periodically structured substrate. The latter can be either asymmetric or symmetric. In the former case, the directed motion can be only unidirectional; it is fixed by the interaction between the substrate and the object following the "ratchet-and-pawl" principle (see, e.g.,[31]). In the latter case, the direction of motion is originally not fixed and is determined dynamically. An example of this kind of a dynamically driven engine was given in [10] and [11]. The models utilized in these works are nothing but a generalized PT-model with oscillating forces.

7. Very thin layers of liquid between crystalline solids have a tendency to undergo layering transitions [34]. Under these boundary lubrication conditions, the fluid takes on the properties of the solid state. The sliding in this case can also be described by a generalized PT-model [35].

8. Further generalizations are very numerous and include, for example, the substitution of a periodic potential by a stochastic one, thus, producing a random PT-model [30]. This allows the transformation of the viscous friction at the nanoscale to a Coulomb-like friction at the macro-scale to be considered by means of a sort of renormalization technique.

4 Conclusion

Ludwig Prandtl is known foremost for his contributions to hydrodynamics. However, like many other accomplished scientists, he provided important contributions to scientific areas which were not the main field of his activities. One of these contributions is the paper on the theory of plasticity analyzed with what we now call the Prandtl-Tomlinson model. Prandtl investigated problems which still remain a subject of scientific investigation until today. The model has played a very prominent role in the history of science, especially tribology, which can be compared with other classical models, such as the contact theory by H. Hertz or the lubrication theory by Petrov and Reynolds.

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