Understanding the friction of atomically thin layered materials

Astrid S. de Wijn

Department of Mechanical and Industrial Engineering,
Norwegian University of Science and Technology, Trondheim, Norway
astrid.dewijn@ntnu.no, astrid@syonax.net

Layered materials such as graphene have interesting frictional properties and are often used as (additives to) lubricants. Experimental Atomic Force Microscopy studies and detailed simulations have shown a number of intriguing effects such as frictional strengthening and dependence of friction on the number of layers covering a surface. We propose a simple, fundamental, model for friction on atomically thin sheets. We use our model to explain a variety of seemingly contradictory experimental and numerical results.

Keywords (from 3 to 5 max): 2d materials, graphene, Prandtl-Tomlinson, strengthening

1. Introduction

AFM experiments on atomically thin sheets, comprised of one or more layers of graphene or other layered materials [1,2], have shown that the friction depends on the number of layers in a surprising way: it is highest for single-layer sheets and decreases with increasing number of layers. In some experiments, an initial strengthening effect has also been observed, where the friction increases slowly at the onset of motion and then reaches a plateau [2]. This effect is also stronger for sheets consisting of fewer layers and appears to be related to the higher friction. These effects appear to be very general and related to the layered structure, as they have been detected in a variety of materials.

A number of mechanisms have been proposed for this peculiar behaviour and have been investigated experimentally as well as in detailed molecular dynamics (MD) simulations. These investigations have led to some controversy and discussion, because different AFM experiments and MD simulations from different authors have produced different suggestions and conclusions about what kind of mechanisms play a role here.

2. Methods

In this work, we propose a new model for friction on atomically thin sheets that we use to explain all these experimental and simulation results. A sketch of the model system we study is shown in Fig. 1. The model is based on the Prandtl–Tomlinson (PT) model, with the addition of one extra degree of freedom, which can represent, e.g. bending or some in-plane degree of freedom such as delamination. We construct this model by systematically expanding the contribution to the potential energy landscape due to the distortion. Because of its simplicity, this model allows us to isolate and understand the dynamics of strengthening and layer-number dependence of friction. We also use it to investigate the influence of various potential mechanisms, the role of the substrate, and thermal noise.

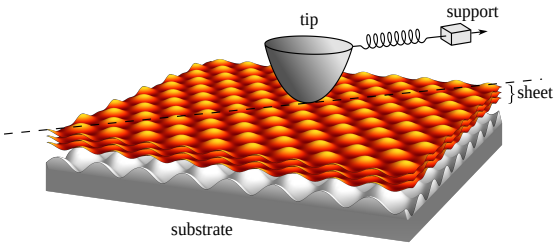

Figure 1: A cartoon of the system under consideration. A tip is dragged via a spring over a sheet comprised of a number of atomically thin layers that lie on a substrate but do not slide on it.

3. Conclusions

With the help of our model, we establish a close connection between the sheet–substrate geometry and the resulting friction response. We show that our model can explain and unify the various experimental and atomistic numerical results and that the seeming contradictions that have been found are simply the result of different degrees of freedom giving rise to similar dynamics.

4. References

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