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ORIGINAL PAPER

A Dislocation-Based Analytical Model for the Nanoscale Processes of Shear and Plowing Friction

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Abstract We describe a friction model to link the continuum-based shear and plowing method of Bowden and Tabor with the atomistic processes that occur at the nanoscale. We show that the interfacial shear component can be modeled via dislocation drag at the interface, and the plowing in terms of power-law creep. We show that without empirical friction measurements, this approach has a strong predictive power for the interfacial sliding of crystalline materials.

Keywords Friction mechanisms · Nanotribology · Contact mechanics

1 Introduction

Tribology is an old discipline that has recently been seeing an increase in attention. Historically, the science behind sliding contact phenomena has been explored in many different ways, but never fully understood due to its complexity and the difficulty of experiments. Recently, however, it has become insufficient to account for friction and wear approximately or empirically. As device engineering trends continue towards reductions in scale, surface effects become relatively more and more important. In addition, increasing concerns about energy and efficiency highlight the significance of frictional losses and the importance of tribology to the lifetime of devices.

There is a long history of using modeling to understand friction. Engineering models, such as those of boundary lubrication, have for decades used contact mechanics and geometry to predict frictional behavior in the presence of lubricants [1–3]. While these methods have been successful in predicting phenomena such as stick–slip [4], more fundamental atomistic analysis on a smaller scale is still desirable. From the earliest atomistic models of Tomlinson [5] and Frenkel-Kontorova [6], we have seen increased understanding from using molecular dynamics, finite-element modeling or similar methods [7–14]. In conjunction with experiments which are able to probe smaller and smaller length scales, we are able to predict more about atomic behavior under stress than we ever have. However, such deterministic methods are inevitably run at small length and time scales, as a result of the many calculations needed to be done per time step.

It is not a new idea to consider the role of dislocations in such small-scale friction processes. In fact, dislocation dynamics has been used effectively to model friction [15] and contact mechanics [16], although again at small scales. It is clear that small scale materials science can be linked to the behavior of sliding asperities, but again the complexity of such models limits their applicability to a wide variety of experiments.

It is possible to describe the behavior of a stressed material in a more general sense, using the idea of deformation mechanisms rather than individual dislocation stresses. One of the earliest attempts to account for the effects of deformation on friction was made by Bowden and Tabor [17], hereafter abbreviated as the BT model. By considering the contact mechanics of an asperity sliding across a flat surface, they realized that not only should there be a shearing component of friction at the interface,

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but the plowing of material in front of the tip should contribute as well. The sum of these two retarding forces was taken to be the effective frictional force experienced by the asperity.

The model is quite simple conceptually, and has only the contact area, shear strength, and flow pressure as parameters. As a result, the BT model has been widely used as a starting point for determining the components of friction. Efforts to introduce material property dependencies into the BT model include work by, e.g. Bull [18], Malzbender and de With [19], and Komvopoulous [20]. However, the relevant terms in these models are often empirical in nature, as they are generally put forth in the context of scratch tests or other tribology experiments. This can result in difficulty when attempting to reproduce or compare results. Attempts have also been made to extend the BT model to take into account additional forms of material deformation, such as asperity creep, asperity deformation in general, etc. These extensions can range from rock friction to aerospace applications [21–24]. This kind of approach has been useful for making sense of more and more complex data sets, but fundamentally it still relies on the experimental data to determine the friction force. In addition, these empirical models present a challenge to understanding the details of a sliding interface at a more fundamental level.

The focus of this paper is to develop a formulation of the BT model in terms of the underlying materials science of bulk plastic deformation. Instead of extending the BT model, we aim to limit the dependence on empirical terms with an analytical formulation. In particular, we equate the shear strength to the retardation of dislocations at the sliding interface, and consider the plowing in front of a rigid asperity as a creep process. We will focus on copper with a grain size of 0.1 mm, but the model is extendable to other materials. The aim of the model is not to exhaustively take into account all mechanisms of friction, but to use dislocation theory to approximate the frictional force of a crystalline material at steady state in terms of well-known bulk deformation mechanisms, and using the substantial existing knowledge on asperity contact mechanics. Due to the non-specific analytical nature, we can then check the model against a wide range of experimental and other results.

2 Model

We will first develop the model by equating the two components of the BT approach to retardation of dislocation motion at the interface, and creep. We will then provide some numerical details of the results.

3 Interface Shear Strength

The BT friction model is a simple summation of shear and plowing forces: $S + P = F$. The shear component of friction in this model essentially considers the normal contact area during sliding interacting with the “shear strength” of the material. This shear term is described by the total contact area (as given by the Hertzian model [25] for a spherical asperity as πa^2 where a is the contact radius) multiplied by the shear strength of the softer material s, so $S = \pi a^2 s$. The empirical shear strength in this case is thought of as the critical stress a material can accommodate before yielding in shear (critical resolved shear stress).

