Final Scientific Report

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visiting Prof. Erio Tosatti, at CNR National Simulation Center DEMOCRITOS in Trieste.

When two crystalline workpieces with incommensurate lattices (or commensurate but not perfectly aligned lattices) are brought into contact, then the minimal force required to achieve sliding vanishes (or is reduced by order of magnitudes), provided that the two substrates are stiff enough. In such a geometrical configuration, the lattice mismatch can prevent interlocking and collective stick–slip motion of the interface atoms, with a consequent vanishingly small frictional force (sometimes called superlubricity). Detailed experimental investigations of superlubricity have been recently performed [1], measuring the friction force between a graphite flake attached to a frictional force microscope tip and an atomically flat graphite surface. Superlow friction forces have been detected for most relative orientations of the flake and the substrate, due to the geometrical out-of-registry feature. For the few commensurate configurations of the contacting surfaces, high dissipative stick-slip dynamics has been recorded.

During this visit, in collaboration with Andrea Vanossi and Erio Tosatti, we extended our recent simulation studies [2,3] of a rigid flake sliding over a flat (graphite) substrate by considering its flexibility. From theoretical point of view, this problem is related to an implementation of tribological models suitable to investigate the behaviour in multi-asperity sliding contacts. The dynamics of the moving flexible flake is governed by both single asperity dynamics as well as ruled by nonlinear collective mechanisms. In the limit of strong stiffness the behaviour of the system is expected to reduce to that of a rigid flake. As previously observed [2,3], there are two competing mechanisms determining friction: the flake can easily slide on top of the substrate thanks to an incommensurate orientation, or it can rotate to specific in-registry angles, restoring high-dissipative stick-slip dynamics. In the opposite limit of high flexibility, the system should behave as a collection of almost independently moving “asperities”, which freely adapt to the substrate potential landscape.

From a numerical view point we worked in the framework of nonlinear equations of motion of Langevin dynamics including thermal effects. The numerical simulations covered quite wide range of the model parameters, in order to reach decisive conclusions. In this short report, preliminary results are presented and summarized in the figures below.

In Fig. 1.a, typical configuration of relatively rigid flake (whose stiffness is controlled by an effective elastic constant K) moving on the substrate potential is shown. The surface is sketched by grey-scale map with darker colour corresponding to deeper valleys of the potential.

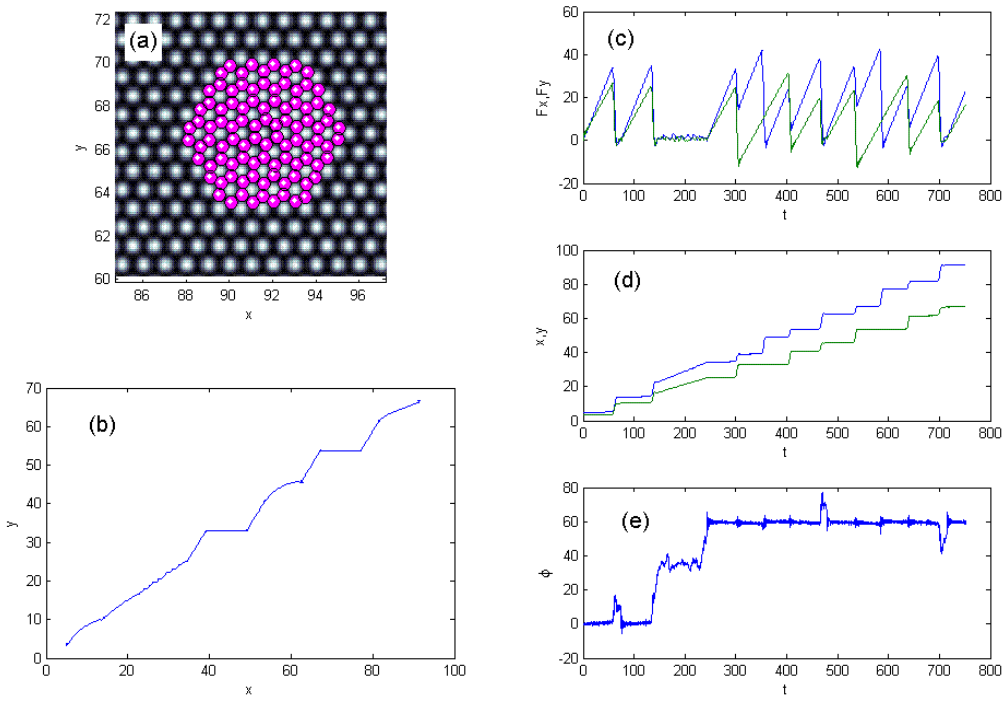

Fig.1

This figure presents a flake containing N=96 graphite atoms. The size of the flake was varied in wide interval. In particular, to get symmetric flakes N has to be taken equal to the following numbers: N = 1, 6, 24, 54, 96, 150. We also checked the dynamical behaviour of different flakes with other, asymmetric, configurations.

