ACSNANO
www.acsnano.org

PERSPECTIVE

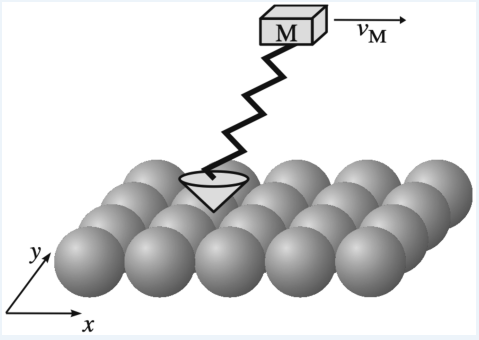
Exploring and Explaining Friction with the Prandtl–Tomlinson Model

Udo D. Schwarz*,† and Hendrik Hölscher‡

†Departments of Mechanical Engineering & Materials Science and Chemical & Environmental Engineering and Center for Research on Interface Structures and Phenomena (CRISP), Yale University, New Haven, Connecticut 06520, United States

‡Karlsruhe Institute of Technology (KIT), P.O. Box 3640, Karlsruhe 76021, Germany

ABSTRACT: **The Prandtl–Tomlinson model of friction, first introduced in 1928 as a "conceptual model" for a single-atom contact, consists of a point mass that is dragged over a sinusoidal potential by a spring. After decades of virtual oblivion, it has recently found impressive validation for contacts comprising tens or even hundreds of atoms. To date, the Prandtl–Tomlinson model enjoys widespread popularity as depicting arguably the most insightful mechanical analogue to atomic-scale effects occurring at sliding interfaces. In this issue of *ACS Nano*, Pawlak *et al.* demonstrate the model's applicability to a true single-atom contact, thereby illustrating that simple mechanical representations can indeed go a long way toward explaining interactions at atomically defined interfaces.**



Friction is an everyday phenomenon we typically think about only when it is (nearly) absent, such as when we slide on ice in the winter.[1] Consequences of vanishing friction may indeed be dramatic, as exemplified by the popular-culture staple of the comedian who slips on a banana peel.[2] Conversely, suppressing friction through proper lubrication is a tremendously important factor for the function of many mechanical devices featuring interfaces that are in relative motion.[3−5] As a result, attempts to control friction are almost as old as civilization.[6]

Despite this long history of *exploring* frictional effects, success in *explaining* their origins is still disappointingly limited. Through the work of Leonardo da Vinci (1452–1519), Guillaume Amontons (1663–1705), and Charles Augustin de Coulomb (1736–1806), three fundamental laws of friction have been established:[7]

i. The frictional force F_{fric} that needs to be overcome to move a slider on a substrate is proportional to the loading force F_{load};
ii. friction is independent of the (apparent) contact area of the slider with the substrate; and
iii. sliding friction is independent of the sliding velocity.

Laws (i) and (ii) are usually expressed as $F_{fric} = \mu F_{load}$, where the "friction coefficient" μ is constant for a given contact. Even though these laws are easy to apply and hold astonishingly well for a wide set of conditions, they do not provide any scientific insight into the underlying principles that govern friction. All parameters affecting friction, such as the nature of the materials involved, surface roughness/preparation, temperature, sliding speeds, and distances are hidden in the empirically determined friction coefficient. While such coefficients may be tabulated for the exact experimental conditions for which they have been determined, it is currently impossible to predict μ for an arbitrary contact.

In a renewed attempt to achieve substantial progress, the field of nanotribology was established in the late 1980s. Through the introduction of novel experimental tools such as the atomic force microscope (AFM), the frictional behavior of nanoscale contacts could be investigated for the first time.[8−10] Researchers anticipated that once the principal mechanisms had been identified in these nanometer-size systems, they could be "scaled up" for better understanding of friction in technologically relevant, macroscopic systems.

> Today, the principles put forward in the Prandtl–Tomlinson model dominate our understanding of atomic-scale friction.

