



Letter

Anomalous friction of graphene nanoribbons on waved graphenes

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HIGHLIGHTS

- The friction increases with the amplitude at a fixed period.
- The friction anomalously increases and then decreases with the period.
- A theory is proposed to explain the simulation results.

ARTICLE INFO

Article history:

Received 3 July 2015

Received in revised form

6 August 2015

Accepted 9 September 2015

Available online 25 September 2015

*This article belongs to the Biomechanics and interdisciplinary

Keywords:

Friction

Small scale

Graphene

Molecular dynamics

ABSTRACT

Friction plays a critical role in the function and maintenance of small-scale structures, where the conventional Coulomb friction law often fails. To probe the friction at small scales, here we present a molecular dynamics study on the process of dragging graphene nanoribbons on waved graphene substrates. The simulation shows that the induced friction on graphene with zero waviness is ultra-low and closely related to the surface energy barrier. On waved graphenes, the friction generally increases with the amplitude of the wave at a fixed period, but anomalously increases and then decreases with the period at a fixed amplitude. These findings provide insights into the ultra-low friction at small scales, as well as some guidelines into the fabrication of graphene-based nano-composites with high performance.

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Friction is very important to the function and maintenance of small scale structures due to their large specific area ratios. Conventionally, the friction is described by the Coulomb law and in linear proportion to the normal compressive force. However, the Coulomb law often fails at small scales because the friction can be coupled with adhesion or be significant even under a normal tensile force [1]. Recently, significant scientific efforts have been devoted to uncover the hidden principles for friction at small scales [2], which, nevertheless, may have already been employed in nature. For example, a large pretension in the spatula pad under gecko toe can be induced through sliding movement, which can lead to highly reversible adhesion of gecko adhesion [3].

Due to the remarkable properties [4–7] and probably also the simplicity, the friction of graphene-based small scale structures has attracted extensive interests [8–12]. With atomic force microscopy (AFM), the friction on SiO₂ covered with a layer of graphene was found to be much lower than that without graphene,

while the adhesion of the former was much larger than that of the latter [13]. The friction between an AFM tip and a graphene substrate was showed to be mainly due to van der Waals force [13]. It was reported that the friction of a supported graphene depends on the supported height with a higher friction at a larger height [14]. Monte Carlo simulation indicated that the friction of a graphene layer manifested with a stick–slip pattern [15]. For multiple layers, the friction was found to be relatively stable and its average value was relatively small [15].

A graphene layer is extremely flexible and can develop waviness on the surface due to thermal fluctuation [16–18]. The waviness can also be introduced in a graphene layer through mechanical compression or through cyclic heating and cooling [19]. Such waviness can dramatically change the properties of graphenes. For example, the electric conductivity of waved graphenes decreased due to the separation of electrons while the ferroelectricity could be highly improved [19]. The local chemistry of a waved graphene can even be different from a flat graphene [19]. Waved graphene layers were also observed in graphene based nano-composites [20].

Here, we employ the molecular dynamics method to simulate the process of dragging graphene nanoribbons (GNRs) on graphene

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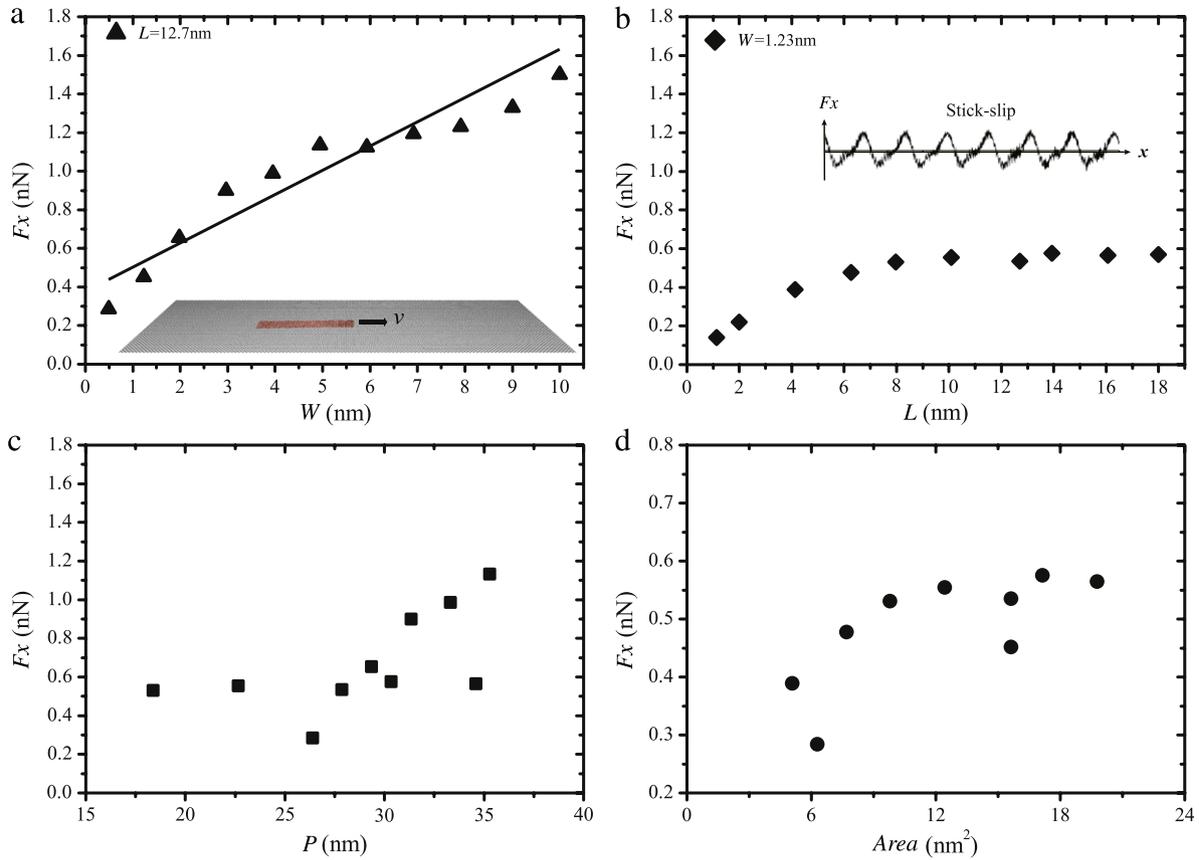


