7th World Tribology Congress, WTC 2022
July 10-15, 2022, Lyon, France

Chemical and Physical Origin of Friction at Atomic Steps

Seong H. Kim,[1)*] Zhe Chen,[1)] Arash Khajeh,[2)] and Ashlie Martini[2)]

[1)] Department of Chemical Engineering and Materials Research Institute, Pennsylvania State University, USA
[2)] Department of Mechanical Engineering, University of California Merced, USA
*Corresponding author: shk10@psu.edu

Whenever solid surfaces are in contact and shear each other, there is a friction. Depending on materials and surrounding environments, friction coefficient can be as small as 0.001 or even larger than 1. What controls such a large variance in friction? To better understand the fundamental mechanism, we study friction at a step edge of graphene on the graphite basal plane using atomic force microscopy (AFM) and reactive molecular dynamics (MD) simulations. The comparison of experimental and computational results provides deeper insights into the chemical and topographic origins of friction.

Keywords (from 3 to 5 max): Origin of friction, atomically flat surface, atomic step, graphite

1. Introduction

A complex set of interfacial processes are involved in friction, their combined effects are often described using a simple phenomenological expression that relates lateral and normal forces via a coefficient of friction (COF). To better understand the mechanisms governing COF, here we study a model system consisting of a sharp silica probe sliding on a chemically and topographically well-defined single-layer graphene step edge on the super-lubricious graphite basal plane.[1-3]

2. Methods

We use AFM experiments and MD simulations and study friction of silica moving across the graphene step edge. A conceptual schematic of the system is shown in Figure 1. The graphene step edge, produced by tape-exfoliation of a graphite substrate in air, is terminated by OH groups through reactions with water molecules impinging from the gas phase.[1]

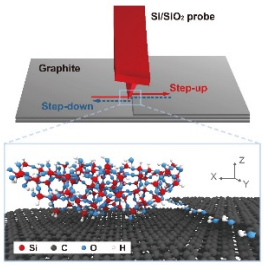

Figure 1: Schematic illustration and atomic-scale rendering of a silica AFM tip sliding up and down a single layer graphene step edge on an atomically flat graphite surface. Figure from Ref. 1.

3. Results

The results of AFM experiments and MD simulations for friction at graphene step edges are shown in Figure 2. The AFM lateral force measured at different steps with the same height (0.34 nm) reveals to the impact of the step edge chemistry on friction. Reactive MD simulations shows the transient chemical bonds and atomic displacements at the step edge during the sliding.

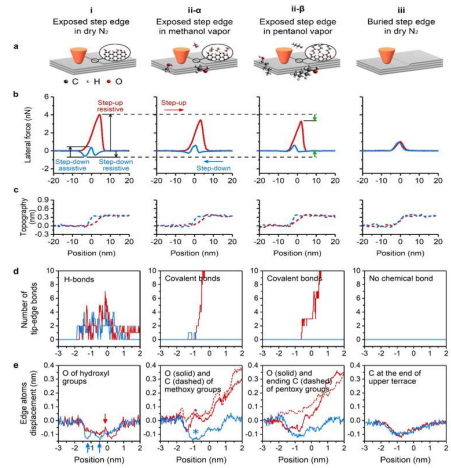

Figure 2: (a) Friction measurements at graphene steps in different conditions. (b,c) AFM lateral and topographic signals. (d,f) Transient chemical bonds and physical deformations at steps observed in MD simulations. Figure from Ref. 3.

4. Discussion

The comparison of AFM and MD results shows that the hysteresis in friction measured during the step-up versus step-down processes in all cases, except the buried step edge, originates from the anisotropic deflection of terminal groups at the exposed step edge, which varies depending on their chemical functionality. The findings explain why friction is high on atomically corrugated and chemically active surfaces, which provides the insight needed to achieve super-lubricity more broadly.

5. References

[1] Z. Chen, A. Khajeh, A. Martini, S. H. Kim "Chemical and physical origins of friction on surfaces with atomic steps" *Science Advances* **2019**, *5*, eaaw0513.

[2] A. Khajeh, Z. Chen, S. H. Kim, A. Martini "Effect of Ambient Chemistry on Friction at the Basal Plane of Graphite" *ACS Appl. Mater. Interfaces* **2019**, *11*, 40800.

[3] Z. Chen, A. Khajeh, A. Martini, S. H. Kim "Identifying physical and chemical contributions to friction: A comparative study of chemically inert and active graphene step edges" *ACS Appl. Mater. Interfaces* **2020**, *12*, 30007.