Among the many scientific advances that nanotribology has enabled, one of the most striking is the observation of individual "hopping events" of atoms moving through a corrugated interface potential featuring atomic periodicity.[11−13] Effectively resulting in a "stick–slip"-type motion, this discovery brought the spotlight back to a much older, but previously unverified "conceptual model" ("Gedankenmodell") that is usually referred to as the *Prandtl–Tomlinson* (PT) model.[14] For historical correctness, however, let us note that the 1929 paper by G. A. Tomlinson[15] credited with impact on

DOI: 10.1021/acsnano.5b08251
ACS Nano XXXX, XXX, XXX–XXX

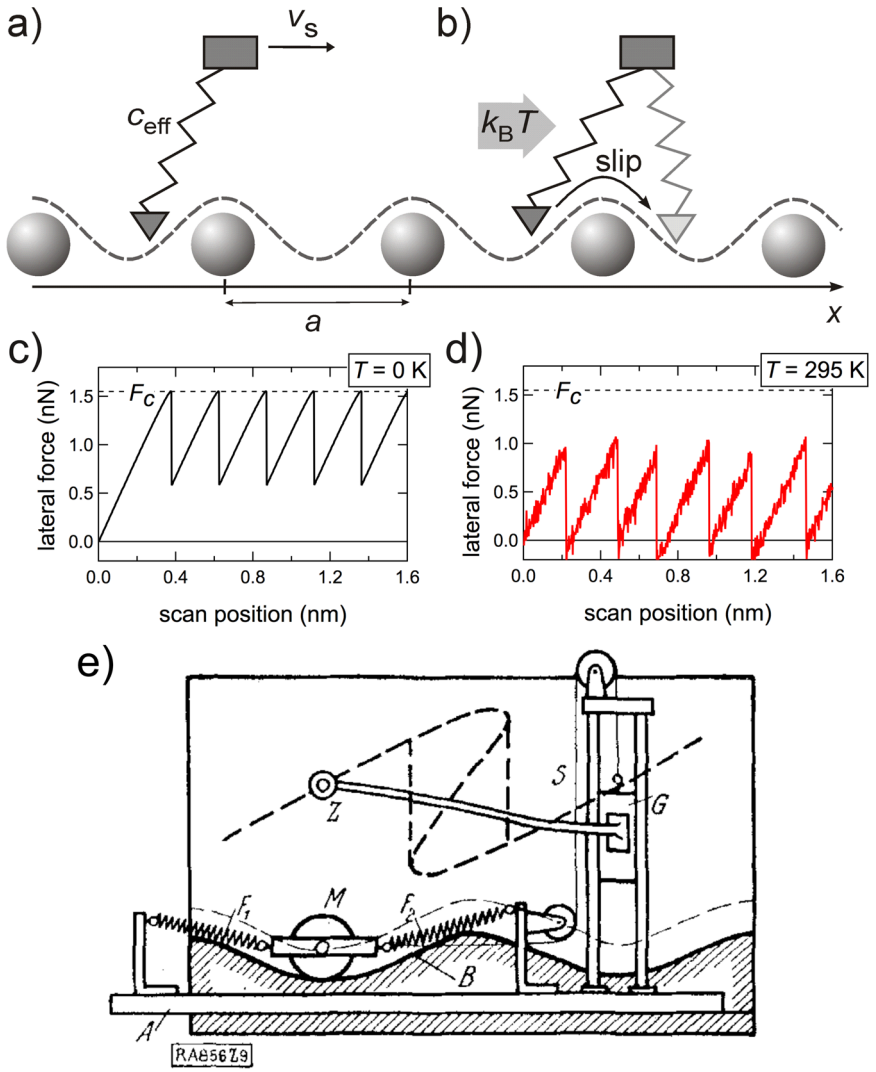


Figure 1. (a) Schematic drawing illustrating the basic principles of the Prandtl−Tomlinson model. A point-like mass is coupled through a spring with spring constant c_{eff} to a supporting body M (gray box) while interacting with a potential $V(x_t)$ featuring a periodicity *a*. During sliding, the body M is moved with velocity v_S in *x* direction. (b) If the spring is soft enough, the resulting tip motion shows a characteristic "stick−slip"-type behavior. Jumps from one potential minimum to another occur when the spring tension has reached a specific critical value. Note that among the many predictive aspects of the model is that temperature effects can easily be introduced by considering thermal oscillations of the tip. (c) If the system moves at *T* = 0 K, the resulting lateral force is a sawtooth-like function and the mass jumps always when the critical force F_c associated with that particular potential and spring constant is reached. Thereby, the lateral force is measured by detecting the spring tension as a function of the location of the body M on the *x* axis (denoted here as "scan position" to highlight its divergence from the position of the tip x_t). (d) For higher temperatures, the mass might jump at values lower than F_c due to thermal activation provided by the energy k_BT (where k_B is Boltzmann's constant). As a consequence, the maxima of the lateral force (and thus the overall measured frictional force) reduce while thermal noise becomes visible on the "rising leg" of the sawtooth function. (e) Sketch of a mechanical model designed by Prandtl[16] to demonstrate the stick−slip like movement of the mass in a sinusoidal potential on the macroscopic scale. Reprinted with permission from ref 16. Copyright 1928 Wiley.

