Low Friction and Wear of Bilayer Graphene: A First Principles Approach

Zaixiu Yang [1], Fatih G. Sen [2], Ahmet T. Alpas [1]

1. Department of Mechanical, Automotive & Material Engineering, University of Windsor, 401 Sunset Ave, Windsor, ON, Canada
2. Argonne National Laboratory, 9700 Cass Ave, Lemont, IL, United States

yang15n@uwindsor.ca

Abstract:

Recent research [1, 2] revealed that multilayered graphene could provide low friction, an effect wich is enhanced in humid atmospheres. Spin polarized density functional theory calculations were employed in this work to investigate the friction reduction mechanisms of graphene under water environment. Van der Waals interactions within the seamless frame of vdW-DF2 were incorporated to accurately simulate the interactions between water molecule and defected graphene, as well as the bilayer graphene. While pristine graphene is rather inert to water, water molecule can be dissociative adsorbed at defect site of graphene (energy barrier 1.27 eV for mono-vacancy graphene). Once the dissociated H and OH from water molecule are attached to the dangling bonds at the mono-vacancy site, it will further promote adsorption of water molecule by increasing adsorption energy of second water molecule to 0.39 eV, compared with that 0.23 eV for whole water molecule adsorbed at mono-vacancy graphene, and 0.12 eV at pristine graphene. To further understand the role of dissociated H and OH in reducing friction between graphene, bilayer AB graphene with OH and H facing each other were investigated. It is found the H and OH in the interlayer can reduce the interlayer adhesion by 20% while increase the interlayer spacing by 0.06 - 0.26 Å compared with pristine graphene. Meanwhile, the dissociative adsorption of water molecule near the vacancy site can lead to the structural disorder of AB graphene which may in turn assist dissociation of water molecule on graphene surface. Thus, the friction reduction of graphene under humidity is initiated by generation of dangling bonds at defect site followed by saturation of dangling bonds H and OH dissociated from water molecule, which leads to the transition of graphene from hydrophobic to hydrophilic and promotes more water molecule trapped to graphene. Then the graphene layer can be easily transferred against each other due to reduced interlayer adhesion and increased interlayer spacing, which would assist the formation of tribolayer at the sliding couterface. Hence, low friction and low wear is achieved. This investigation sheds light on the application of graphene as protective coatings.

References

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Figures