Quantum Molecular Dynamics Simulations Elucidate the Tribochemistry of Graphene-Based Materials

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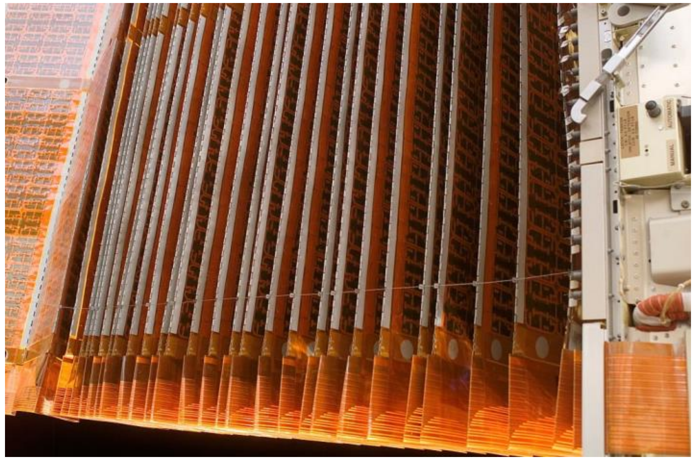
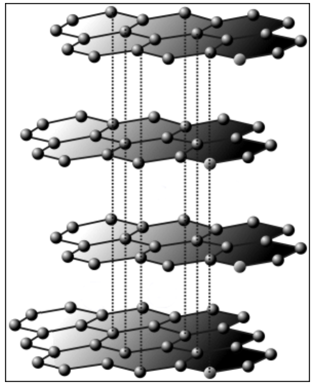
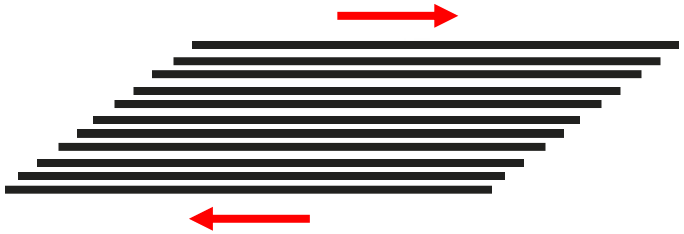
Tribology

Tribology is the science and engineering of understanding friction, lubrication and wear phenomena for interacting surfaces in relative motion



Graphite as a Lubricant

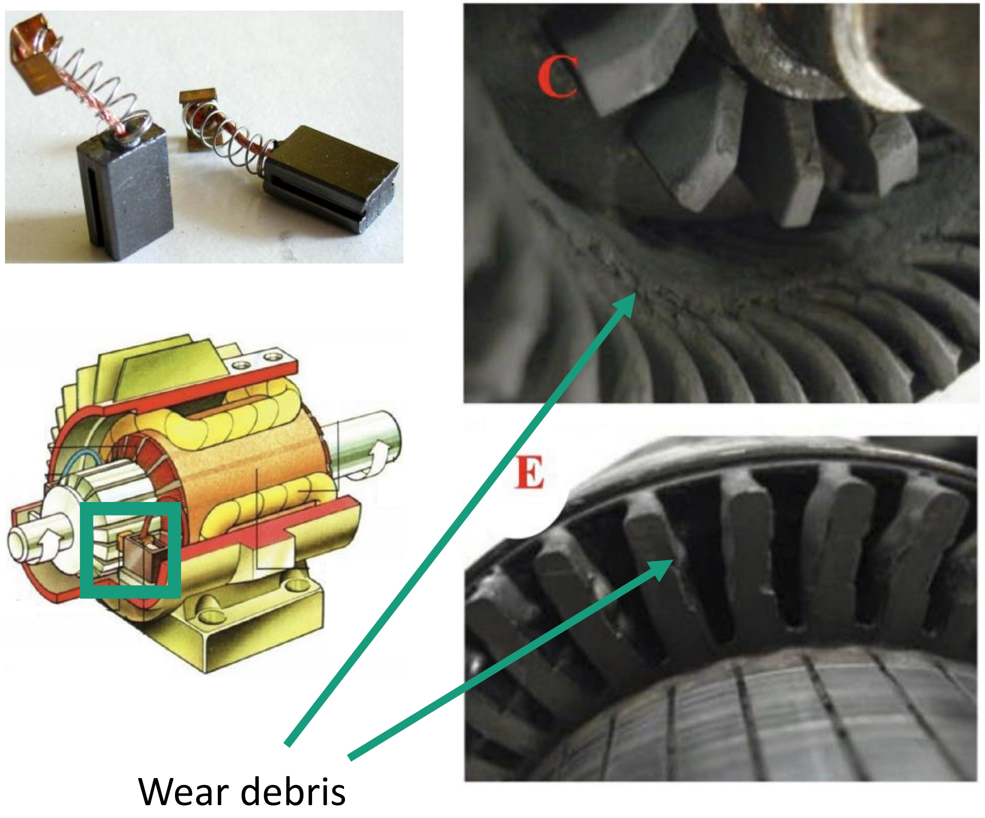




Why is graphite a good lubricant?

