

FRICITION AND WEAR MECHANISMS OF PTFE BY ATOMISTIC SIMULATIONS: TRANSFER FILM FORMATION AND THE SYNERGY BETWEEN PTFE AND PEEK

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ABSTRACT

Polytetrafluoroethylene (PTFE) is a widely used material for tribological applications due to its low friction properties, chemical stability, and high temperature resistance [1]. Its slipperiness, resulting from the weak adhesion between the molecular layers composing this solid lubricant, facilitates the formation of transfer films when PTFE comes into contact with a counter surface [1, 2]. However, this mechanism, which contributes to the remarkably low friction coefficients, is also associated with significant wear of the solid lubricant.

This talk focuses on two possible ways to address this issue. We will first discuss how the constant replenishment of PTFE on the surfaces via the double transfer mechanism can be used to compensate for the wear losses. To better understand the transfer film formation at steel interfaces, we performed classical molecular dynamics simulations (MD) of PTFE-lubricated iron oxide interfaces using a newly developed non-reactive force field based on density functional theory. The adhesion of PTFE to iron oxide drives the transfer film formation, while shear-induced chain alignment within PTFE results in reduced friction. These results agree with ball-on-disc tribological experiments enhanced by a pin-on-disc sliding contact that transfers PTFE to the steel surface (Figure 1a) [2].

Another possibility to extend the lifetime of PTFE-lubricated contacts is by blending PTFE with other polymers that are better resistant to wear. For instance, PTFE/polyetheretherketone (PEEK) blends exhibit significantly lower wear than pure PTFE and PEEK alone [3]. Our MD simulations indicate that sliding drives the phase separation between the two polymers, and shear is accommodated between crystalline PTFE layers, rather than in PEEK or at the PTFE/PEEK interface (Figure 1b) [4].

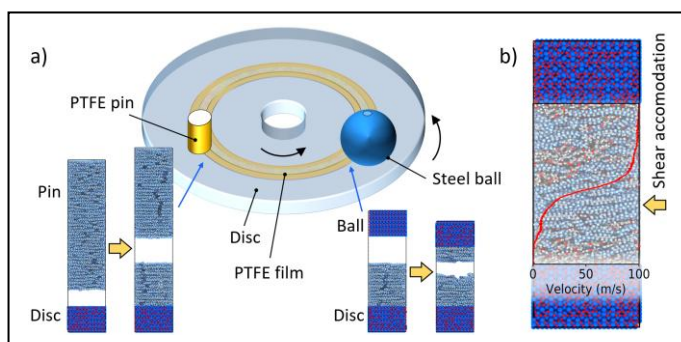


Figure 1 – a) Double transfer film mechanism of PTFE and b) shear accommodation in the PTFE/PEEK blend.

The friction performance of the blend, as well as of the pure polymers, will be compared to the one of polyethylene, which is structurally similar to PTFE, and discussed in detail.

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