Relating atomic-scale surface structure to friction via multiscale simulations: the cases of PTFE and B-doped diamond-like carbon

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Abstract

Friction in dry and boundary lubrication conditions is strongly influenced by the atomic structure of the sliding surfaces. In general, a stable passivation of surface dangling bonds is a prerequisite for low friction and wear. However, even subtle changes in surface chemistry can cause the friction coefficient of passivated interfaces to vary by an order of magnitude (1). In this talk, I will present the results of multiscale simulation studies that combine density functional theory, non-reactive molecular dynamics and contact mechanics to shed light on the relationships between the chemical structure of surfaces and friction.
The first case study involves fluorinated carbon materials. Some of these materials, like PTFE, have exceptional tribological properties. However, their chemical stability poses serious problems because of their accumulation in the environment and in biological systems. Therefore, regulations in this area aim to their replacement and understanding the mechanisms responsible for their friction properties may help in this non-trivial process. The results of our multiscale simulations allow us to answer some fundamental questions in this context: Why are perfluorinated carbon materials polar and hydrophobic (2)? Why are they more slippery than their hydrogenated analogues (3)? Why is PTFE non-sticky but forms transfer films on PTFE-lubricated steel surfaces (4)?

In the second case study, I will focus on friction of boron-doped diamond-like carbon coatings in humid air. While boron typically reduces wear in cutting applications, some B-doped coatings show poor tribological performance compared with undoped films. Our simulations suggest that the friction increase could be related to a subtle change in surface chemistry caused by boron atoms (5). Hydroxyl groups that normally passivate carbon surfaces in humid environments can be activated by boron and form B–O dative bonds across the tribological interfaces, leading to a mild friction increase.

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