Atomic-scale sliding friction on contaminated surface

Supplementary Information

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1 Normal load dependence of friction force at zero coverage

We have performed friction simulations for a direct contact between the tip and substrate (see Figure S1), in the absence of adsorbates. We found that the friction force is much smaller than that in the presence of adsorbates, because the tip and substrate surfaces are incommensurate.

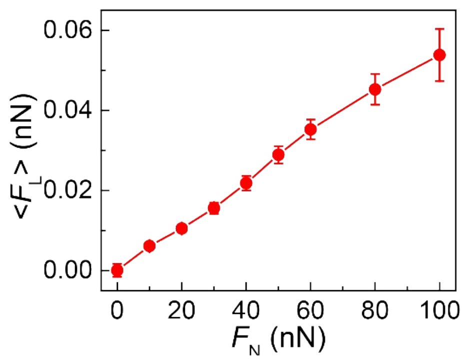

Figure S1. The friction force ($\langle F_L \rangle$) as a function of normal load (F_N) calculated for direct contact between tip and substrate. The parameters are the same as that in Fig. 2 in the main text.

2 Effect of coverage on the adsorbate diffusion

As illustrated in Figure S2

Figure S2, the adsorbate diffusion coefficient decreases with the coverage rapidly, while the number of particles interacting with tip sharply grows with the coverage for $\theta < 0.1$ and levels of for $\theta > 0.1$. Here the procedure for calculation of this number is similar to that proposed by Pastewka and Robbins.[1] Namely, the adsorbate is considered to be in direct contact with the tip when the minimal distance between the adsorbate and the tip atoms is smaller than the equilibrium one, which for the LJ interaction equals to $2^{1/6}\sigma$. In this case, the adsorbate feels a repulsive force from the tip.

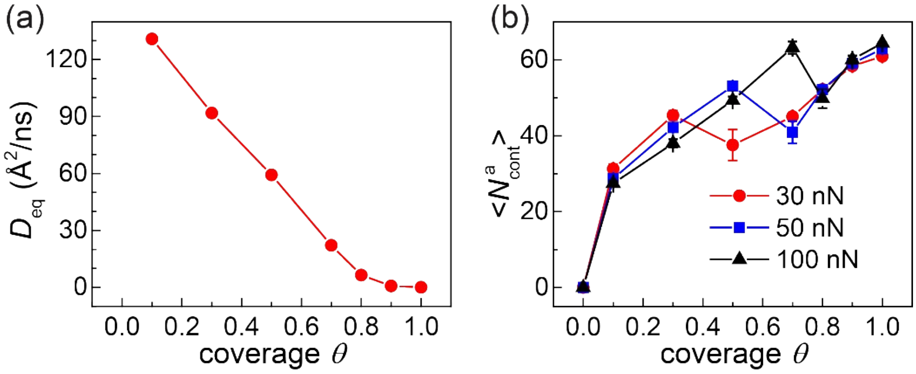

Figure S2. (a) Coverage dependence of diffusion coefficient of adsorbed particles at the substrate surface (D_{eq}) in the absence of tip. (b) The average number adsorbed particle being in direct contact with the tip ($\langle N^{a}_{cont}\rangle$) as a function of coverage calculated for different normal loads. Here, T = 300 K, U_0 = 0.38 eV. Other parameters are the same as that in Fig. 2 in the main text.

3 Effect of damping coefficients on friction force

We have checked the effect of damping coefficients on the simulation results. We have carried out additional simulations of friction in a broad range of damping coefficient, ranging from 0.1 ps^{-1} to 10 ps^{-1}. Figure S3 shows the coverage dependence of friction force calculated for three different values of damping coefficients (0.1, 1 and 10 ps^{-1}) and a normal load of 50 nN. It can be seen that the choice of the damping coefficient has a minor effect on the friction force, and the non-monotonic dependence of friction on the adsorbates coverage is retained for all considered values of damping. This can be explained considering that in the stick-slip regime of motion discussed here, the frictional energy dissipation is determined by the heights of potential barriers at the adsorbate-substrate and adsorbate-tip interfaces, and the "viscous" term makes only a small contribution to the overall energy dissipation.

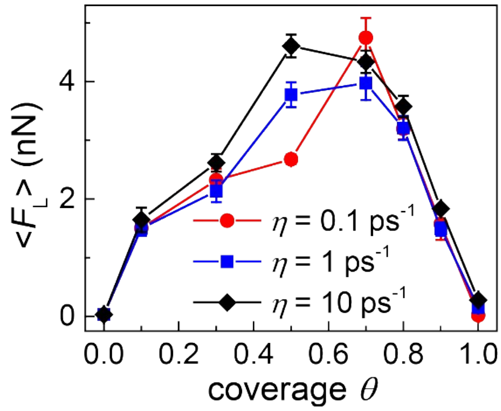

Figure S3. Friction force ($\langle F_L \rangle$) as a function of coverage calculated for different damping coefficients. Here $U_0 = 0.38$ eV and $T = 300$ K. Other parameters are the same as that in Fig. 2 in the main text.

4 The number of particles interacting with the tip

As shown in Fig. 3 in the main text, for coverages $\theta \leq 0.8$ the tip penetrates deeper into the adsorbed layer with increasing normal load, and the friction force increases significantly. In Figure S4, we present a load dependence of the number of adsorbates in direct contact with the tip. Figure S4 shows that this number grows significantly when the tip penetrates into the adsorbed layer, resulting in the increase of the friction force. In particular, for $\theta = 0.3$ the number of adsorbates in contact with the tip exhibits a maximum at the normal load of 20 nN, for which the friction force also reaches a maximum. A similar behavior, if less pronounced, is found for $\theta = 0.5$.

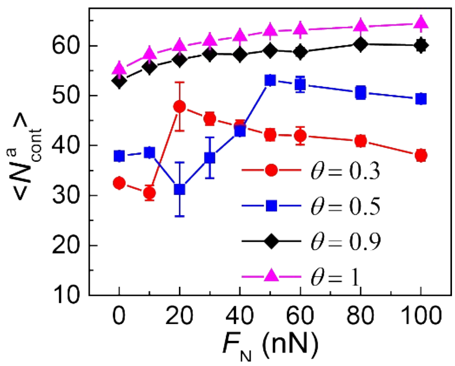

Figure S4. The number of adsorbates that interact with the tip ($\langle N^a_{cont} \rangle$) as a function of normal load (F_N) calculated for four different coverages (θ = 0.3, 0.5, 0.9, 1). Here $U_0 = 0.38$ eV and $T = 300$ K. Other parameters are the same as that in Fig. 2 in the main text.

Reference

1. L. Pastewka and M. O. Robbins, *Proc. Natl. Acad. Sci.*, 2014, **111**, 3298-3303.