Supplementary information

Lifted graphene nanoribbons on gold: from smooth sliding to multiple stick-slip regimes

L Gigli,[a] N Manini,[b] E Tosatti,[a,c,d] R Guerra,[b,e] A Vanossi[d,a]

Abstract

To enhance the online version of the research article, we include here four movies, extracted from Molecular Dynamics simulation data, showing the driven dynamical behavior of the GNR at different lifting heights, specifically highlighting the transition from smooth-sliding at low z_0 (= 1nm) to multiple stick-slip regimes at high z_0 (= 10 nm), for both forward and backward scan directions.

We also include for comparison the force traces obtained for $z_0 = 10\,\text{nm}$ with the same simulation setup described in Sect. 2, and those with a 4 times larger value of the interaction amplitudes ($\epsilon_C = 10\,\text{meV}$ and $\epsilon_H = 2.5\,\text{meV}$), see Fig. 1 Suppl..

Fig. 2 Suppl. highligths, instead, the similarity of the GNR frictional behavior in the presence of a very soft (10^5 times smaller k_z) vertical spring constant.

We finally show the time-evolution of the kinetic friction force F_k and the effective contact length L_eff, calculated via Eq. 5 (main manuscript), in case of a very large value of lifting $z_0 = 22.5\,\text{nm}$ and in backward driving. The results show that the peeling tendency registered at intermediate liftings (Fig. 7 of the main paper) is more pronounced at higher lifting heights, as expected.

Movies "GNR_forward_1nm.mp4" and "GNR_backward_1nm.mp4"
The two movies show, for both forward and backward driving, the stationary smooth sliding regime of the GNR lifted at $z_0 = 1\,\text{nm}$. The corresponding frictional force traces, reported in Fig. 2 (left panel), exhibit an identical symmetric response in the two opposite scanning directions.

Movies "GNR_forward_10nm.mp4" and "GNR_backward_10nm.mp4"
The two movies show, for both forward and backward driving, the GNR steady multiple stick-slip regime dominated by the nanoribbon bending elasticity at a lifting height $z_0 = 10\,\text{nm}$. Here, the different GNR mechanical response under driving for the two opposite scan directions gives rise to inequivalent forward/backward force traces, as shown in Fig. 3 (bottom panel).

[a] *International School for Advanced Studies (SISSA), Trieste, Italy*
[b] *Dipartimento di Fisica, Università degli Studi di Milano, Italy*
[c] *The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy*
[d] *CNR-IOM Democritos National Simulation Center, Trieste, Italy*
[e] *Center for Complexity and Biosystems, University of Milan, Italy*