the PT model (so much so that the PT model is sometimes simply denoted as the "Tomlinson model"[14]) does not contain the theory of the PT model as it is used today. This mistake was compounded by the fact that the 1928 paper by Ludwig Prandtl (1875−1953),[16] where the theory was actually presented, was written in German and therefore not accessible for large parts of the scientific community. This situation changed relatively recently, when in 2012, a translation into English was published by the same journal in which the original 1928 article appeared.[14] It may also be interesting to note that Prandtl developed the model many years before he published it. In 1913, one of his former graduate students, Theodore von Kármán, and Prandtl's own Ph.D. advisor (and father-in-law) August Föppl outlined its basic aspects in a review on the 'physical foundations of the mechanics of materials' [that was also written in German; see ref 17], remarking: "Since the Prandtl theory is to date unpublished, we will present it in some more detail based on communications from the author himself. Full publication by Prandtl... is expected at a later time." In his 1928 article, Prandtl himself stated that he did not have time to publish his work earlier because he was too occupied with his work on aerodynamics.[16]

Today, the principles put forward in the PT model dominate our understanding of atomic-scale friction. Consisting of a point mass driven over a periodic potential (see Figure 1 for details), it readily explains observations in a large number of

DOI: 10.1021/acsnano.5b08251
ACS Nano XXXX, XXX, XXX−XXX

cases: flat surfaces,[11] flat surfaces with different types of atoms,[18] velocity dependence,[19,20] temperature dependence,[21] atomic-scale steps,[22] and even ions in a trap.[23] But its predictive capabilities do not end here; despite its origins as a single-atom model, the PT model also delivers intuitive rationalizations for many fundamental properties of dry friction. For example, the fact that we must apply a certain minimum force to the slider before any movement is initiated (macroscopically well-known as the "force of static friction") corresponds in this atomic-scale image to a "pretensioning" of the spring between point mass and slider before the first slip occurs. Once in motion, the slider will continue to move even if a force smaller than the force of static friction is applied because the slider's inertia helps overcome potential barriers. This result again elegantly connects atomic-scale insight with the macroscopic finding that kinetic friction is almost always less than static friction.

Despite the PT model's successes, one of its most apparent weaknesses was that it was never directly confirmed for the 'single-atom-attached-to-a-slider-by-a-mechanical-spring' case that it is envisioned to describe. Atomic force microscope tips sliding in intimate contact over a substrate, as previously used,[11,18−22] produce nanocontacts that comprise at least tens, but more often even hundreds of atoms at the interface due to the experimental difficulty of balancing attractive and repulsive forces adequately.[24,25] As a result, AFMs previously measured the *collective behavior of an ensemble of atoms* rather than directly reflecting the behavior of an individual atom.

Pawlak *et al.* were able to demonstrate through a combination of experiment and simulation that the movement of the nitrogen apex atom—and the molecule as a whole—exactly follows the behavior that the PT model predicts for the single-atom case.

The article by Pawlak *et al.* in this issue of *ACS Nano* now fills this important conceptual void.[26] Two experimental advances made this possible. First, Pawlak *et al.* attached a porphyrin molecule to the tip of an AFM. At low temperatures (5 K), where the experiments were conducted, adhesion is sufficient to keep the molecule firmly "glued" to the tip end. The internal rigidity of the molecule then provided both a single-atom tip apex that is robust enough not to deteriorate while being dragged over the surface (in the form of a nitrogen atom terminating a downward-pointing carbonitrile end group of the porphyrin) as well as the "spring attachment" of the atom to the slider (through the internal flexing and bending degrees of freedom of the molecule). Second, they used a control scheme developed for high-resolution atomic force microscopy[27] that enables them to "hover" the tip over the surface at any desired distance while the force fluctuations acting on the molecule during sliding are monitored with ultimate accuracy. With these ingredients in place, Pawlak *et al.* were able to demonstrate through a combination of experiments and simulations that the movement of the nitrogen apex atom—and the molecule as a whole—exactly follows the behavior that the PT model predicts for the single-atom case.[26]

OUTLOOK AND FUTURE CHALLENGES

With the PT model's applicability to a true single-atom contact established, work has just begun. One interesting direction to follow would be to study the influence of the chemical activity of different end groups with a variety of substrates or structural features such as defects, surface steps, and impurities. Additionally, changing the strength of the elastic attachment of the end group to the tip by sampling more complex, custom-designed molecules could lead to other notable insights.