- Bragg 1928: X-ray diffraction experiments
  → Lamellar structure
- Weak bonding between layers
- Idea: layers slide against each other

Graphite Brushes in Electric Motors and Generators



Holle et al., Advanced Composites and Hybrid Materials 4, 162 (2021)

- Commutator brushes in electric generators
- 1930s: Rapid wear when used in planes flying higher than ~6000 m
- 1947: Humidity is crucial for graphite wear

High-Altitude Brush Problem

D. RAMADANOFF
MEMBER AIEE

S. W. GLASS
NONMEMBER AIEE

THE rapid development of military aircraft during the past three years has been accompanied by an equally vigorous development and use of electric motors and generators necessary for their operation and control. This dynamoelectric equipment covers not only the d-c and a-c applications but also a wide range of small brushes. These are the brushes which were showing rapid wear during flights.

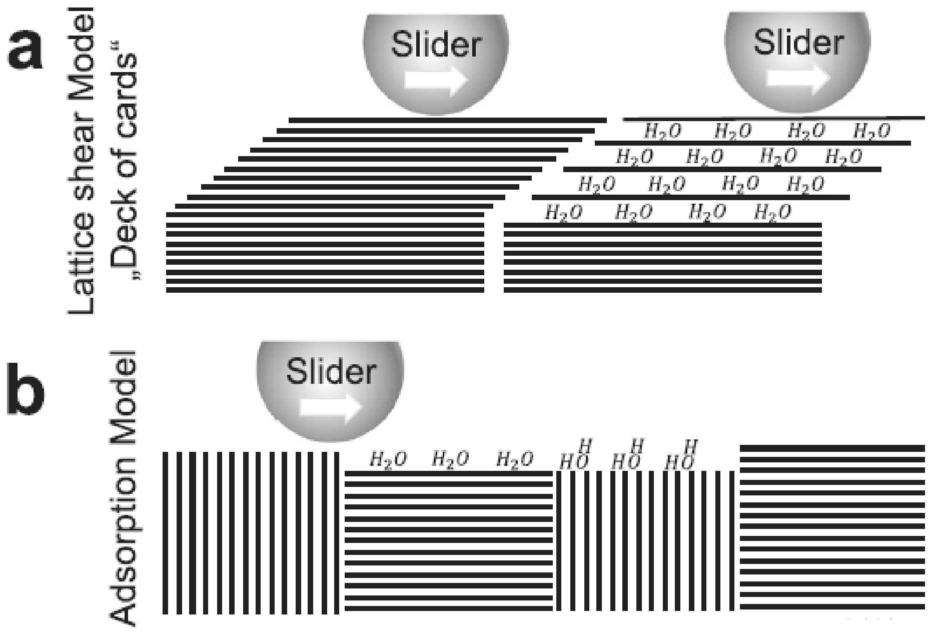
For the first approach of the problem the testing was conducted with equipment made from an actual propeller brush housing and holder (Figure 1). By these means it soon was established that brush

Trans. AIEE 63, 825 (1944)