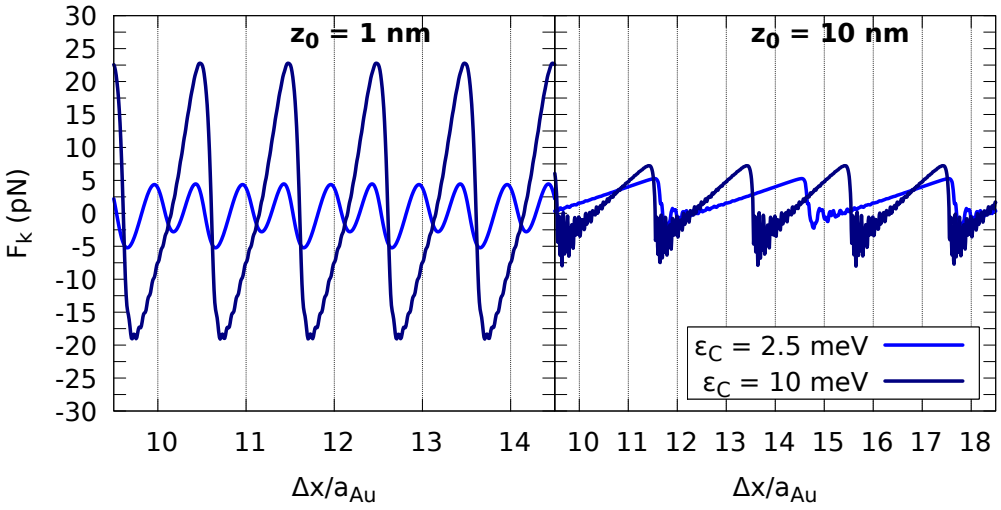

Figure 1: Comparison between the GNR sliding dynamics for two different values of the C-Au interaction amplitudes $\epsilon_C = 2.5\,\mathrm{meV}$ and $\epsilon_C = 10\,\mathrm{meV}$ (the H-Au interaction amplitude is scaled proportionally) for $z_0 = 1.0\,\mathrm{nm}$ and $z_0 = 10\,\mathrm{nm}$ in the forward motion. The qualitative system behavior, particularly the emergence of a clear stick-slip dynamics with a z_0-dependent perioditicy, is not significantly affected by scaling up the interaction amplitudes by a factor 4. Quantitatively, the observed transitions from smooth sliding to single and multiple stick-slip regimes may occur at slightly different lifting values of the GNR edge.

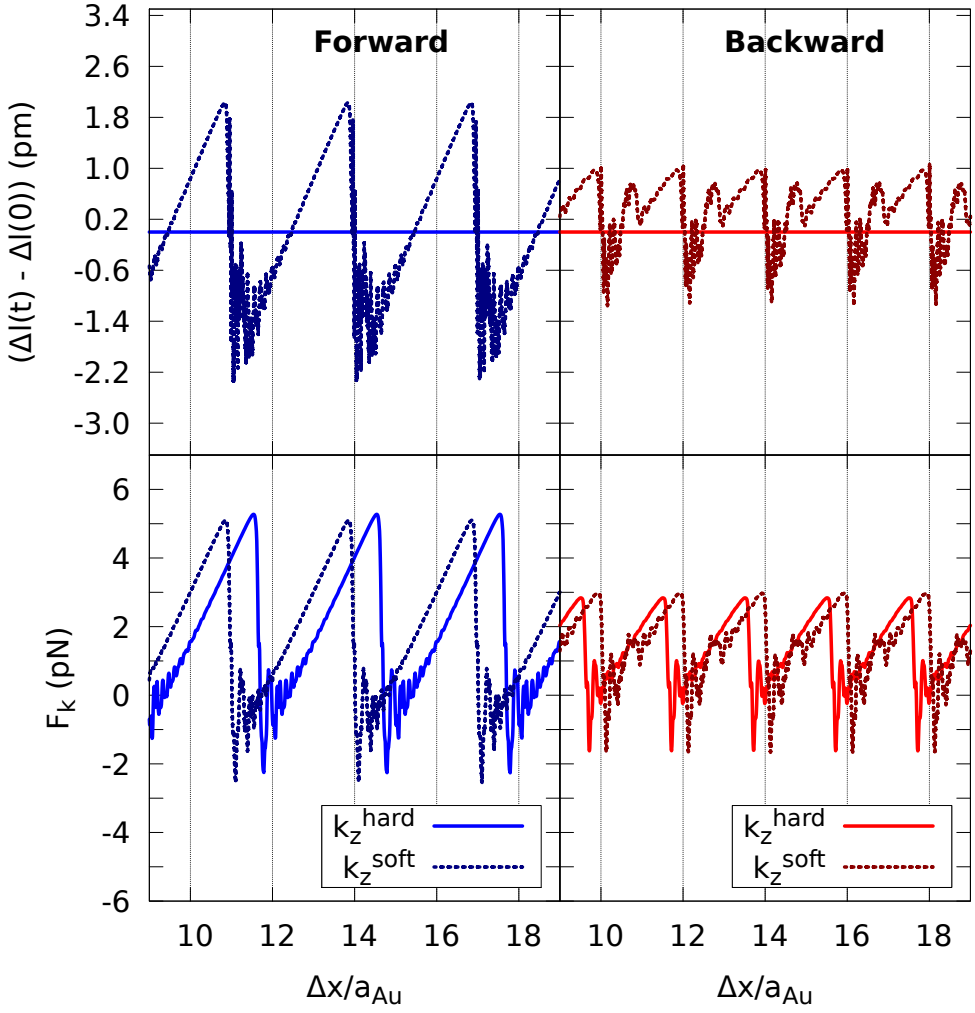

Figure 2: Comparison between the GNR sliding dynamics for $z_0 = 10\,\mathrm{nm}$ with two different vertical springs ($k_z^{\mathrm{hard}} = 1.6 \cdot 10^5\,\mathrm{N/m}$ and $k_z^{\mathrm{soft}} = 1.8\,\mathrm{N/m}$). The lower panels show the force traces in the forward (left) and backward (right) motion, while the upper panels show the time variation of the vertical spring elongation with respect to the equilibrium configuration of the lifted GNR. The vertical tiny oscillations of the soft-spring lifted end of the GNR do not affect appreciably the stick-slip frictional dynamics.

