Simulation on structure and properties of diamond-like carbon films

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Diamond like carbon (DLC) film has excellent characteristics such as high hardness, low friction, good wear resistance, and corrosion resistance, which has attracted great attention as a surface protective film for key moving parts of automobiles, machinery, and marine equipment. However, DLC films suffer from key bottlenecks such as high residual stress, poor adhesion between film and substrate, and high dependence on friction environment. In addition, there is insufficient in-depth research on the relation between composition, structure, and friction properties of films due to the lack of essential understanding at the atomic/electronic scale, which limits their widespread applications. Therefore, we have conducted systematic research on the surface/interface structure modulation, controllable preparation, and property evaluation of DLC films through a combination of theoretical calculations and experiments, mainly including: 1) the stress reduction mechanism of metal-doped DLC films; (2) Composite structure design and structure-property relationship of co-doped DLC films; (3) Theoretical study on surface/interface structure modulation and friction behavior of DLC films under dry and oil lubrication conditions.

Keywords: Diamond-like carbon; surface/interface structure modulation; anti-friction and wear-resistance; friction mechanism