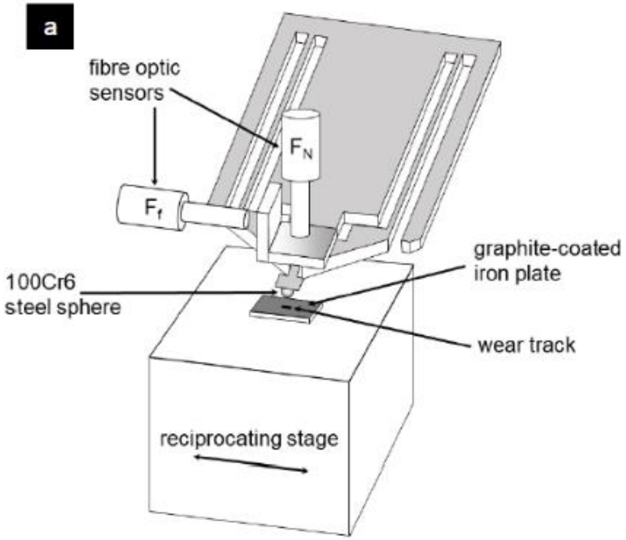
Graphite Lubrication Models

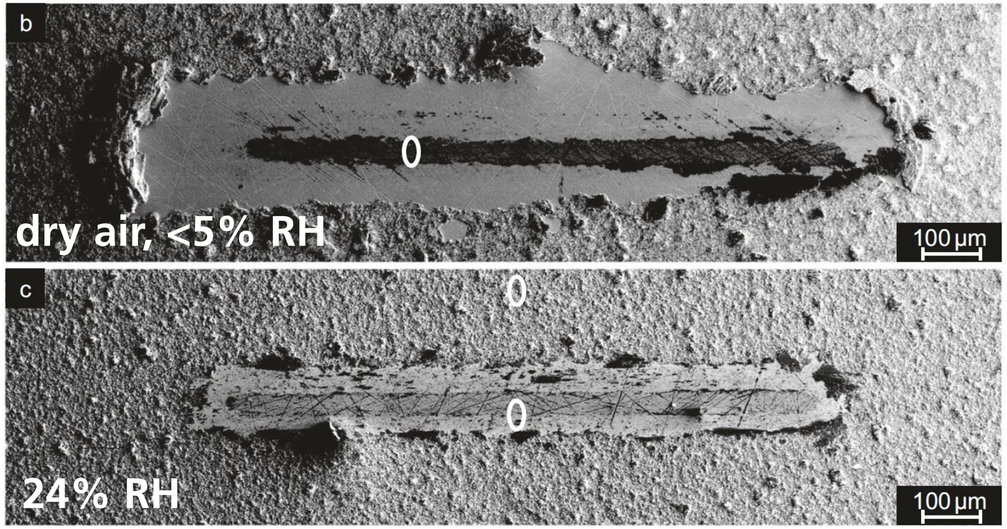
- Friction mechanism unknown → depends on ambient humidity
- Deck-of-cards model
  - No explanation for humidity dependence
  - Water intercalation?
- Adsorption model
  - Thin water film on the surface
  - Passivation of dangling bonds

