# Friction at the nanoscale

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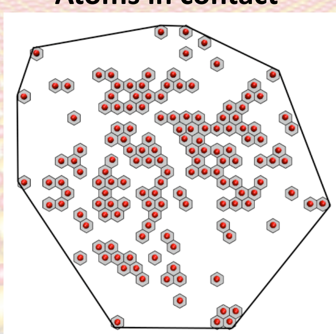
**Motivation:** Understanding of fundamental mechanisms of friction and wear of ultrananocrystalline diamond (UNCD). Promising material for coating drill bits for oil recovery.

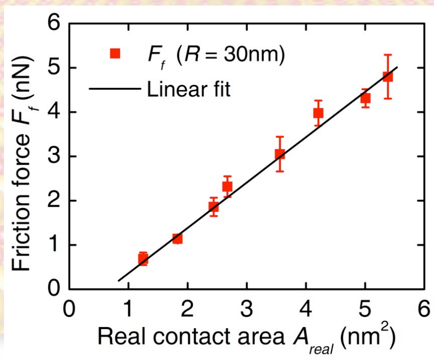
**Approach:** Massively parallel molecular dynamics simulations using realistic potentials (background picture)

**Discovered friction laws at the nanoscale. Determined dependence of friction force on load and contact area.**

**Atoms in contact**

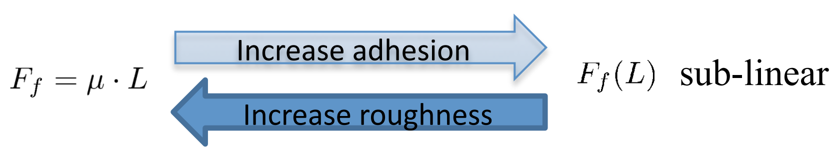


**Friction force – Real contact area**




- **We demonstrated that behavior of nanoscale contacts is described by roughness theories instead of continuum mechanics**
- **Friction force is controlled by the short range chemical interactions.** $F_f = \tau \cdot A_{real} = \tau \cdot N_{at} \cdot A_{at}$  $F_f = \mu \cdot L$

**Demonstrated a transition from a linear to sublinear friction – load dependence. Explained previously reported experiments.**

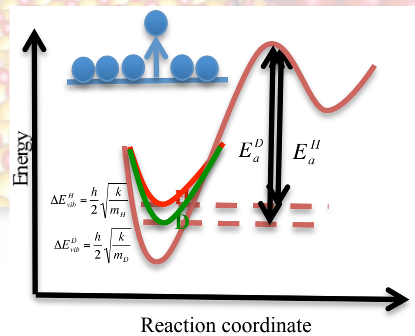



Mo, Turner, and Szlufarska, *Nature*, **457**, 1116 (2009)

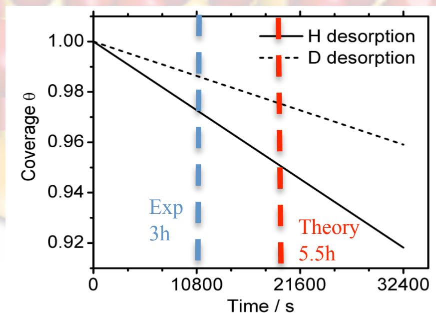
**Proposed a physical explanation for experimentally observed isotope effect on solid friction.**

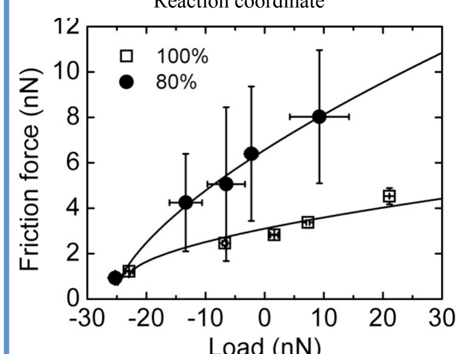
**Motivation: Experiment reported friction reduction of 20% by passivating diamond with deuterium instead of hydrogen**

**D is chemically more stable than H on diamond surface**




**Surface coverage of H/D decreases during annealing**




- **The isotope effect on solid friction is consistent with differences in chemical stability of H and D on diamond**
- **A few percent of surface vacancies has a large effect on friction.**

Mo, Müser, and Szlufarska, *Physical Review B* (in press)

Discovered friction laws at the nanoscale. Proposed a physical explanation of why deuterium lowers friction of diamond