However, if we look at this model from the point of view of the deformation mechanics, we know that the interfacial sliding has to do with dislocation motion, and indeed we can consider the forces on the dislocations to be representative of the macroscale forces on the material [26]. Using this interpretation, we can redefine the empirical shear term S as a viscous dislocation drag force F_D (see below). Both terms effectively try to capture the interfacial resistance generated by sliding one material over another.

The problem of viscous drag of dislocations in the bulk is well established, and when applied to a sliding interface [26] gives a macroscale friction force due to the dislocation drag F_D if:

$$F_D = \frac{N_d(\sigma_p b)(\sin\theta + \cos\theta)}{2} \coth\left[\frac{2(\sigma_p b)\sin\left(\frac{\Delta\theta}{2}\right)}{B_{tot} v}\right] \qquad (1)$$

where v is the velocity of the dislocation, b the Burgers vector of the dislocation, σ_p is the Peierls stress, N_d is the number of dislocations in the contact area, θ is the misorientation angle from a commensurate surface, and B_{tot} is the sum of the electronic, flutter, and phonon wind contributions to dislocation drag. For our purposes, we can consider only incommensurate surfaces and set θ to be a constant 10° angle. Then, for a given velocity of relative motion, we need only to determine B_{tot} and N_d.

For the calculation of B_{tot} (which can be decomposed into different quasiparticle excitations by the moving strain field of a dislocation), the reader is referred to the paper by Merkle and Marks [26] and references therein. N_d is simply determined by multiplying the areal density of dislocations by the contact area πa^2, as determined by force equilibrium:

$$\frac{F_N}{\pi a^2} = H \Rightarrow a = \sqrt{\frac{F_N}{\pi H}} \qquad (2)$$

where F_N is the normal load and H is the generalized hardness, or resistance to plastic deformation, which combines the elastic and plastic material responses.

Increasing H will reduce the contact area for a given normal load. For copper, yield strengths may vary widely, but 500 MPa was chosen as a typical value of H for this model.

4 Plowing

The plowing component of friction deals with the force necessary to physically push the material in front of the asperity aside. The plowing term in the BT model is given by the cross-sectional area of the groove track caused by the asperity, multiplied by the "flow pressure" (i.e. the necessary instantaneous stress to cause or continue plastic deformation).

Rather than analyzing this along the same lines as in the original BT model, we use a more standard materials science approach and deal with the plastic deformation as creep. For high-temperature, power-law creep, we know the semi-empirical relationship between shear strain rate and shear stress:

$$\dot{\gamma} = A_2 \frac{D_v G b}{kT}\left(\frac{\sigma_s}{G}\right)^n \tag{3}$$

where D_v is the diffusion coefficient (neglecting dislocation core diffusion), b is the relevant Burgers vector, G the shear modulus, σ_s is the shear stress, n is the power-law creep exponent, and A_2 is the appropriate Dorn constant. For $n = 3$ and $A_2 = 1$, this relation is quite general and can be derived from physical models of dislocation mechanics. However, most materials require variation of these two parameters to fit experimental data, for reasons which are not completely clear. As a result, we must look to experimental data for bulk copper to determine A_2 and n [27].

We build in a temperature dependence in an Arrhenius fashion for the diffusion constant, and the modulus has a temperature dependence as well [27]:

$$D_v = D_{0v} e^{-\frac{Q_v}{RT}} \tag{4}$$

$$G = G_0\left(1 + \frac{T - 300}{T_m}\right)\frac{T_m}{G_0}\frac{dG}{dT} \tag{5}$$

For a given asperity velocity and shape we will be able to geometrically determine the shear strain rate in the material. This rate is solely dependent on the velocity and the relevant distance over which the dislocation deforms the material. In this case, we take the reference length as the distance from the dislocation core exhibiting 1% strain. In the pressure–temperature regime where power-law creep is the dominant deformation mechanism, then we can equate the shear strain rates. In the case of a cone-shaped asperity:

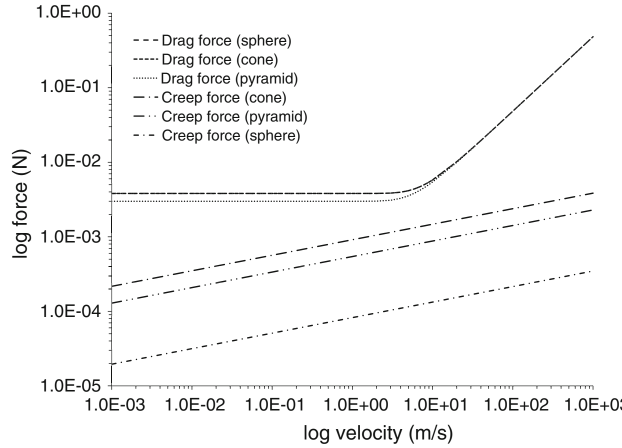

Fig. 1 Creep and drag forces versus sliding velocity and asperity shape. Normal load 100 μN, temperature 0.8 T_m, cone/pyramid angle 20°, and sphere radius of curvature 1 μm

$$\begin{aligned} \dot{\gamma} &= A_2 \frac{D_v G b}{kT}\left(\frac{\sigma_s}{G}\right)^n = \frac{\pi^2 v}{4 \cdot 50 b}; \\ \left(\sigma_s^n\right)^{\frac{1}{n}} &= \sigma_s = G \cdot \left(\frac{kT\pi^2 v}{200 A_2 D_v G b^2}\right)^{\frac{1}{n}} \end{aligned} \tag{6}$$

In the above equations, we have derived a mathematical formulation in which we couple the conventional creep model with the shear stress σ_s acting on the interface. Similar forms exist for spherical and square pyramidal asperities. The frictional force due to plowing can then be easily written using the contact radius a, determined by force balance between the normal load and the indented material, and corresponding indentation depth d:

$$\begin{aligned} F_C &= \sigma_s A \\ &= G a^2 \cot\theta \cdot \left(\frac{kT\pi^2 v}{200 A_2 D_v G b^2}\right)^{\frac{1}{n}} \end{aligned} \tag{7}$$

$$= G a^2 \cot\theta \cdot \left(\frac{\sqrt{2} kT\pi v}{100(2+\sqrt{2}) A_2 D_v G b^2}\right)^{\frac{1}{n}} \tag{8}$$

$$\begin{aligned} &= G \cdot \left(\frac{kT\pi^2 v}{200 A_2 D_v G b^2}\right)^{\frac{1}{n}} \cdot \\ &\times \left[R^2 \cos^{-1}\left(\frac{R-d}{R}\right) - (R-d)\sqrt{2Rd - d^2}\right] \end{aligned} \tag{9}$$

where Eq. 7 is for a cone with angle θ, Eq. 8 is for a square pyramid with angle θ, and Eq. 9 is for a sphere with radius of curvature R. See Goddard and Wilman [28] for an analysis of the contact mechanics of differently shaped asperities.

These equations for the creep force F_C combine with the F_D term given by Eq. 1 to give the friction coefficient μ:

$$\mu = \frac{F_D + F_C}{F_N}. \quad (10)$$

5 Results and discussion

We find in general that modeling the plowing component of friction as a result of material deformation, in this case, power-law creep, is a feasible approach. As we will see below the trends and values are in general consistent with the literature.

Figure 1 compares the drag (adhesive) and creep (plowing) components to total friction. The dislocation model predicts a transition (curved region on the plot) where the dominant source of drag goes from radiative to viscous effects. The influence of plowing friction is most felt in this regime, where the total friction deviates most from the adhesive force. Also note, under similar circumstances, the spherical asperity produces less plowing due to the higher aspect ratio of the cone and square pyramid. In general, the ratio of plowing to adhesive components of the friction coefficient falls within the reported range for measured metal-on-metal friction [29].

We can see by virtue of the shear term alone that there is a sharp transition in the friction force, which corresponds with the onset of viscous drag effects on dislocations. Comparison with the deformation mechanism maps for copper shows that this transition also has a good correlation with the stress necessary to leave the climb-mediated creep deformation regime and enter a regime of power-law breakdown, where the glide rate becomes the controlling factor [27]. In effect, it is postulated that once the material can no longer easily deform via dislocation motion, there are sharp increases in the friction from the change in deformation mechanism. We can further speculate that because wear rates are analytically linked directly to friction [28], the inability for a material to deform easily via dislocations leads to a sharp increase in the material ejected from the interface as wear.

We find that at high normal loads, shown in Fig. 2, the increase in net friction force becomes directly proportional, meaning the coefficient of friction becomes a constant. The increasing normal load in this model is tied to increasing contact area, and it is evident that at high loads, the increase in the drag force becomes dominated by the increase in contact area, and corresponding increase in the number of dislocations at the sliding interface. The creep force has the same dependence on the horizontal projected contact area regardless of the force, so this result is to be expected.