→ Experiments and atomistic simulations



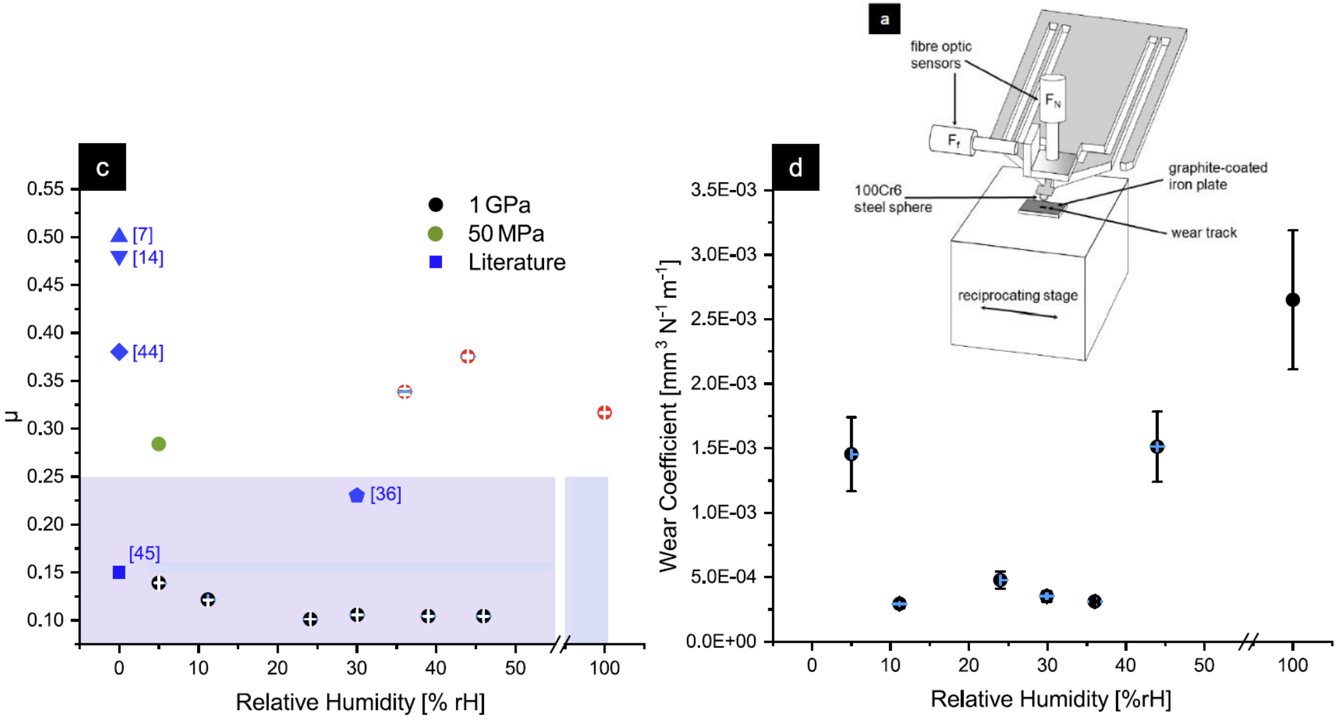
Experiments – Graphite coated steel

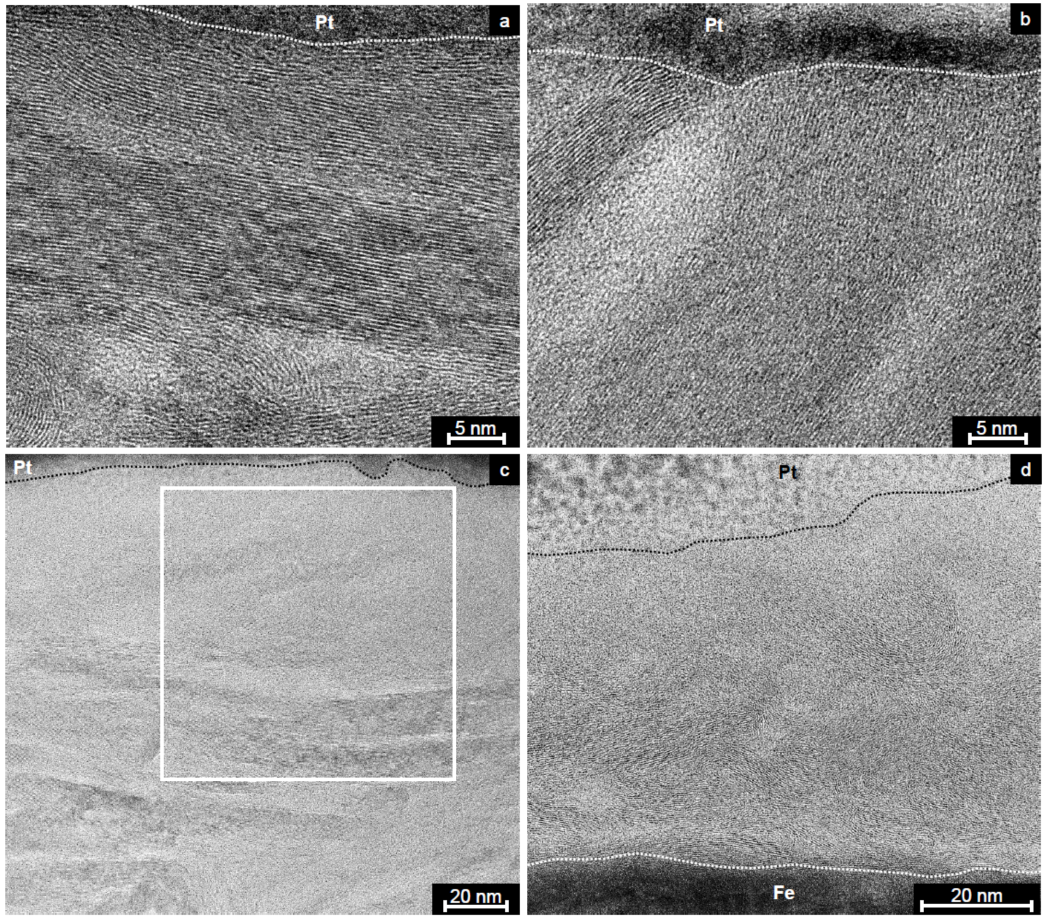




- Tribometer experiments: Steel sphere sliding on graphite coated iron
- Experiments in controlled atmosphere
- Surface analysis using SEM and TEM