The real challenge lies, however, in answering the question of how to extrapolate the findings from nanometer-sized contacts to the macroscopic scale. Initial attempts included considering a large number of atoms, which are elastically coupled to the slider as well as among each other. Such a model, which has its main use in describing dislocation-based plastic deformation in crystals, was proposed by Frenkel and Kontorova in 1938 and has been improved since in later studies.[28] Most interestingly, provided the internal coupling is above a certain threshold value, friction is predicted to increase with contact area only in a sublinear fashion for incommensurate interfaces since the effective overall energy barrier to move across the interaction potential will eventually approach zero.[29] This effect, which has often been called "structural lubricity" or even "superlubricity",[13] has, in fact, not only been observed for contacts comprising up to hundreds of thousands of atoms,[30] but its friction-area scaling laws were successfully traced back to a product between a *purely structural factor* and the *diffusion barrier* that a *single adsorbed atom* has to overcome while moving from one potential minimum to another.[31] Nevertheless, the bigger, more complex question of how "upscaling" to realistic, rough contacts would work remains largely unsolved. At least for now, the above-cited expectation that, from understanding of the atomic fundamentals of friction, macroscopic friction could be explained with the help of statistics (*i.e.*, by the summation of the interactions of a large number of small individual contacts that form the macroscopic roughness of the contact interface) has not yet been fulfilled.

AUTHOR INFORMATION

Corresponding Author

*E-mail: udo.schwarz@yale.edu.

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

U.D.S. acknowledges the support of the Yale Materials Research Science and Engineering Center (MRSEC) under the National Science Foundation grant No. NSF DMR-1119826.

REFERENCES

(1) Rosenberg, R. Why Is Ice Slippery? *Phys. Today* **2005**, *58*, 50−55.
(2) Mabuchi, K.; Tanaka, K.; Uchijima, D.; Sakai, R. Frictional Coefficient Under Banana Skin. *Tribol. Online* **2012**, *7*, 147−151.
(3) Hsu, S. M. Molecular Basis of Lubrication. *Tribol. Int.* **2004**, *37*, 553−559.
(4) Holmberg, K.; Andersson, P.; Erdemir, A. Global Energy Consumption Due to Friction in Passenger Cars. *Tribol. Int.* **2012**, *47*, 221−234.
(5) Schwarz, U. D. Tracking Antiwear Film Formation. *Science* **2015**, *348*, 40−41.
(6) Dowson, D. *History of Tribology*; Wiley-Blackwell, 2009.

