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Simulated sliding of surface deposited islands and nanoclusters: from static pinning to high speed ballistic friction[1]

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The physics of friction of surface adsorbed molecules, nanoclusters, and rare gas islands is incompletely understood. We present two case studies aimed at improving this state of affairs. The static friction of rare gas islands, as revealed, e.g., in Quartz Crystal Microbalance experiments, is known to persist, unexpectedly, even on incommensurate and defect-free crystal surfaces, where sliding should theoretically be free. Through atomistic simulations mimicking Kr islands on Au(111), we show that surprisingly the island edges may be the ultimate culprits. An edge-originated energy barrier blocks the motion of solitons (tiny density and corrugation modulations with the beat periodicity between adsorbate and surface), keeping the whole island pinned. As the critical static friction force is reached, the barrier vanishes at one point on the edge, and here solitons enter and sweep the island, which becomes depinned. Surface smoothness and high temperature facilitate edge depinning. But the island's thermal expansion also leads to changeable commensurability upon heating, giving rise to the possibility of re-entrant static friction. On a different note, we address the high speed kinetic friction of sliding metal clusters. Simulating the motion of kicked Au clusters on graphite, we characterize a novel ballistic friction regime at high speed, and demonstrate the crossover from this to frictional drift at low speed. Consistent with simple theory, we find that the temperature dependence of the cluster slip distance and slip time is opposite in these two regimes. Crucially to both regimes, rotations and translations are shown to be correlated in slow drift but anti-correlated in fast sliding. This interplay, besides turning the kicked cluster trajectories from straight to curved, controls the crossover between the two sliding regimes. Despite the deep difference with drift, the speed dependence of ballistic friction is, like drift, viscous.

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