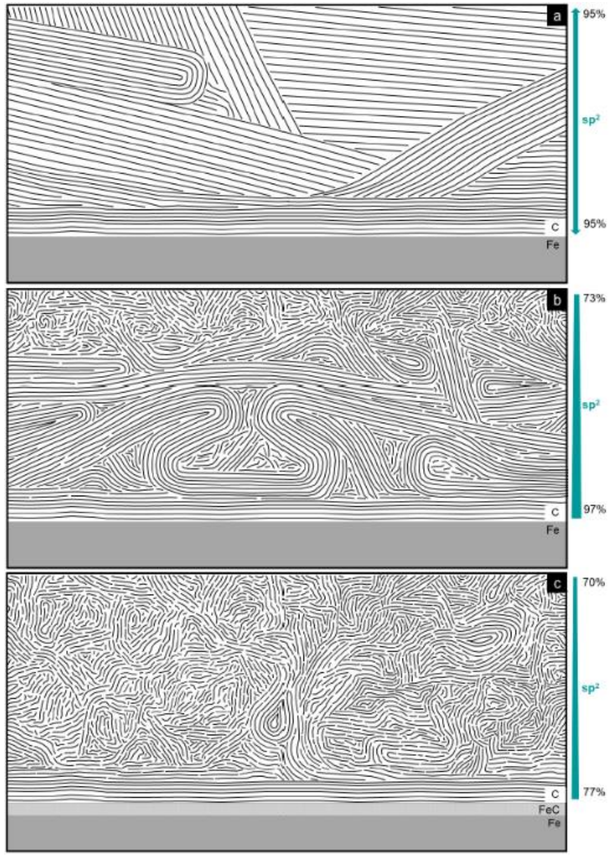
Experiments – Graphite coated steel

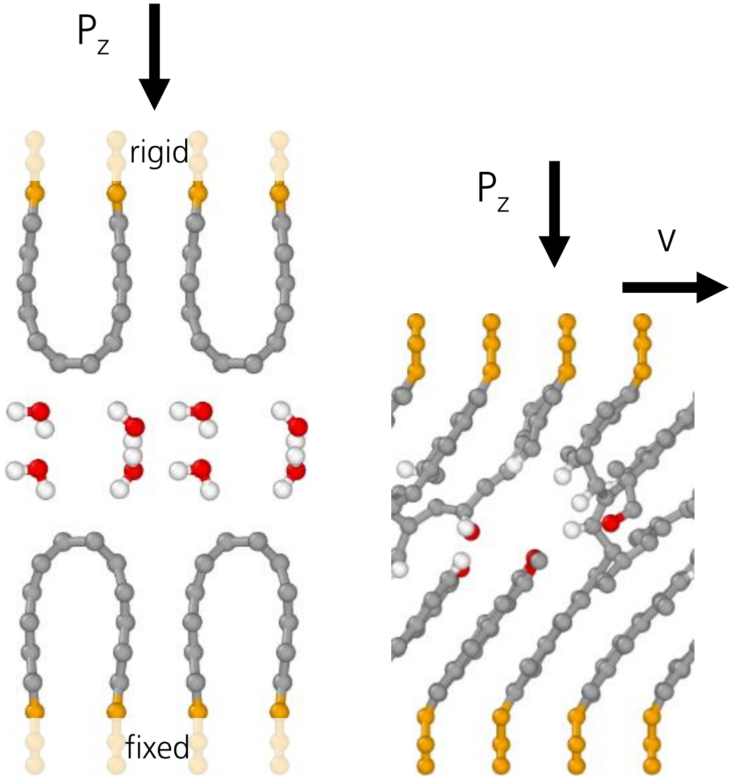




- Friction and wear depend on ambient humidity
- TEM: Shearing within the graphite layer, formation of turbostratic carbon
  → not covered by the deck-of-cards and the adsorption model

