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Comment on "friction between incommensurate crystals"

A. P. MERKLE and L. D. MARKS*

Department of Materials Science and Engineering,
Northwestern University, Evanston, IL 60208, USA

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We present results from an independent analysis of friction that more generally addresses all crystalline materials by an extension of coincident site lattice theory and dislocation drag. Calculations for graphitic friction are carried out and agree in magnitude with experimental friction forces. More interestingly, static, dynamic and anisotropic friction forces, incommensurability effects and superlubricity are explained by a more rigorous analysis of the dislocation structure at a sliding interface.

In a recent paper, Friedel and de Gennes [1] elegantly framed the problem of friction between atomically flat and impurity-free crystalline surfaces. This topic has recently received much theoretical interest, largely because of the highly sensitive experimental capabilities developed to measure friction in controlled environments [2–5]. Extremely low friction forces have been measured, and although these low forces are not exclusively measured between crystalline materials, they occur between crystalline bodies only at incommensurate orientations. We believe that Friedel and de Gennes [1] have successfully identified some of the key components missing in many theoretical studies on solid friction: the motion of and interaction between intrinsic interfacial dislocations when a shear stress (e.g. sliding) is applied. They correctly identify a number of physical phenomena related to a finite-sized flat crystalline contact, including dislocation arrays (misfit dislocations found in bicrystals), surface waves (Rayleigh–Love) and phonon drag processes. They conclude that superlubrication is not a surprise in the weak-coupling regime, but that significant complications exist, including dislocation and electronic bonding structure.

We have independently performed a similar analysis [6], but in a more general context not just limited to materials such as graphite and MoS_2. We believe it is important to go beyond the analysis of Friedel and de Gennes [1], in particular to extend it to include several well established literature fields.

(i) Grain boundary dislocations need to be considered within the well established coincident site lattice (CSL) model.

*Corresponding author. Email: l-marks@northwestern.edu

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(ii) The difference between what they refer to as strong and weak coupling is really the question of whether or not the interfacial dislocations are extended or localized.
(iii) It is very important to differentiate between static friction, which is the resistance to motion at infinitesimally small velocities, and dynamic friction and any full analysis should consider both.
(iv) The question of friction with an incommensurate system is intimately linked to the well established Aubry transition, where there are some very recent experimental observations [5] directly demonstrating very low friction in some cases.

In more detail, in their paper Friedel and de Gennes [1] use what they refer to as 'ladders of dislocations' to accommodate the misfit at a grain boundary. We will argue that one should instead use conventional CSL theory [7–9] to model the grain boundary structure. An interface between two hexagonal planes results in a dislocation network of hexagonally symmetric in-plane screw dislocations [10, 11]. Frank's formula solves for the inter-dislocation spacing, and instead of having two orthogonally oriented sets of dislocations we have three in-plane sets for the hexagonal case that are oriented 120° from each other. Details of the structure of dislocations in the basal plane of graphite have been studied by transmission electron microscopy techniques [12]. Dislocations that have a Burgers component in the direction of sliding will experience drag, leading to anisotropic forces as a function of sliding direction (see figure 1).

Friedel and de Gennes [1] also argue that for rigid layers, instead of discrete full or partial dislocations one can think about a larger set of infinitesimally small dislocations. Whereas this is reasonable in some senses as a mathematical limit, what they are really referring to is the question of whether the dislocation core is extended or not. It is well known that as a screw dislocation width (core) is expanded, its Peierls stress is dramatically reduced [13], in this case leading to lower static friction forces.