Figure 3 shows the isolated effect of increased plowing severity while holding the drag force constant. A similar plot will be obtained if you plot the data vs. penetration depth. As the cone angle decreases for a given load, the asperity must penetrate deeper into the material to maintain force balance. Under significant plowing (0.1 radians corresponds to a 355 μm penetration depth), the plowing force will dominate. This trend is consistent with reported experimental and theoretical penetration depth dependence, considering an asperity with finite penetration depth would result in a constant creep force once the cone angle becomes small enough [19, 30]. It is also clear that increasing temperatures not only increase the absolute contact areas, increasing friction overall, but increase the creep component of the total friction. At higher temperatures, the material deforms more easily by creep, resulting in lower frictional forces.

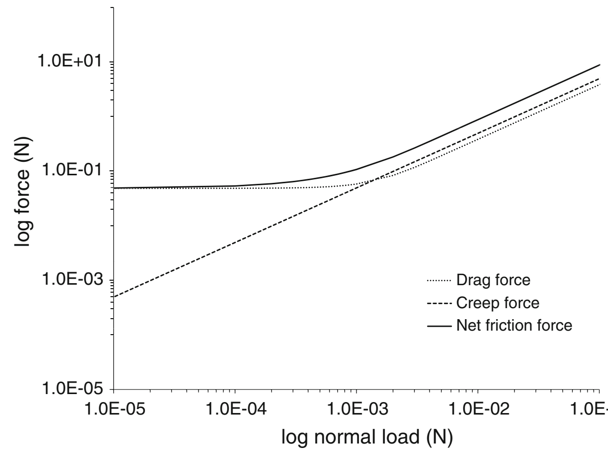

Fig. 2 Friction force versus normal load. 100 m/s sliding velocity, and cone angle 10°

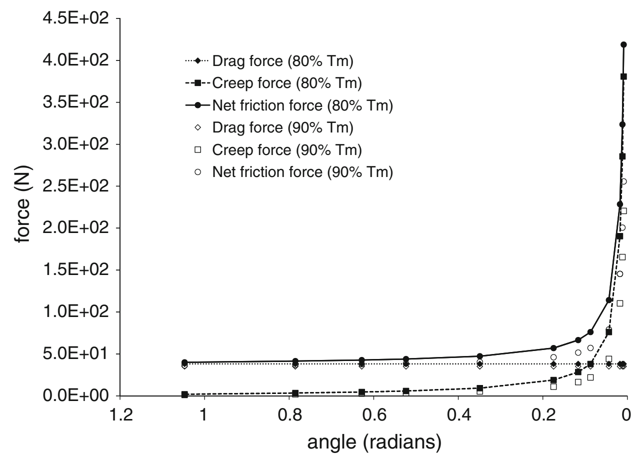

Fig. 3 Friction force versus cone angle and temperature. For a cone-shaped asperity, 1 m/s, 1 N load. A decrease in the cone angle corresponds directly to an increase in the penetration depth of the asperity, for the same normal load

6 Conclusions

We have presented a very straightforward dislocation-based interpretation of the BT shear and plowing model. Our formulation uses an analytical continuum approach to predict the steady-state friction forces to first order at a sliding interface, with only a few well-known experimentally derived parameters necessary. The predictions from this model—in particular, the power-law creep mechanism for plowing friction—have a good correspondence with measured results, and using only dislocation-based deformation mechanisms we can account for a good deal of tribological behavior. Not only is this approach easily modifiable and extendable to other materials, but it is able to offer alternative explanations for known phenomena in a materials science context. In that sense, we have seen that this approach can be quite effective in understanding fundamental trends in friction behavior and therefore, how they can be affected by materials design.

Furthermore, the structure of the model—and its basis in the BT approach—provides the ability to easily incorporate additional phenomena, such as asperity deformation [31], shear-localized chip formation [32], dislocation pinning, grain boundaries, and other energy dissipation mechanisms. Modeling dynamic processes using dislocation theory might also be a fruitful approach to expand this model.