Atomistic simulations

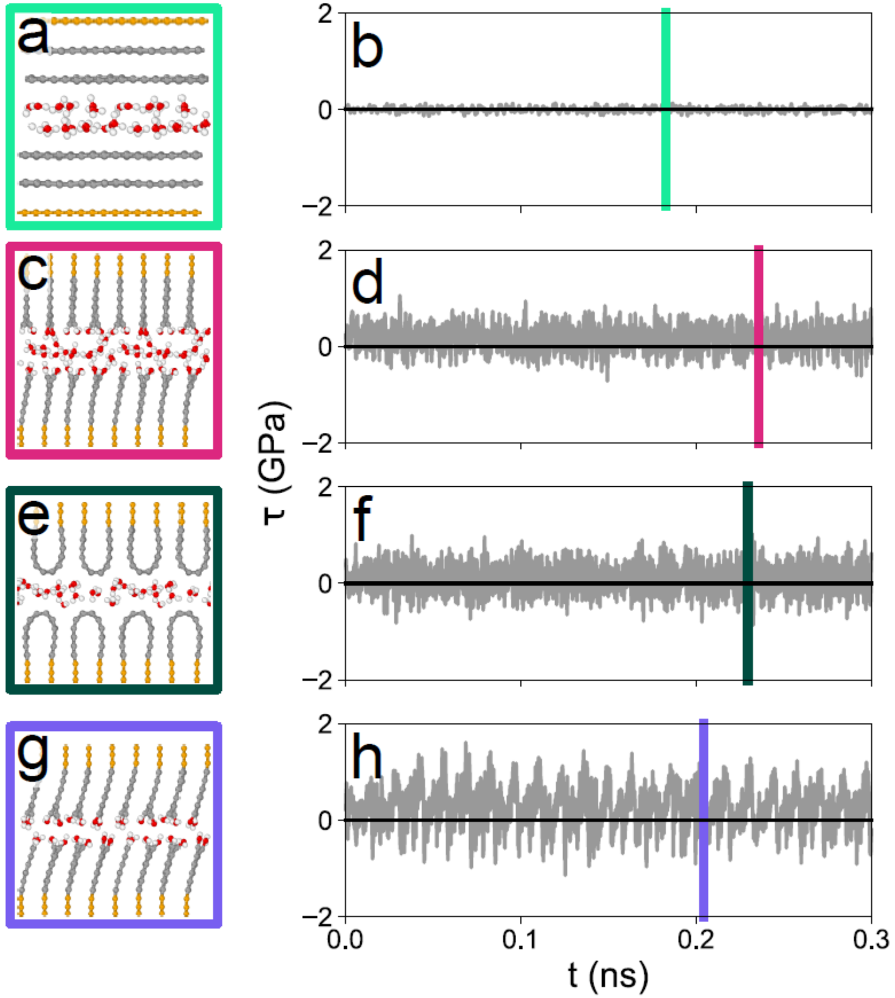


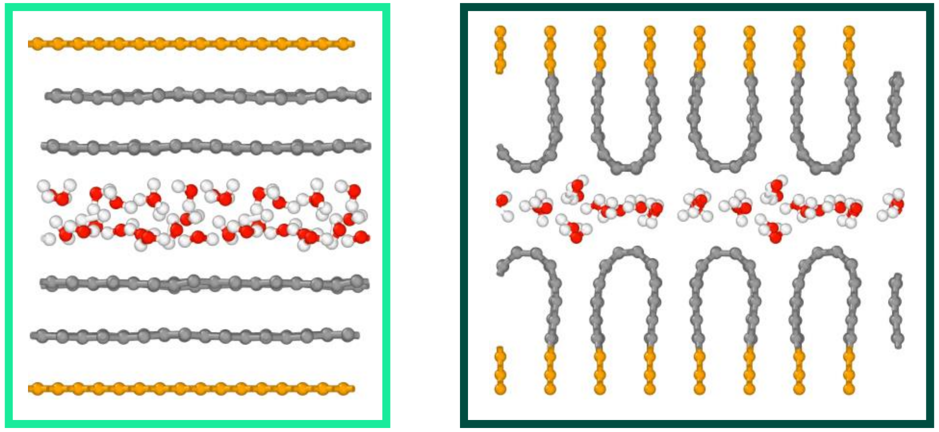


- Structural transformation cannot be observed in-situ → Atomistic simulations

- Tight-Binding MD
- v = 100 m/s, T = 300 K
- P_z = 500 MPa – 5 GPa
- 0-32 water molecules
- simulated time up to 0.8 ns

