

## Atomistic Insights into Friction at Diamond-Rock Interfaces

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The interactions between polycrystalline diamond compact (PDC) drill bits and rock-surfaces is not fully understood. We perform molecular simulations to investigate the interactions in diamond-rock systems. Using nonequilibrium molecular dynamics (NEMD) simulations, we explain the increased friction properties observed experimentally at diamond-calcite interfaces compared to diamond-quartz. We consider both dry and aqueous environments using new reactive force field (ReaxFF) parameters, which have been verified against first principles calculations. We monitor mechanochemical processes within these systems such as tip-substrate bond formation and structural changes within both the tip and the substrates. These successfully rationalise the experimentally-observed tribological behaviour.

**Keywords (from 3 to 5 max):** mechanochemistry, ReaxFF NEMD simulations, shear-induced chemical reactions

### 1. Introduction

Recent estimates have suggested that friction and wear account for around 40% of energy losses in the energy industry, for example to extract oil and gas. The development and application of improved drill bit material is therefore essential to meet future energy requirements in a sustainable manner. Polycrystalline diamond compact (PDC) bits proved to be extremely effective in drilling soft to medium rock formations, however the rates of penetration (ROP) and bit life is significantly reduced in harder formations (e.g. calcite and granite). Rock chemistry can also greatly influence PDC bit performance, in particular, for carbonate-containing rocks, rock powder strongly adheres to the wear flat [1].

### 2. Methods

We employ the reactive force field (ReaxFF) and LAMMPS to examine diamond-granite and diamond-limestone systems. Although rocks have a very heterogenous surface chemistry,  $\alpha$ -quartz(0001) and calcite{10.4} are broadly representative of granite and limestone respectively and have been shown with density functional theory (DFT) to be the most thermodynamically stable surfaces. ReaxFF is a bond order based that was originally developed by van Duin et al. [2] to study the dissociation and reactions of small hydrocarbon molecules. The version of ReaxFF implemented in LAMMPS uses the functional form which was outlined by Chenoweth et al. [3].

#### 2.1. Basic equation

$$r_y = A \exp\left(-\frac{E_a - \Delta x^* F}{k_B T}\right) = A \exp\left(-\frac{E_a - \sigma \Delta V^*}{k_B T}\right) \quad (1)$$

The reaction rate or yield can be examined through this Arrhenius-type equation, which emphasizes the catalytic nature of an external mechanical stress.

#### 2.2. Results

Both dry and aqueous systems capture the trends observed experimentally where we observe increased

friction properties at diamond-calcite interfaces compared with diamond-quartz. NEMD simulations show that material loss during sliding varies linearly with normal load and sliding distance, which is consistent with Archard's law.

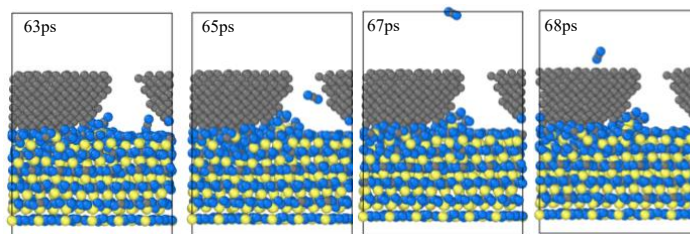


Figure 1: CO<sub>2</sub> molecule evolving from the calcite surface. C – grey; O – blue; Ca – yellow.

### 3. Discussion

Friction results show that the friction force increases linearly with normal force, which is in agreement with Amontons' friction law. The indentation depth for on the  $\alpha$ -quartz(0001) surface is significantly shallower compared to the calcite{10.4} due to its increased hardness. This results in more ploughing of the surface and thus increased friction properties at the diamond-calcite interface. ReaxFF data shows drastic chemical rearrangements in the surface chemistry of both systems with both showing a strong diamond-oxygen affinity.

### 4. References

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