Comment on "Transition from Thermal to Athermal Friction under Cryogenic Conditions"

In a recent Letter, Zhao *et al.* [1] reported on the temperature dependence of friction at a silicon nitride/MoS_2 interface using a variable temperature atomic force microscope (AFM); similar techniques were used previously on a variety of other interfaces [2–5]. The Arrhenius analysis of the data in [1] and other models of friction [6–8] implicitly assume that the interface is near thermal equilibrium and can be characterized by a single temperature which governs the transition probabilities and fluctuating forces. The purpose of this Comment is to point out that this assumption will be strongly violated in a conventional variable temperature AFM, and the data are therefore very difficult to interpret.

The commercial variable temperature UHV AFM used in [1] cools the sample by means of a thermal link to a continuous flow cryostat. The rest of the instrument including the scan head is thermally isolated from the cold stage and remains near room temperature to avoid thermal drift in the scan piezos [9]. When the tip is not in contact with the substrate, the cantilever temperature is determined by a balance between radiation to the environment and conduction to the base of the cantilever which is near room temperature. Simple calculations as well as direct measurements show that radiation is negligible, and the temperature of the cantilever remains near room temperature even when the tip is a few nanometers above a surface near 100 K [10,11]. When the tip is in contact, the temperature profile can be estimated by modeling the tip as a truncated cone with half angle α in contact with the substrate with a disk of radius R. The heat flow through the tip is determined by the total temperature difference ΔT between the base of the cone and the substrate, and the conductance of the tip and the boundary. The heat flow across the boundary q in Watts is given by $q = \pi R^2 \sigma \Delta T_{\text{boundary}}$, where σ is the boundary conductance which has typical values of $10^8\ \text{W/m}^2\,\text{K}$ at room temperature and decreases at low temperatures [12]. The existence of a boundary conductance implies that the temperature profile is not continuous at the interface, but rather has an atomically sharp discontinuity measured by $\Delta T_{\text{boundary}}$. The temperature inside the tip obeys Laplace's equation with a zero flux condition on the side walls. The solution is $T = T_{\text{base}} - \frac{R}{r}\Delta T_{\text{cone}} \csc(\alpha)$, where ΔT_{cone} is the temperature drop across the conical tip, T_{base} is the temperature at the base of the cone which is attached to the end of the cantilever, and r is a spherical polar coordinate with origin at the apex of the cone. The heat current associated with this temperature distribution is $q = \beta\kappa R \Delta T_{\text{cone}}$, where κ is the thermal conductivity of the tip material and $\beta = 4\alpha \csc(\alpha)$ is a geometrical factor. Requiring continuity of the heat current yields expressions for the temperature drops:

$$\Delta T_{\text{boundary}} = \frac{\beta\kappa\Delta T}{\beta\kappa + \pi R\sigma}, \qquad \Delta T_{\text{cone}} = \frac{\pi R\sigma\Delta T}{\beta\kappa + \pi R\sigma}. \quad (1)$$

This result can be used to compute the temperature profile near the tip contact. Using values characteristic of the Si_3N_4 cantilevers of Ref. [1] with $\kappa = 3$, $\Delta T = 170$ K, $\alpha = 35°$, $R = 20 \times 10^{-9}$, and $\sigma = 10^8$ in SI units yields $\Delta T_{\text{boundary}} = 113$ K and $\Delta T_{\text{cone}} = 57$ K. Most of the temperature drop is due to the boundary conductance and occurs within a few atomic diameters of the contact. The total heat current through the contact is only a few μW, but the heat flux is over $10^9\ \text{W/m}^2$, which is comparable to the heat flux in an arc welder. This large heat flux generates a hot spot in the substrate under the tip of magnitude $\approx$ 50 K; the details of the calculation are given in Ref. [13]. Conventional thermal analysis shows that very large thermal gradients exist in this system and the temperature of the tip can differ from the substrate temperature by more than 100 K. The measurement of an activation energy and the transition temperature to athermal behavior reported in Ref. [1] must be reassessed in light of these considerations.

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