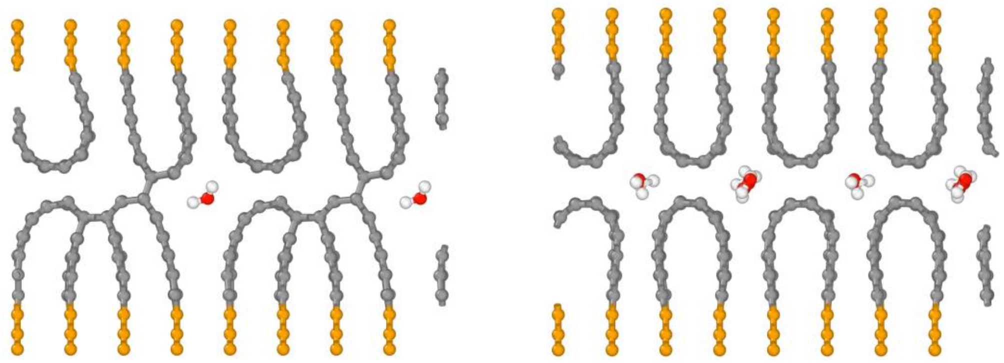
Graphite – H_2O – Graphite



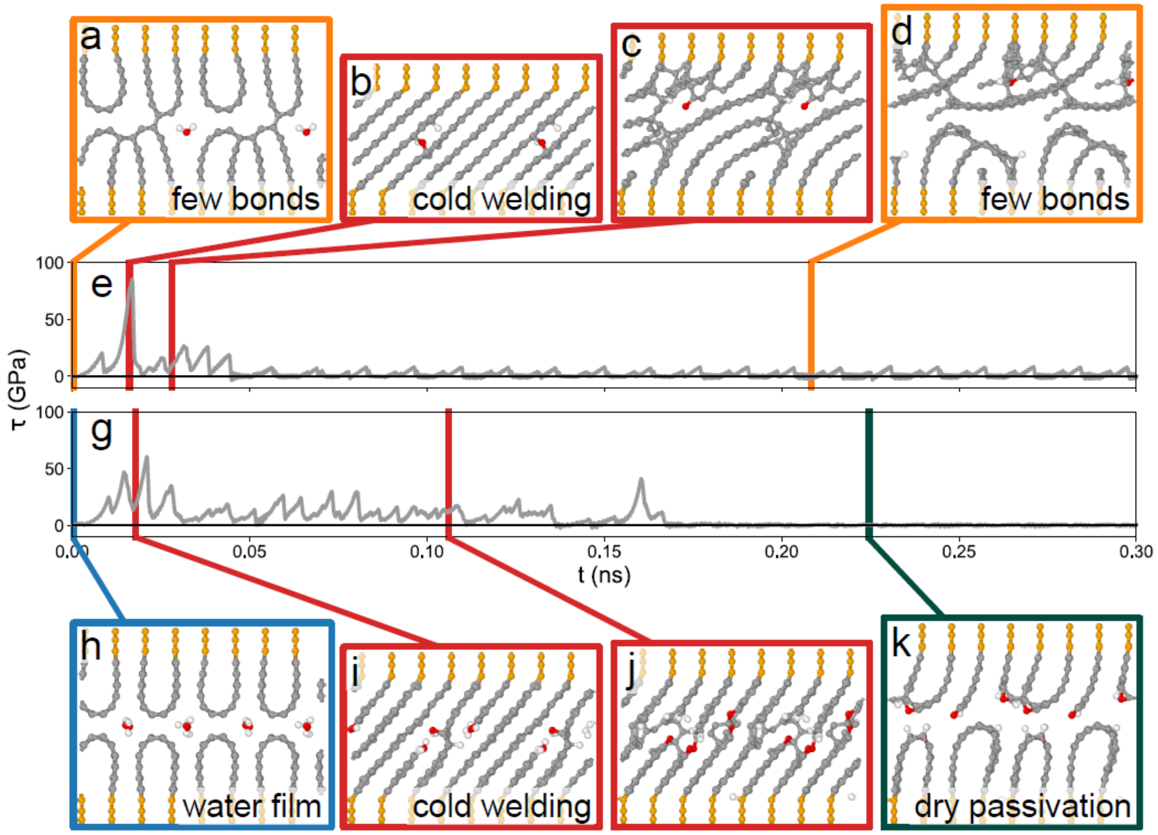


- Study with different graphite orientations
- Several possible graphite particle edge structures
- No reactions between water and graphite in most of the systems
- Strong dependence of system behavior in (e,f) on water content and normal load

Graphite – H_2O – Graphite



- Graphene planes perpendicular to sliding direction, small amount of water
- Reactions between surfaces
- Cold welding, surface passivations (complete or with remaining bonds), water films
- Detailed parameter study



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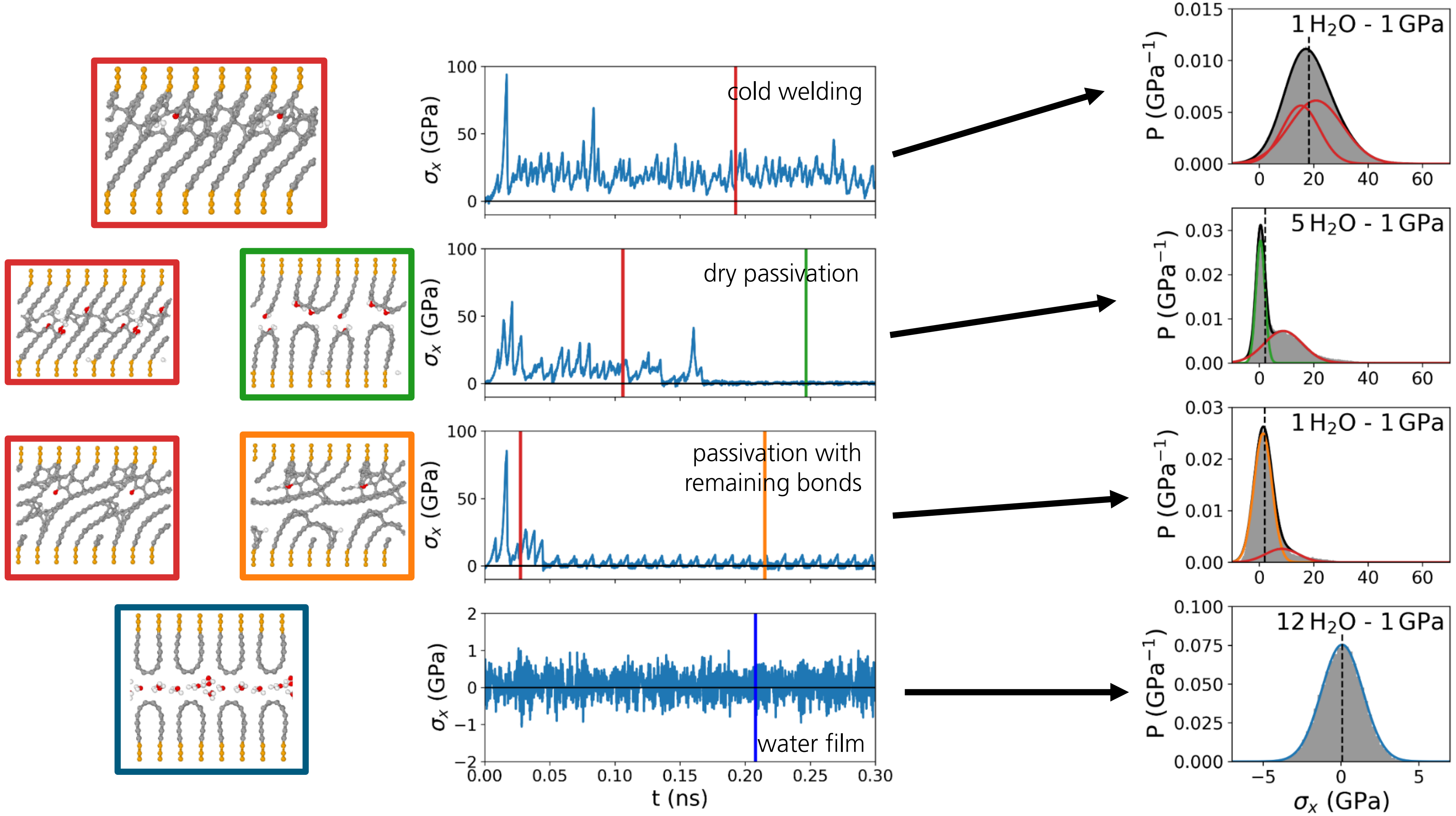