Typical trajectory of the center of mass of the flake is depicted in the subplot (b). At arbitrary angle of the driving force the flake performs either "jumps" along one of the symmetry axes or long slips parallel to the external force (depending on the orientation angle of the flake to the surface potential). The particular scenario corresponding to the given trajectory generates $F_{x,y}$ projections of the friction force and time evolution of the (x,y)-coordinates shown in Fig1(c) and (d) by blue and green colors, respectively. It is easily to see direct correspondence between long sliding interval in the subplot (d) and low friction in (c). The behavior of the relative flake-substrate orientation angle ϕ is reported in panel (e) of the same figure.

Analogous results for a very flexible flake are shown in the Fig.2. According to the experimental situation, the flake is attached to the AFM tip through its central part (6 atoms in our simulation cases). Due to flexibility, this may produce a flake deformation especially occurring during substrate pinning. as in Fig.2(a). Differences in trajectories and corresponding frictional forces are clearly visible comparing the two figures. The flexible flake executes much shorter "jumps", during which it

starts to rotate around local energy minimum in angle-space (but rarely performing large rotations to other in-registry angles: $\phi = \pm 60^0, \pm 120^0$, ...).

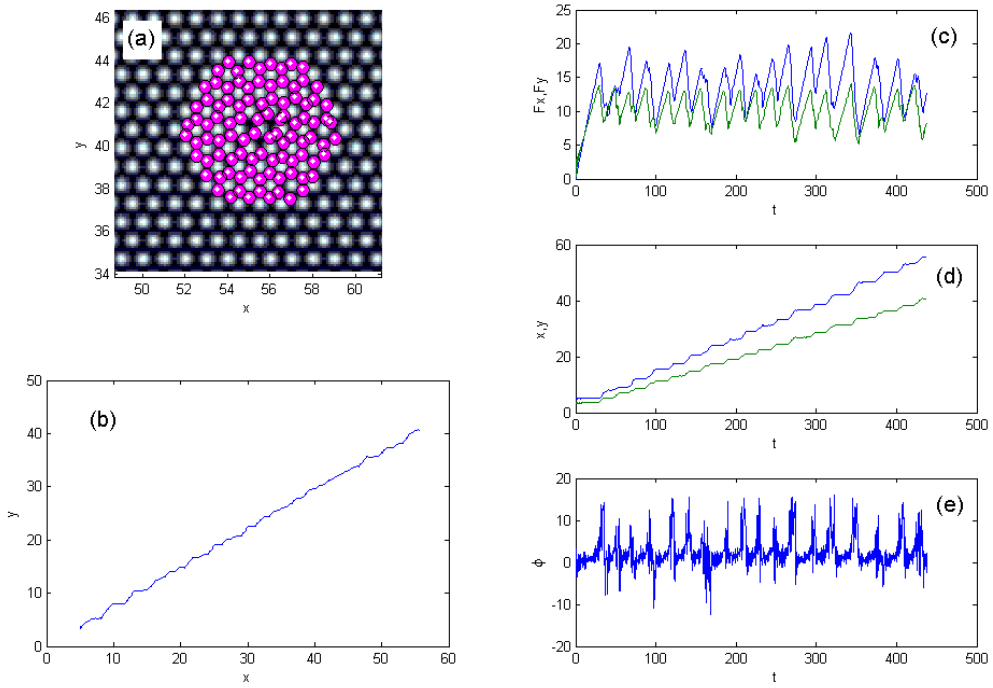

Fig.2

Friction force dependence (normalized to the number of atoms N) on the flexibility constant K, for different flake sizes N = 6, 24, 54, 96, is shown in Fig.3(a)-(d) (open squares). Full colored circles represent the corresponding standard deviations of the friction force, usually assuming large values in the case of stick-slip regime of motion. A decrease of the mean friction force at low values of K is always quite well pronounced. Long periods of sliding for relatively rigid large flakes (N≥54) lead to the strong fluctuations of the mean force which can vary from a minimum almost coinciding with the force of sliding to a maximum which is close to mean force at perfect stick-slip. These deviations are marked in the subplot (d) by two horizontal dashed lines.

Decrease of the friction with the flexibility is found to be more pronounced for the smaller flakes, but mean friction force at higher rigidity is smaller for the bigger ones. In all the cases, the friction force per atom for the flakes is much smaller than the control value $< F_{fric} > \approx 1.57$ found for the solitary atom in Tomlinson model at the same parameters.