DOI: 10.1021/acsnano.5b08251
ACS Nano XXXX, XXX, XXX−XXX

(7) Popova, E.; Popov, V. L. The Research Works of Coulomb and Amontons and Generalized Laws of Friction. *Friction* **2015**, *3*, 183–190.
(8) Bhushan, B.; Israelachvili, J.; Landman, U. Nanotribology - Friction, Wear and Lubrication at the Atomic-Scale. *Nature* **1995**, *374*, 607–616.
(9) Carpick, R.; Salmeron, M. Scratching the Surface: Fundamental Investigations of Tribology with Atomic Force Microscopy. *Chem. Rev.* **1997**, *97*, 1163–1194.
(10) Bhushan, B. Nanotribology and Nanomechanics. *Wear* **2005**, *259*, 1507–1531.
(11) Mate, C. M.; McClelland, G. M.; Erlandsson, R.; Chiang, S. Atomic-Scale Friction of a Tungsten Tip on a Graphite Surface. *Phys. Rev. Lett.* **1987**, *59*, 1942–1945.
(12) Hölscher, H.; Schwarz, U. D.; Wiesendanger, R. Simulation of a Scanned Tip on a NaF (001) Surface in Friction Force Microscopy. *Europhys. Lett.* **1996**, *36*, 19.
(13) Hölscher, H.; Schirmeisen, A.; Schwarz, U. D. Principles of Atomic Friction: From Sticking Atoms to Superlubric Sliding. *Philos. Trans. R. Soc., A* **2008**, *366*, 1383–1404.
(14) Popov, V. L.; Gray, J. A. T. Prandtl–Tomlinson Model: History and Applications in Friction, Plasticity, and Nanotechnologies. *Z. Angew. Math. Mech.* **2012**, *92*, 683–708.
(15) Tomlinson, G. A. A Molecular Theory of Friction. *Philos. Mag.* **1929**, *7*, 905–939.
(16) Prandtl, L. Ein Gedankenmodell Zur Kinetischen Theorie Der Festen Körper. *Z. Angew. Math. Mech.* **1928**, *8*, 85–106.
(17) Von Kármán, Th.; Föppl, A. Physikalische Grundlagen der Festigkeitslehre: 24. Hysteresis und Nachwirkung in Kristallen und kristallinischen Haufwerken. *Encyl. d. math. Wiss.* **1913**, *4–4*, 767–770.
(18) Hölscher, H.; Raberg, W.; Schwarz, U. D.; Hasbach, A.; Wandelt, K.; Wiesendanger, R. Imaging of Sub-Unit-Cell Structures in the Contact Mode of the Scanning Force Microscope. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1999**, *59*, 1661.
(19) Gnecco, E.; Bennewitz, R.; Gyalog, T.; Loppacher, C.; Bammerlin, M.; Meyer, E.; Guntherodt, H. Velocity Dependence of Atomic Friction. *Phys. Rev. Lett.* **2000**, *84*, 1172–1175.
(20) Riedo, E.; Gnecco, E.; Bennewitz, R.; Meyer, E.; Brune, H. Interaction Potential and Hopping Dynamics Governing Sliding Friction. *Phys. Rev. Lett.* **2003**, *91*, 084502.
(21) Jansen, L.; Hölscher, H.; Fuchs, H.; Schirmeisen, A. Temperature Dependence of Atomic-Scale Stick-Slip Friction. *Phys. Rev. Lett.* **2010**, *104*, 256101.
(22) Hölscher, H.; Ebeling, D.; Schwarz, U. D. Friction at Atomic-Scale Surface Steps: Experiment and Theory. *Phys. Rev. Lett.* **2008**, *101*, 246105.
(23) Gangloff, D.; Bylinskii, A.; Counts, I.; Jhe, W.; Vuletic, V. Velocity Tuning of Friction with Two Trapped Atoms. *Nat. Phys.* **2015**, *11*, 915–919.
(24) Mo, Y.; Turner, K. T.; Szlufarska, I. Friction Laws at the Nanoscale. *Nature* **2009**, *457*, 1116–1119.
(25) Luan, B.; Robbins, M. O. Contact of Single Asperities with Varying Adhesion: Comparing Continuum Mechanics to Atomistic Simulations. *Phys. Rev. E* **2006**, *74*, 026111.
(26) Pawlak, R.; Ouyang, W.; Filippov, A.; Kalikhman-Razvozov, L.; Kawai, S.; Glatzel, T.; Gnecco, E.; Baratoff, A.; Zheng, Q.-S.; Hod, O.; Urbakh, M.; Meyer, E. Single-Molecule Tribology: Force Microscopy Manipulation of a Porphyrin Derivative on a Copper Surface. *ACS Nano* **2015**, DOI: 10.1021/acsnano.5b05761.
(27) Garcia, R.; Perez, R. Dynamic Atomic Force Microscopy Methods. *Surf. Sci. Rep.* **2002**, *47*, 197–301.
(28) Braun, O. M.; Kivshar, Y. *The Frenkel-Kontorova Model*; Springer: Berlin, Heidelberg, 2004.
(29) Muser, M. H.; Wenning, L.; Robbins, M. O. Simple Microscopic Theory of Amontons's Laws for Static Friction. *Phys. Rev. Lett.* **2001**, *86*, 1295–1298.
(30) Dietzel, D.; Ritter, C.; Mönninghoff, T.; Fuchs, H.; Schirmeisen, A.; Schwarz, U. D. Frictional Duality Observed During Nanoparticle Sliding. *Phys. Rev. Lett.* **2008**, *101*, 125505.
(31) Dietzel, D.; Feldmann, M.; Schwarz, U. D.; Fuchs, H.; Schirmeisen, A. Scaling Laws of Structural Lubricity. *Phys. Rev. Lett.* **2013**, *111*, 235502.

DOI: 10.1021/acsnano.5b08251
ACS Nano XXXX, XXX, XXX–XXX