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References

1. Bowden, F.P., Tabor, D.: The Friction and Lubrication of Solids. Clarendon Press, Oxford (1958)
2. Hamrock, B.J., Schmid, S.R., Jacobson, B.O.: Fundamentals of Machine Elements. McGraw-Hill Higher Education, Boston (2004)
3. Bhushan, B., Israelachvili, J.N., Landman, U.: Nanotribology: friction, wear and lubrication at the atomic scale. Nature **374**, 607–616 (1995)
4. Weiss, M., Elmer, F.-J.: Dry friction in the Frenkel–Kontorova–Tomlinson model: dynamical properties. Z. Phys B Condens Matter **104**, 55–69 (1997)
5. Tomlinson, G.A.: A molecular theory of friction. Philos. Mag. **7**, 905–939 (1929)
6. Kontorova, T., Frenkel, Y.I.: On the theory of plastic deformation and twinning. Zh. Eksp. Teor. Fiz. **8**, 1340 (1938)
7. Persson, B.N.J.: Theory of friction and boundary lubrication. Phys. Rev. B Condens. Matter **48**, 18140–18140 (1993)
8. Persson, B.N.J.: Theory and simulation of sliding friction. Phys. Rev. Lett. **71**, 1212–1215 (1993)
9. Singer, I.L.: Friction and energy-dissipation at the atomic-scale—a review. J. Vac. Sci. Technol. A **12**, 2605–2616 (1994)
10. Krim, J.: Atomic-scale origins of friction. Langmuir **12**, 4564–4566 (1996)
11. Mulliah, D., Kenny, S.D., McGee, E., Smith, R., Richter, A., Wolf, B.: Atomistic modelling of ploughing friction in silver, iron and silicon. Nanotechnology **17**, 1807–1818 (2006)
12. Carpick, R. W., Agrait, N., Ogletree, D. F., Salmeron, M. Measurement of interfacial shear (friction) with an ultrahigh vacuum atomic force microscope. J. Vac. Sci. Technol. B **14**, 1289–1295 (1996)
13. Bellemare, S., Dao, M., Suresh, S.: The frictional sliding response of elasto-plastic materials in contact with a conical indenter. Int. J. Solids Struct. **44**, 1970–1989 (2007)
14. Prasad, A., Dao, M., Suresh, S.: Steady-state frictional sliding contact on surfaces of plastically graded materials. Acta Mater. **57**, 511–524 (2009)
15. Deshpande, V.S., Needleman, A., Van der Giessen, E.: Discrete dislocation plasticity analysis of static friction. Acta Mater. **52**, 3135–3149 (2004)
16. Polonsky, I.A., Keer, L.M.: Scale effects of elastic-plastic behavior of microscopic asperity contacts. J. Tribol. **118**, 335–340 (1996)
17. Bowden, F.P., Moore, A.J.W., Tabor, D.: The ploughing and adhesion of sliding metals. J. Appl. Phys. **14**, 80–91 (1943)
18. Bull, S.J.: Can scratch testing be used as a model for the abrasive wear of hard coatings? Wear **233–235**, 412–423 (1999)
19. Malzbender, J., de With, G.: Sliding indentation, friction and fracture of a hybrid coating on glass. Wear **236**, 355–359 (1999)
20. Komvopoulos, K.: Sliding friction mechanisms of boundary-lubricated layered surfaces: part II—theoretical analysis. Tribol. Trans. **34**, 281–291 (1991)
21. Scholz, C.H., Engelder, J.T.: The role of asperity indentation and ploughing in rock friction–I : asperity creep and stick-slip. Int. J. Rock Mech. Min. Sci. Geomech. Abstr. **13**, 149–154 (1976)
22. Nam, P.S.: Tribophysics. Prentice-Hall, Englewood Cliffs (1986)
23. Jaffer, F.: Experimental evaluation of sliding friction coefficients for aerospace applications. Master's thesis, University of Toronto, Toronto (2001)
24. Tas, N.R., Gui, C., Elwenspoek, M.: Static friction in elastic adhesion contacts in MEMS. J. Adhes. Sci. Technol. **17**, 547–561 (2003)
25. Hertz, H.: Ueber die Berührung fester elastischer Körper. J. Reine. Angew. Math. **92**, 156–171 (1882)
26. Merkle, A., Marks, L. D.: A predictive analytical friction model from basic theories of interfaces, contacts and dislocations. Tribol. Lett. **25**, online (2007)
27. Frost, H.J., Ashby, M.F.: Deformation-mechanism maps : the plasticity and creep of metals and ceramics. Pergamon Press, New York (1982)
28. Goddard, J., Wilman, H.: A theory of friction and wear during the abrasion of metals. Wear **5**, 114–135 (1962)
29. Szeri, A.Z.: Fluid Film Lubrication – Theory and Design. Cambridge University Press, Cambridge (1998)
30. Liu, Z., Sun, J., Shen, W.: Study of plowing and friction at the surfaces of plastic deformed metals. Tribol. Int. **35**, 511–522 (2002)
31. Bhushan, B.: Handbook of Micro/Nanotribology. CRC Press, Boca Raton (1995)
32. Komanduri, R.: Some clarifications on the mechanics of chip formation when machining titanium alloys. Wear **76**, 15–34 (1982)