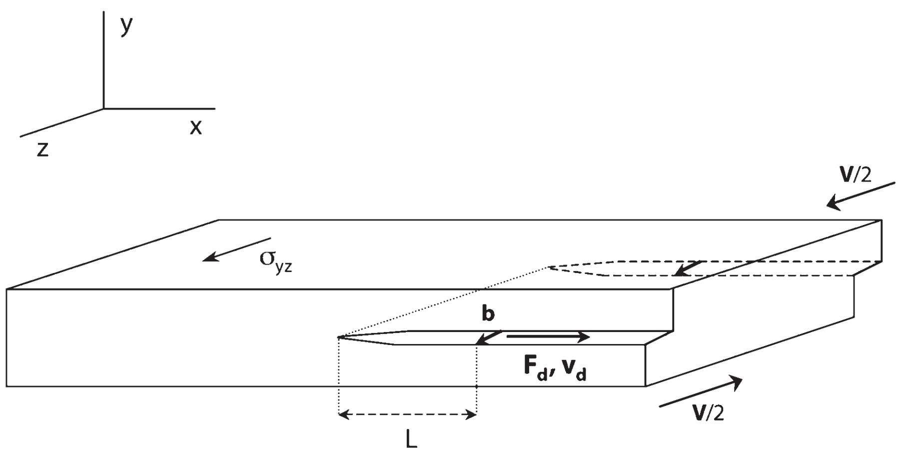

Figure 1. Forces on a screw dislocation in response to a shear.

Turning to the question of viscous friction, Friedel and de Gennes [1] use a relatively simple model based upon that of Sokoloff. We believe that this needs to be generalized. Following Alshits [14], one can write for the force resisting the motion of dislocations,

$$F = \sigma_{\mathrm{p}} b \coth\left(\frac{\sigma_{\mathrm{p}} b}{B v_{\mathrm{d}}}\right) \tag{1}$$

where B is a viscous damping term which can be expanded in a number of different contributions as

$$B = B_{\mathrm{w}} + B_{\mathrm{fl}} + B_{\mathrm{e}} \tag{2}$$

where B_{fl} is the flutter term [15], B_{w} is the phonon wind term [16] and B_{e} is the electron drag coefficient [17]. This force on dislocations closely matches friction behaviour in a number of ways. In the limit to zero velocity, equation (1) approaches the Peierls stress of the material, in effect a static friction. It also contains a continuous transition from radiative (Peierls-type) friction to viscous friction (see figure 2), as seen recently in friction measurements between polymers over a large range of velocities [18].

Graphite sliding on graphite has been observed to give low friction forces for incommensurate orientations. A calculation of friction forces was carried out using the above model applied to the sliding conditions in the experiment by Dienwiebel *et al*. [3]. For a load of 18 nN, sliding velocity of 20 nm s^{-1} and tip radius of 80 nm, and using a measured shear stress value of graphite [19], we arrive at a Σ1 kinetic

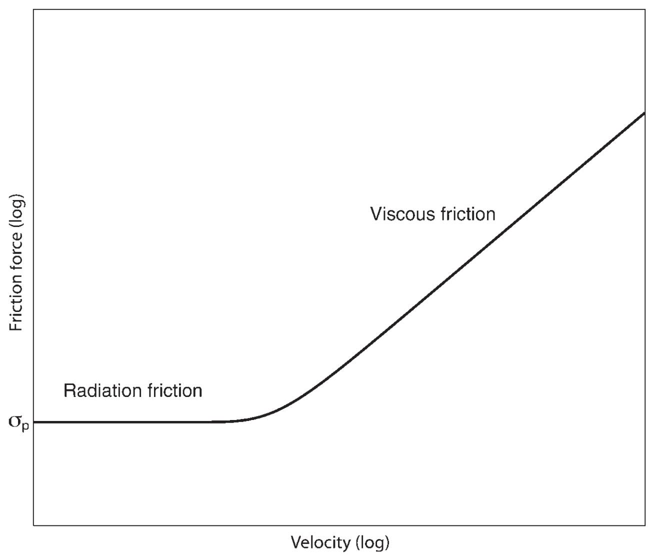

Figure 2. Functional form of friction via dislocation drag as a function of sliding velocity (arbitrary units), indicating the transition from a Peierls dominated regime to viscous friction.

