Supporting Information

Edge orientation dependent nanoscale friction

Hongwei Zhang,^{a,b} Tienchong Chang^{*c}

^aSchool of Science, Xi'an Polytechnic University, Xi'an 710048, China ^bState Key Laboratory of Ocean Engineering, School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiao Tong University, Shanghai 200240, China ^cShanghai Institute of Applied Mathematics and Mechanics, Shanghai Key Laboratory of Mechanics in Energy Engineering, Shanghai University, Shanghai 200072, China

* Corresponding Author: T. Chang (tchang@staff.shu.edu.cn)

Shown in Fig. S1 are the model and results for a graphene flake with its armchair edge oriented perpendicular to the sliding (*z*-axis) direction. The bond of the graphene substrate perpendicular to the flake sliding direction is oriented in the zigzag direction, so that the interfacial registry between the flake and the substrate is incommensurate. The simulation conditions are same as those used in the case for a flake with its zigzag edge perpendicular to the sliding direction (see Fig. 1). Similar conclusion to that observed in Fig. 2(d) and (e) can be drew – the friction force depends strongly on the length of the edge perpendicular to the sliding direction.

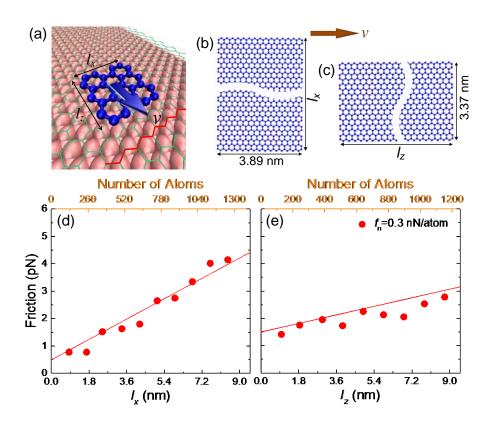


Fig. S1 (a) Schematic illustration of a flake with its armchair edge perpendicular to the sliding direction. (b) and (c) Model size. (d) and (e) The friction versus the lateral and the longitudinal edge lengths.

Fig. S2 shows the friction as functions of the lateral and the longitudinal edge length at zero normal load (the model and the simulation conditions are same as those used in Fig. 1). The results indicate again that the friction force is strongly dependent on the lateral edge length but less dependent on the longitudinal edge length. Moreover, the molecular dynamics simulations data can be well reproduced by eqn (1) in which the interlayer contact pressure p=0, indicating that the present friction formula is capable of predicting the interlayer friction force between graphene layers at zero normal load.

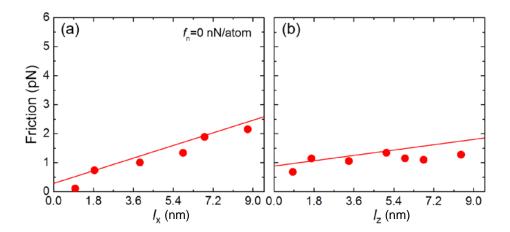


Fig. S2 Friction versus (a) the lateral edge length and (b) the longitudinal edge length at zero normal load. The solid lines represent the fit of the simulation data to the proposed nanoscale friction formula (eqn (1)).

Fig. S3 depicts the temperature effect on the interlayer friction. The simulation conditions except temperature are same as those used the case shown in Fig. 1. As we can see, a higher temperature results in a higher friction force. To consider the temperature effect on the interlayer friction in the proposed new friction formula fit the simulation data to the model and obtained that λ_{\Box} (=28.0 nm) and $\lambda_{//}$ (=10.6 nm) are unchanged, while the friction coefficient μ is linearly dependent on temperature and can be expressed as μ =(0.0854+0.000557*T*)×10⁻⁶ in which *T* is the system temperature. Based on these parameters, the proposed friction formula can well reproduce the interlayer friction for two flakes with nearly the same area but different aspect ratio sliding on the same substrate, as shown in Fig. S4.

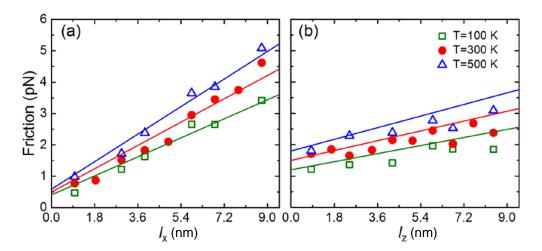


Fig. S3 Friction versus (a) the lateral edge length and (b) the longitudinal edge length, at the various temperatures of 100, 300 and 500 K under a normal load f_n =0.3 nN per atom. The solid lines represent the fit of the simulation data to the proposed nanoscale friction formula (eqn (1)).

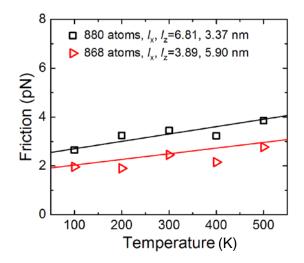


Fig. S4 Friction versus temperature under a normal load $f_n=0.3$ nN per atom. Two flake samples with nearly the same area but different aspect ratio are considered. The solid lines represent the fit of the simulation data to the proposed nanoscale friction formula (eqn (1)).