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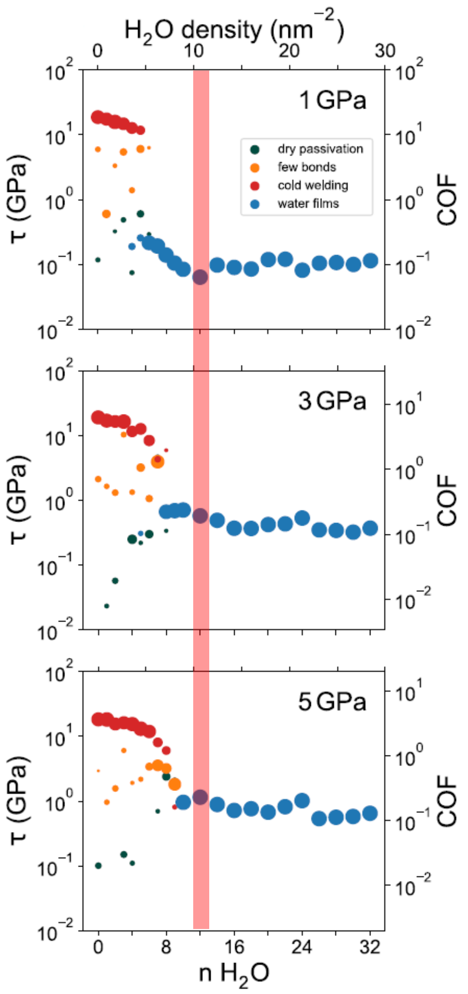
Graphite – H_2O – Graphite



- Dominating effects
  - Cold welding
  - Water films
- Transition shifts with increasing pressure

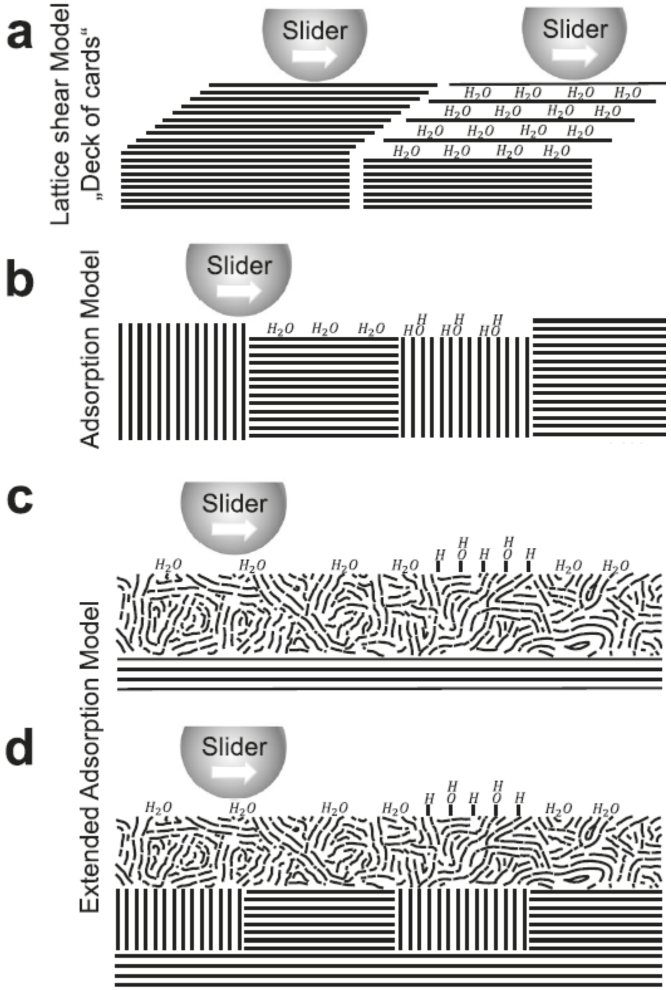
- Water monolayer $\rho_{H_2O} \approx 12\, nm^{-2}$
- Condensation from ambient humidity

- Explanation for the good lubrication properties of graphite in laboratory air
- Contacts might run dry every now and then (locally) → turbostratic carbon
- Transition to cold welding regime in dry air

Summary

- Deck-of-Cards sliding only at the interface to the substrate possible
- Shearing within the graphite layer → turbostratic carbon
- Not explained by the adsorption model

- Extension:
  Formation of turbostratic carbon and surface passivations



C. Morstein, A. Klemenz, M. Moseler, M. Dienwiebel: Graphite lubrication of highly loaded contacts: humidity-dependent friction and structural transition to turbostratic carbon, Nature Communications 13, 5958 (2022)

Thank you for your attention!