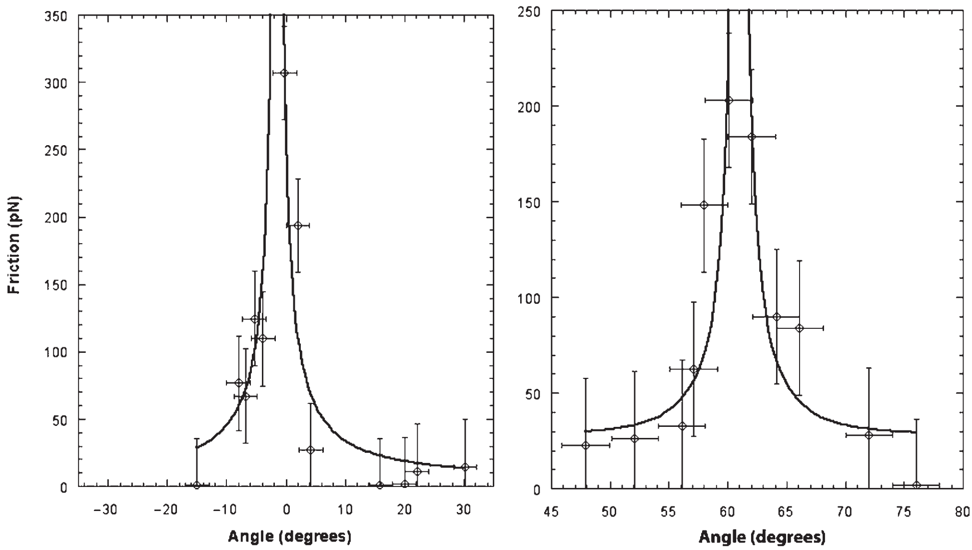

Figure 3. Fit to Dienwiebel friction data (graphite–graphite sliding) using the analytical expression for dislocation drag. The fit to the viscous drag coefficient gives a mean value of $0.0012 \pm 0.0001\,\mathrm{N\,s\,m^{-1}}$.

friction range of $\mu = 0.001$–0.026 for dislocation spacing limits of 5 and 25 nm. The experimental kinetic friction coefficient for commensurate contact conditions was 0.017, in agreement with our calculated range. Performing a fit of equation (1) (see figure 3), accounting for all experimental and contact parameters including sliding velocity, partial dislocation structure and materials constants, we can give an estimate of the effective viscous drag coefficient and Peierls stress for the contact. By using a $600\,\text{Å}^2$ sliding flake, fits to both peaks yield an average value of $0.0012 \pm 0.0001\,\mathrm{N\,s\,m^{-1}}$ for B. Since the sliding conditions are within the viscous drag regime, the fits are somewhat insensitive to the value of the Peierls stress, but an order of magnitude fit places it at 1 Pa. We acknowledge that in this analysis, a simple estimate was used to account for the finite size effects of the graphite flake by solving for a fraction of a dislocation. This is not generally correct, and remains an active field of research, particularly in the investigation of dislocation-mediated deformation of nanograined materials. Experiments have shown [20] that nanoparticles forming twist boundaries with a crystalline substrate rotate to form commensurate contact in a thermally activated process, whereas molecular dynamics simulations [21] have indicated that for particles smaller than 5 nm this phenomenon occurs athermally. A significant amount of additional work must be carried out to complete the analysis of smaller contacts, identifying the precise structure of dislocations at nanometre-sized grain boundaries, but we believe that this order of magnitude estimate is nonetheless useful; the principals of the model do not change, only the specific dislocation structure. We note that Dienwiebel's experiment [3] represents the most sensitive and thorough set of experimental data for any system in regards to friction anisotropy at the nanoscale. However, in order to more

