BALLISTIC TO DIFFUSIVE CROSSOVER IN THE SLIDING OF KICKED CLUSTERS

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Some deposited metal clusters deposited on particularly smooth surfaces -- in particular Au/graphite -- are known, despite a size of as many as 100-1000 atoms, to diffuse thermally as rigid bodies. That free cluster diffusion has been well understood and also reproduced by molecular dynamics (MD) simulations. However, no work has been devoted yet to the interesting possibility that these clusters could be pushed around, either inertially as in a quartz crystal microbalance (QCM)experimental setup, or even laterally kicked by e.g., a fast moving tip. when forced to slide over the substrate the clusters will cause a friction, which can be characterized by a velocity and temperature dependent slip time \tau. Under the hypothesis of viscous friction, the slip time in principle measures at each temperature T the exponential decay time of the initially imparted velocity v. In this work we will present theoretical arguments and MD simulations demonstrating two very different regimes in the sliding of a cluster. At sufficiently low velocities, such as those attained in a QCM, the clusters will drift diffusively. In this regime and within linear response the drift mobility -- and thus the slip time -- is simply proportional to the two-dimensional diffusion coefficient D through Einstein's relation. Since, as is generally the case, D is thermally activated and exponentially increasing with T, so will the slip time.[1] At the opposite limit of a strongly kicked cluster and for sufficiently high lateral kick velocities, the diffusive picture no longer applies and the cluster sliding will turn ballistic. In that regime friction should arise primarily from collisions of the cluster contact surface against the thermally excited vibrational rugosity of the substrate. Since the high temperature instantaneous surface square vibration amplitude increases roughly linearly with T, the ballistic slip time of sliding clusters is predicted to drop as 1/T. We will present MD simulations of Au clusters on graphite demonstrating this behavior for large velocities around 100 m/s, and also demonstrate a very gradual ballistic-diffusive crossover for lower velocities.

[1] S. Pisov, E. Tosatti, U. Tartaglino, and A. Vanossi, J. Phys.:Condens. Matter, {2007) (it in press).