Final Scientific Report

CNR Short-term mobility program 2009

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

During this visit, in collaboration with Andrea Vanossi and Erio Tosatti, we investigated frictional properties of quasicrystals. Early experimental measurements showed that the intriguing quasicrystal structure goes hand-in-hand with physical properties (e.g., hardness) that are unusual, in light of their chemical composition. Due to their long-range atomic order but no spatial translational invariance, they have lately attracted much attention as a class of increasingly interesting tribological materials, showing anomalously low coefficients of friction and high scratch resistance. To unravel the most intriguing hypothesis that their frictional response could be related to the exotic atomic structure of the bulk material, friction force microscopy (FFM) experiments have been recently done [1,2] in the regime of "wearless" friction, where no irreversible changes such as broken chemical bonds or permanently displaced atoms take place at the contacting interface. A significant anisotropy in friction has been observed by dragging the FFM tip along the periodic and aperiodic directions of a twofold decagonal Al-Ni-Co quasicrystal surface. While most known quasicrystals are icosahedral, with quasiperiodic bulk structure in all three dimensions, the decagonal quasicrystals have a structure presenting both periodic and aperiodic atomic arrangements in the same surface [7], allowing appropriate in situ experimental comparisons of friction along crystalline and quasicrystalline directions.

During my visit we investigated through numerical simulations the fundamental aspects of quasicrystal wearless friction related to their intrinsic peculiar morphology. By implementing an on-site substrate potential, closely mimicking the structural features of the twofold decagonal Al-Ni-Co surface (see Fig.1), and in the framework of a Tomlinson model, we were able to reproduce the experimentally observed anisotropic tribological response of the FFM tip sliding along different directions (see Fig.2).

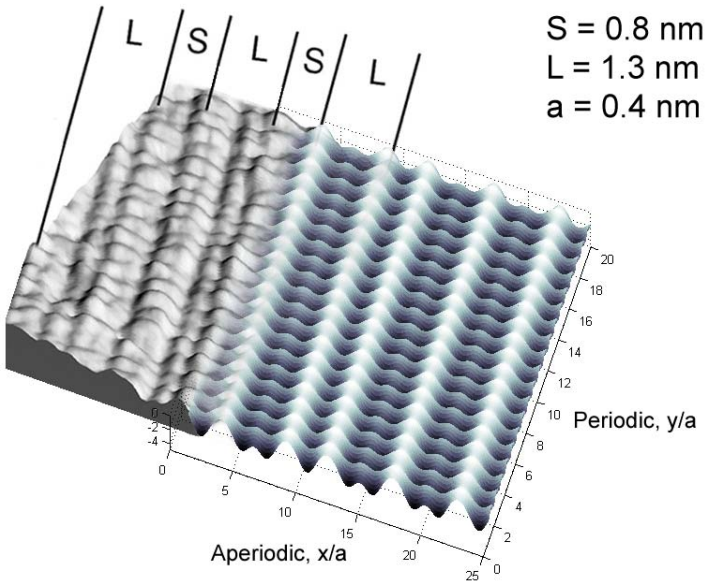

Fig.1. Collage of the STM image of a fragment of twofold Al-Ni-Co surface with the numerically generated potential used in simulations. Al atomic rows along the periodic *x*-axis exhibit periodicity of *a=0.4 nm*. In the aperiodic *y*-direction, these rows are separated by short and long distances ($S = 0.8nm, L = 1.3nm$) following the Fibonacci sequence. The surface topography is well reproduced by a surface potential composed of a set of anisotropic Gaussian functions.

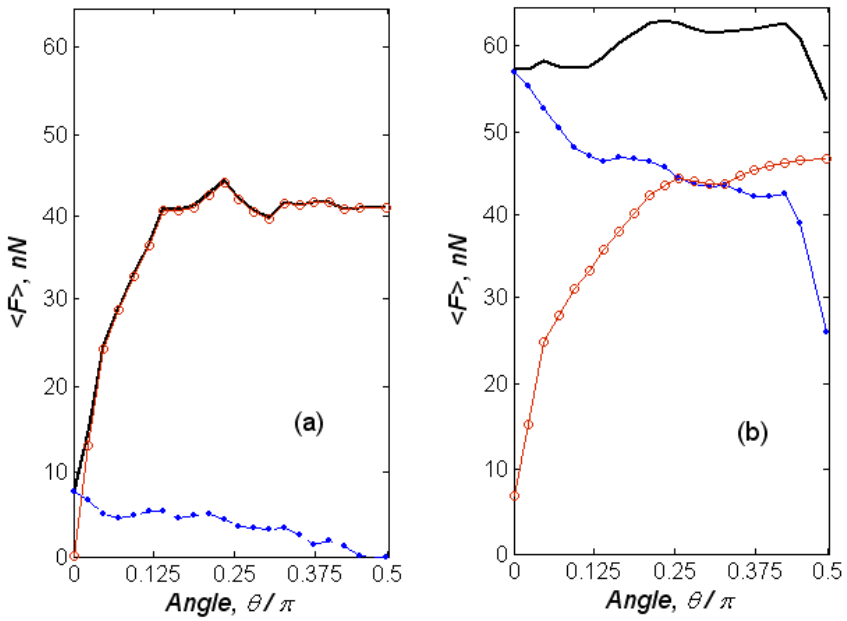

Fig.2 Dependence of the mean friction force (bold curves) and its projections on the periodic (open circles) and aperiodic (dots) axes on the pulling direction. (a) numerical results for the twofold Al-Ni-Co surface shown in Fig. 1; (b) numerical results for a model quasicrystal surface which exhibits identical corrugation lengths along the periodic and aperiodic directions, i.e., $S \equiv a = 0.4nm$ and $L = \tau S$.

We have found the distinct stick-slip patters in the lateral force occurring for the periodic and quasiperiodic directions, specifically exploring the temperature dependence that governs the transitions between single and multiple slip regimes of motion.

Our simulations demonstrated that the observed anisotropy of friction can be explained by a difference in length scales of the potential corrugation in the aperiodic and periodic direction. The model also predicted different temperature dependencies of friction for pulling along aperiodic and periodic directions. It should be noted that an additional contribution to the friction anisotropy may arise from a possible difference in the rates of energy dissipation along the aperiodic and periodic direction, which enter the model though the damping coefficients, γ_x and γ_y, assumed here to be equal. For example, the phonon dispersion bands in the aperiodic directions might show energy gaps due to the Fibonacci sequence of distances and masses, making energy losses by generation of phonon modes less favorable than along the periodic direction.

This short term visit, sponsored by CNR, has fruitfully reinforced the scientific collaboration with Prof. E. Tosatti and Dr. A. Vanossi: (i) a joint paper on friction at quasicrystal has been submitted to Physical Review Letters; (ii) future joint researches have been planned and started.

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References

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[2] J.Y. Park, D.F. Ogletree, M. Salmeron, R.A. Ribeiro, P.C. Canfield, C.J. Jenks, and P.A. Thiel, Phys. Rev. B **72**, 220201(R) (2005).