INSIGHTS INTO THE NANOSCALE TRIBOLOGICAL PROPERTIES OF GRAPHITE IN WATER

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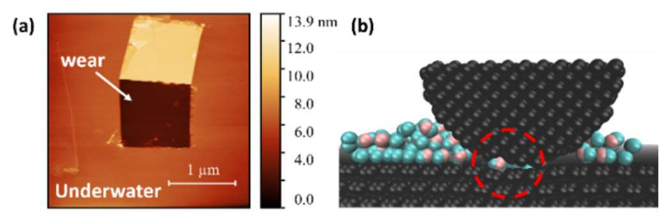
ABSTRACT

Graphite, possessing remarkable friction reduction capabilities due to easy shearing of its weakly bonded single atomic thin graphene sheets, emerges as an attractive material for numerous tribological applications. However, the intricate interplay between its tribological properties and the surrounding environment, such as water vapor, oxygen, or gases, significantly affects its lubrication longevity and frictional performance. Graphite exhibits low friction and wear in the presence of condensable vapors under humid environment in comparison to vacuum or dry environment.[1] In fact, in a recent nanoscale investigation, it is found that graphite demonstrates a nonmonotonic behavior of friction with varying humidity and offered low friction only above a threshold humidity.[2] Another study demonstrates that the initiation of wear on graphite surfaces predominantly occurs at step-edges, where dangling bonds are abundant, while the interior regions demonstrate greater resilience against nanoscale scratches.[3] Intriguingly, recent research reports that step-edge defects on the graphite surfaces exhibit improved wear resistance in humid environment, attributing to the passivation of dangling bonds of the step-edge carbon atoms by condensed water molecules.[4]

Understanding the dynamic behavior of tribological properties of graphite in response to environmental variations necessitates a deeper comprehension of the interactions between the graphite surface and the surrounding molecules during sliding, a facet that remains poorly understood. To bridge the gap, we conducted a comprehensive investigation, combining atomic force microscopy (AFM) experiments and molecular dynamics (MD) simulations, to make a comparative analysis of friction and wear behavior of graphite under two different environmental conditions: the ambient (air) and underwater condition. The experimental results note a significant distinction in the friction and wear behavior of graphite between the two environments. The presence of water in underwater conditions not only increases the friction but also considerably reduces the wear resistance of the graphite surface (Fig. 1(a)). Insights from MD simulations elucidate that the increased friction of graphite in underwater condition arises from the resistance posed by surrounding water molecules during sliding. These molecules get trapped at the contact interface at increased loads, inducing high localized stresses, and ultimately lead to the failure of C-C bonds of the graphite surface (Fig. 1(b)).

Fig.1(a) Zoom-out topography of the wear region of graphite surface in underwater condition (b) MD snapshot of water molecule trapped between tip and substate during sliding.



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