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Structural Superlubricity Meets Grain Boundaries

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The quest to scale-up structural superlubricity at graphitic interfaces to micro- and macro-scopic dimensions implies the inevitable presence of polycrystalline surfaces. This in turn introduces grain boundaries that may contribute excess friction. The study of the underlying frictional mechanisms and identification of way to control them is the focus of the present study.

Keywords: tribology, graphene, grain-boundaries, structural superlubricity

1. Introduction

Structural superlubricity is a promising route to achieve ultra-low friction and wear at dry rigid incommensurate interfaces.[1] Its demonstration at pristine nanoscale graphene contacts,[2] has risen hopes of achieving superlubricity at micro-[1,3] and even macro-scale graphitic interfaces. However, in the quest of scaling up superlubricity, new challenges appear, that have to be carefully examined and thoroughly understood. With this respect, an important challenge is the appearance of grain boundaries that are often corrugated and may introduce excess friction. In this study,[4,5] we investigate unique dissipative mechanisms occurring at graphene grain boundaries and identify ways to control and reduce the corresponding excess friction. We first focus on the dynamical processes occurring when a finite few-layered graphene flake crosses a single grain boundary defect. Then we turn our attention to tribological mechanisms characterizing extended grain boundary models.

2. Methods

To study the frictional mechanisms of graphitic grain boundaries we construct fully atomistic periodic models of polycrystalline surfaces supported by few-layered pristine graphene (see Fig. 1). The intra-layer interactions are modeled using the second-generation reactive empirical bond order potential potential,[6] and the inter-layer interactions are modeled using the registry-dependent inter-layer potential.[7] Shear dynamics is introduced by driving a (finite-sized or periodic) tri-layer graphene slider across the polycrystalline surface and external pressure is introduced by applying a normal load to the atoms of the slider's top layer. To avoid overheating of the system, damped dynamics ($T = 0K$) or Langevin thermostats ($T > 0K$) are applied to the internal layers of the slider and the substrate.

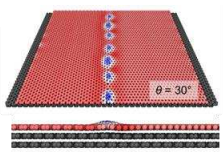

Figure 1: A corrugated graphene grain boundary with misfit angle of 30° supported by a pristine graphene bilayer. The lower layer serves as a rigid support during the simulation. Periodic boundary conditions are applied in the lateral directions.

3. Discussion

For finite graphitic flakes sliding over individual grain boundary defects unique physical mechanisms of frictional energy dissipation are revealed including: (i) variations of compressibility along the surface; (ii) heat produced during defect (un)buckling events; and (iii) elastic energy storage in irreversible buckling processes. These mechanisms lead to the occurrence of negative average differential friction coefficients.

For extended grain boundaries we identify a non-monotonic behavior of friction with respect to normal load and temperature. At low temperatures the friction force initially increases with normal load and, after reaching a maximal value, it is found to decrease. At higher temperatures negative differential friction coefficients are obtained for the entire normal load regime considered. The underlying mechanism involves an initial increase in dissipative defect buckling events due to reduction of the corresponding energy barrier followed by buckling inhibition due to a high-load "ironing" effect of the grain boundary defects.

4. References

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