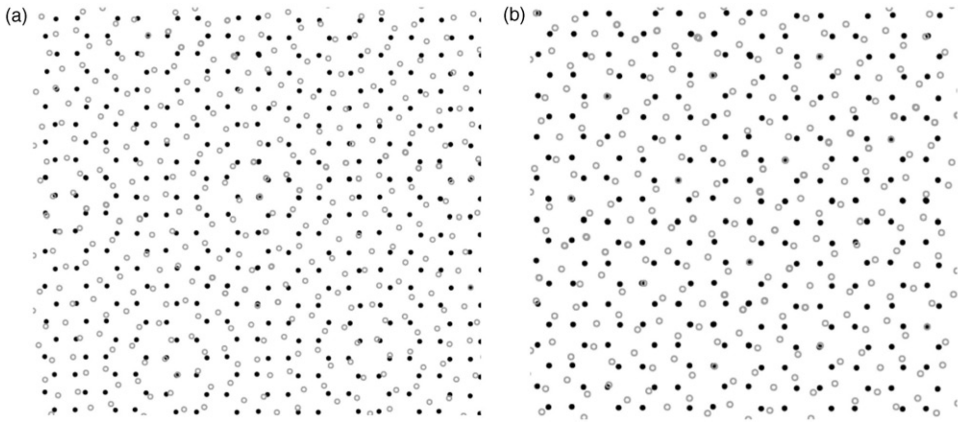

Figure 4. Hexagonal CSL showing a 6° misorientation (a) forming a hexagonal network of misfit cores and the Σ7 boundary (38.21°) (b).

accurately fit the anisotropy peak widths to an analytical model for dislocation friction, at least an order of magnitude improvement in force resolution must be made to the experimental data. This can be achieved in part by increasing the normal load, taking care not to increase to the point where the flake detaches from the tungsten tip.

It is worth mentioning that for hexagonal CSL orientations there are in other special twist orientations (see figure 4) between 0° and 60°, including Σ7 at 38.21°, Σ13 at 27.79°, Σ19 at 46.82° and Σ21 at 21.78°. Although much weaker than the commensurate six-fold symmetry, we expect that these peaks could be experimentally resolved. Dissociated dislocations [22] at these orientations will lead to a friction value at least an order of magnitude weaker than commensurate contact. The measurements by Dienwiebel *et al.* [3] show a slight bump at the Σ21 orientation, but the expected friction value is within the associated experimental error. A significant peak is resolved at $50 \pm 2°$, and could reasonably represent the Σ19 boundary. It would be worthwhile to perform this experiment with better force and angular resolution, if necessary at higher normal loads and contact areas.

Lastly, in terms of incommensurate systems, it is important to recognize that this has been analyzed in detail within the context of the Frenkel–Kontorovva model. The classic case is the Aubry transition; below a certain coupling constant the interfacial dislocations completely dissociate leading to a nominally zero static friction [23]. In terms of equation (1) this corresponds to vanishing of the Peierls stress associated with the motion of these dislocations. Note, however, that this does not mean that there will be zero dynamic friction because there will still be drag effects due to the motion of the elastic deformation field including surface waves.

A recent study by Park *et al.* [5] has shown strongly anisotropic friction forces on the surface of a decagonal Al–Ni–Co quasicrystal. This unique surface attains periodicity in one direction, whereas in another it is quasiperiodic, following the stacking sequence of Fibbonacci. It was found that friction increases by a factor of eight in the periodic direction as compared to the quasiperiodic direction. We believe this experiment has convincingly isolated the issue of the role of periodicity on friction, and can be explained by the behaviour of dislocations. By maintaining a constant contact orientation, the sliding direction was changed, meaning that the initial interfacial dislocation structure was essentially unchanged. Only the motion of interfacial dislocations behaves differently. When sliding in the periodic direction, regularly spaced dislocations with Burgers vectors along the direction of motion experience a drag force. When sliding is performed in the quasiperiodic direction, the dissociated aperiodically spaced dislocations are now the only remaining contributors to drag, resulting in a greatly reduced friction force.

Friction between crystalline bodies is a complex issue that has only recently become amenable to direct experimental investigation. We point out that a relatively simple analysis of the structure and motion of interfacial dislocations can account for observed friction phenomena. We believe the motion of dislocations at interfaces plays a large role in the dissipative forces associated with friction, and encourage further experimentation to uncover anisotropic, velocity, temperature and structure (incommensurability) dependencies.

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