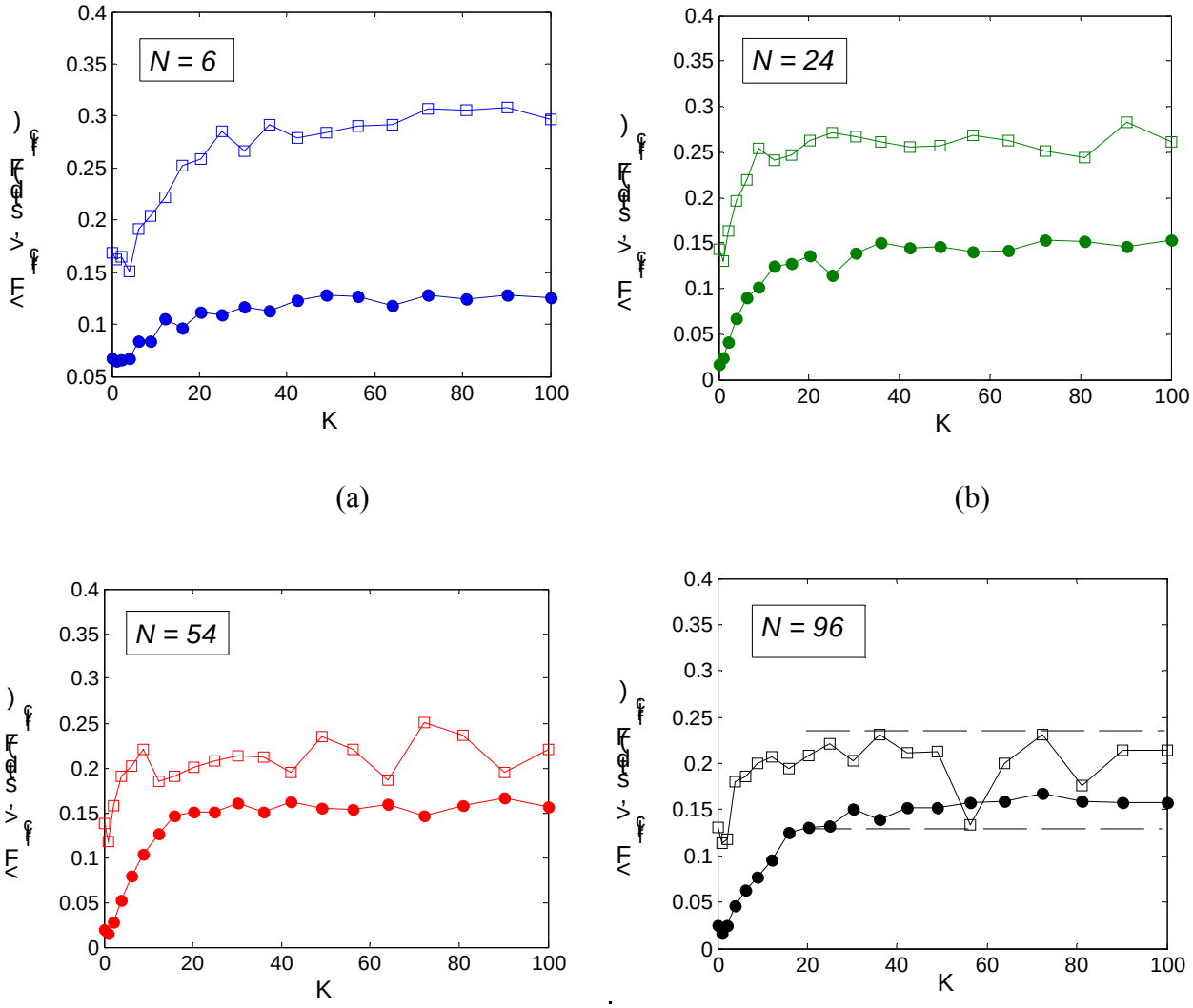

Fig.3

This short term visit, sponsored by CNR, has fruitfully reinforced the scientific collaboration with Prof. E. Tosatti and Dr. A. Vanossi, allowing to plan future joint research strategies on problems related to simulation of friction at the nanoscale.

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References

[1] M. Dienwiebel et al., Phys. Rev. Lett. **92**, 126101 (2004).

[2] A.E. Filippov, M. Dienwiebel, J.W.M. Frenken, J. Klafter, and M. Urbakh, Phys. Rev. Lett. **100**, 046102 (2008).

[3] A.E. Filippov, A. Vanossi, and M. Urbakh, Phys. Rev. E **79**, 021108 (2009).