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Multi-scale simulations of PEEK tribointerfaces

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A multiscale simulation method to quantify friction phenomena at neat PEEK interfaces is presented and compared to tribometer experiments. At the molecular scale, atomistic simulations provide insights on structural transformations in the polymer, i.e. nano-roughness flattening, chain alignment and onset of transfer film formation. Nanoscale friction laws are formulated, which are then integrated over the real contact area from elastoplastic contact mechanics to determine the macroscopic dry friction coefficient μ. Good agreement between experiments and simulations is found at high loading conditions, where μ≈0.5-0.7. Physisorbed water reduces significantly intersurface adhesion, likely leading to reduced friction (μ≈0.2) at lower loads.

Keywords: molecular dynamics, contact mechanics, multi-scale simulations, PEEK

1. Introduction

Polymers are increasingly being used as tribomaterials due to their low friction, corrosion resistance, biocompatibility and cost efficiency. Numerical modeling of polymer friction must account for several phenomena and complex material properties [1]. For instance, a critical parameter remains the shear strength of adhesive junctions [2], which depends strongly on surface chemistry or physiosorbed molecules. In this work we present a multiscale approach coupling atomistic to macroscopic simulations and assess its capability to predict the friction coefficient from experiments.

2. Methods

2.1. *Non-reactive Molecular Dynamics* shear simulations of PEEK-PEEK or PEEK-steel interfaces with or without physisorbed water were performed at varying pressures P and sliding speeds U. Atomic trajectories reveal structural transformations at the sliding interface, and the shear stress in steady state is quantified through a nanoscopic friction law $\tau(P,U)$.

2.2. *Elasto-plastic contact mechanics* simulations based on AFM topography data and material properties from nanoindentation experiments provide the relative contact area $A_{rel.}/A_{app.}$ for rough geometries representative of the experimental samples.

2.3. *Reciprocating tribometer experiments* are performed on a sphere-plane setup at low sliding speed (2 mm/s). Normal loading is varied from low values up to pressures close to the material plasticity limit (P_{Hertz} = 10-75MPa).

3. Results and discussion

Atomistic simulations of PEEK-PEEK interfaces reveal flattening of nano-roughness and reorientation of the polymer chains along the sliding direction. Against rough steel countersurfaces PEEK chains deposit in the asperity valleys, which may indicate transfer film onset.
In dry conditions, the shear stress is high due to large intersurface adhesion, and of the order of the shear strength of bulk PEEK. It varies linearly with pressure and is independent on the sliding velocity, which is summarized by: $\tau(P,U) = 0.18P + \tau_{adh.}$. The adhesion-related shear stress $\tau_{adh.}$ is strongly reduced by the presence of physisorbed water films. Integration of the nanoscopic friction law over the contact area gives the macroscopic friction coefficient $\mu = 0.18 + \frac{\bar{\tau}_{adh.}}{P_{ext.}}\frac{A_{real}}{A_{app.}}$. For dry interfaces, $\mu \approx 0.5 - 0.7$ depending on the PEEK penetration hardness, whereas $\mu = 0.18$ if adhesion is suppressed, e.g. by water at lower loads. These values are in good agreement with the friction coefficient from experiments.

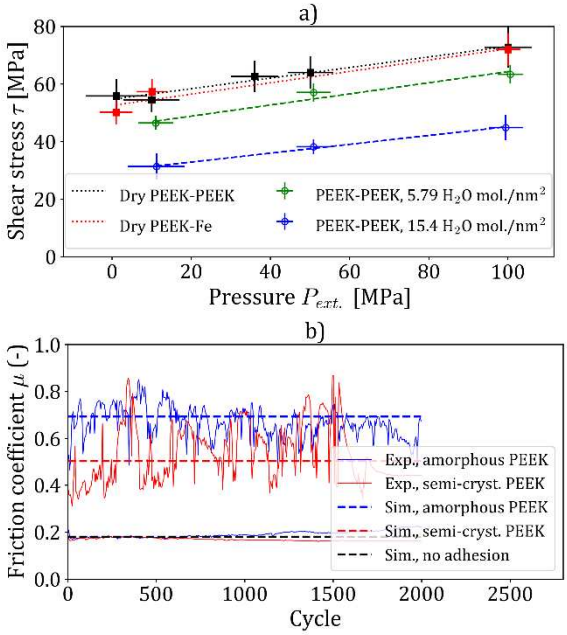

Figure 1: a) Shear stress dependence on pressure at the nanometer scale, and b) Comparison of the friction coefficient from the multi-scale approach and experiments.

4. References

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