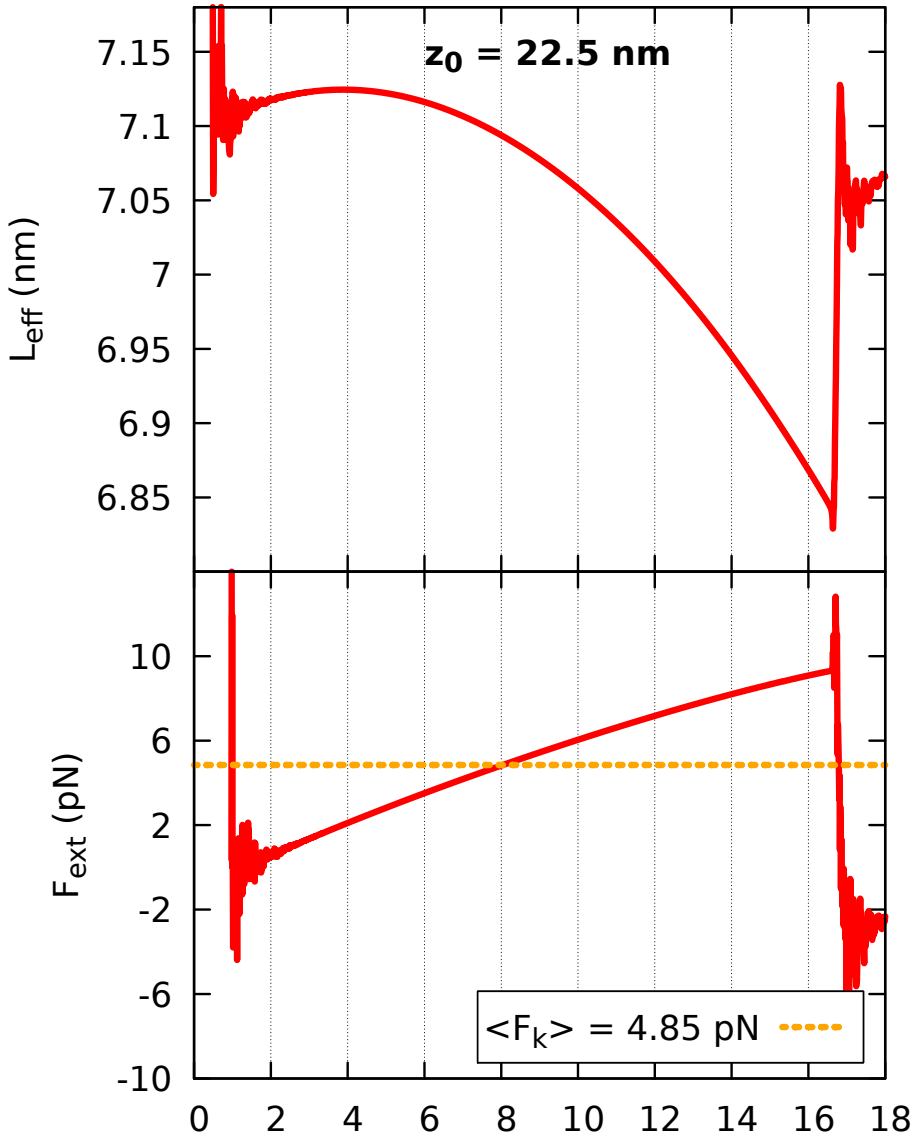

Figure 3: Time-evolution of the kinetic friction force F_{k} (lower panel) and the effective GNR-substrate contact length L_{eff} (upper panel), as defined in Eq. 5 in the manuscript, for high lifting ($z_0 = 22.5\,\mathrm{nm}$). The peel-off dynamics of the GNR from the substrate is signaled by the large decrease of L_{eff} in the stick phase.