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Edge effect in structural superlubricity

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Structural superlubricity, which promises an ultralow sliding friction thanks to the cancellation of the lateral force between two incommensurate interfaces, is a fundamental phenomenon in modern tribology. However, the edge of the superlubric system, a natural existing defect, has complex effects on the friction behavior. Thus, the key to achieve its application is understanding the origin of friction. Inspired by observation from experiments, we perform large-scale molecular dynamics simulation to study the edge effect, and the edge-dominated friction origin is revealed. The hydrogen bond in the paralleled edge is responsible for the edge effect. We believe this work provide guidelines in designing future superlubric devices.

Keywords: superlubricity, edge effect, graphene, molecular dynamics simulation

1. Introduction

Structural superlubricity is a state where the ultralow sliding friction is achieved due to the cancellation of the lateral force between two rigid incommensurate interfaces. The ultralow friction coefficient and undetectable wear promise structural superlubricity of extensive importance in classical engineering, data storage, and energy industries [1]. A large number of studies emerged in the last decade, which reveal the friction behaviors different from the traditional friction laws. For example, the negative friction coefficient, the atypical size, velocity, and temperature dependence.

The latest experiments and molecular dynamics simulation show that the edge of the superlubric graphite system, a natural existing defect, contributes most of the friction, and can further affect the friction behaviors [2]. However, it remains to be a difficulty in determining the atomic structure of the edge in experiments. At the same time, quantities of theories and simulations neglect/weaken the edge effect by using periodic boundary conditions or hydrogen passivation, which leads to a large gap in the current understanding of the edge effect.

2. Methods

In this work, we explore the sliding friction of graphite mesa system by using full atomic molecular dynamics (MD) simulations, which has been proved to be superlubric experimentally. The simulation model is shown in Figure 1a. The system consists of 4 flexible graphene layers. The lower two layers are substrate, and the upper two layers are slider. The misfit angle between the substrate and the slider is θ=30 °, which promises a stable superlubricity. In order to restore the edge effect in experiments, we added functional groups to the edge of the slider (Figure 1a).

The MD simulations are performed using LAMMPS code. The interlayer interaction among each graphene layer is described by registry-dependent anisotropic interlayer potential (ILP). The carbon-carbon intralayer interaction is computed by REBO force field. Langevin thermostat is applied to the bottom layers of the slider with a fixed temperature T and damping coefficient η=1ps^{-1}. The spring with the spring constant K=100 N/m is tethered to the centroid of the top layer. The other end of the spring moves with a constant velocity v along y direction. The friction force of three different cases is studied here, including the clean, parallel, and perpendicular cases.

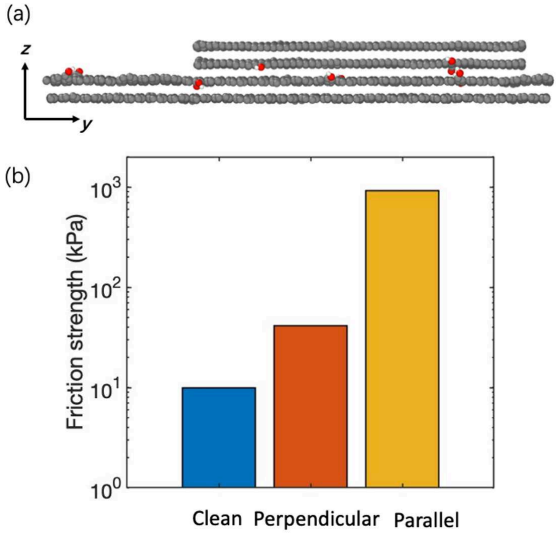

Figure 1. Simulation model and result. a, The sideview of the system. b, The shear strength for different cases.

3. Results and discussion

The friction force of three different cases is shown in Figure 1b. The friction stress of the clean case is in the order of 10 kPa, which agrees well with our former simulation and experiments. Interestingly, the friction stress of the -OH terminated cases, especially the parallel case, is of two orders magnitude larger than the clean case.

Our results provide insights in the origin of friction for structural superlubricity and benefit its application on a wide range of science and engineering fields.

4. References

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