Fig. 1. Variation of the friction with the width of the GNR at a fixed length, $L = 12.7$ nm (a), with the length of the GNR at a fixed width, $W = 1.23$ nm (b), with the perimeter of the GNR (c) and with the area of the GNR (d). Solid line in plot (a) is a linear fit to the simulation results. Inset in plot (a) illustrates the dragging of a GNR on a flat graphene substrate. Inset in plot (b) displays the stick-slip phenomenon observed in the simulation.

substrates with or without waviness. We find that the friction of GNRs on a suspended graphene layer without waviness is ultra-low and proportional to the width of a GNR. We show that, on waved graphenes, the friction generally increases with the amplitude of the waves at a fixed period, but anomalously increases and then intriguingly decreases with the period at a fixed amplitude. We further develop a theory to explain the simulation results.

The molecular dynamics simulations are carried out with LAMMPS. In all simulations, the reactive empirical bond order (REBO) potential is adopted to describe the carbon-carbon interaction within each layer [21], while the Lennard-Jones potential with $\sigma_{cc} = 3.4$ Å and $\epsilon_{cc} = 0.00284$ eV [22] is used to describe the carbon-carbon interaction between neighboring layers. In the simulation, the temperature of the system is maintained at ~ 300 K.

We firstly investigate the dragging of a GNR on a flat graphene substrate. The GNR has a width of W and a length of L . As shown in the inset of Fig. 1(a), the right edge of the GNR layer is horizontally pulled at a constant velocity of 0.1 Å/ps. The calculated total resisting force on the GNR along the pulling direction (inset of Fig. 1(b)) has a period close to the size of the crystal lattice of a graphene. Though local out-of-plane bending of nanoribbons may be very small, local non-uniform in-plane shearing deformation of nanoribbons is clearly observed in the simulation. In the slip phase, local interaction energy between the nanoribbon and graphene substrate is considered to be downhill, which leads us to believe that the force trace shown in the inset of Fig. 1(b) involves unstable slip motion. The friction calculated from the average value of the negative peak of this resisting force along the pulling direction within multiple periods is very small. Figure 1(a) shows that the friction increases almost linearly with the width of the GNR at

a slope of ~ 0.15 nN/nm. Such a linear relation is robust. For example, when $W = 20$ nm, the simulated friction is 3.11 nN. As shown in Fig. 1(b), the friction initially increases with the length of the GNR until it saturates for long GNRs. The dependence of friction on perimeter or area will be affected by how these two parameters change in the simulation. As indicated in Figs. 1(c) and (d), the friction significantly scatters around a fixed perimeter or around a fixed area, which leads us to conclude that the friction does not correlate with either the perimeter or the area of GNRs.

We then investigate the dragging of a GNR on a waved graphene substrate, as illustrated in the inset of Fig. 2(a). The waviness is described by

$$z = A \sin \frac{2\pi}{\lambda} x - A, \quad (1)$$

where A is the amplitude and λ is the period. We vary A and λ in the simulation. The total resisting force on the GNR along the pulling direction is obtained in the simulation, which also exhibits a stick-slip phenomenon (Fig. 2(b)). When A is relatively small, the period of the stick-slip is close to the size of the crystal lattice of a graphene. For a relatively large A , the period of the stick-slip is close to the period of the wave. The friction is subsequently calculated from the average value of the negative peak of the resisting force along the pulling direction within multiple periods. Similarly, we find that the friction is also very low. As shown in Fig. 2(b), the friction generally increases with the amplitude of the waves at a fixed period. As shown in Fig. 2(c), the friction increases and then decreases with the period at a fixed amplitude. Figures 2(b) and (c) indicate that the friction of GNRs on waved graphenes can be several times higher than that on flat graphene.

Recently, the peeling of a thin film adhering on a corrugated substrate was investigated [23]. For the special case of a thin film

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