The Structure and Sliding Friction of Diamond-like Carbon Surfaces from Molecular Dynamics Simulations

Qing Zhang, Adri Van Duin, Tahir Cagin, and William A. Goddard, III
Materials and Process Simulation Center (MSC), MC 139-74
California Institute of Technology, Pasadena CA, 91125

Abstract

Using the ReaxFF reactive force field in molecular dynamics (MD) simulations we have predicted the three-dimensional structure of diamond-like carbon (DLC) at densities ranging from 2.4-3.4 g/cm³. The structures for these solid amorphous systems were generated by melting a cell with 512 atoms, followed by rapid quenching from the liquid phase. The energetically most favorable DLC structure has a density close to the experimental value (3.24 g/cm³). At this density we find that 70% of the atoms have sp³ character in a good agreement with experiment (70% from the Martin group in Lyon). We find that all of the sp³ atoms connect to form a percolating tetrahedral network to which are attached isolated sp2 atoms or short chains of sp² atoms. DLC surfaces were constructed by determining the lowest energy surface for cutting the bulk DLC cell. We found that the surface C atoms react readily with glycerol to form a very smooth carbon surface containing OH-terminated groups, which enhanced by sliding. This agrees with experiments from the Martin group in Lyon.

Using MD simulations we examine the friction properties for various DLC surface: bare surface, H-terminated, OH-terminated, and the passivated surface after reaction with glycerol. We found that the bare DLC surface has a very high friction coefficient (~ 1.0), whereas the DLC surface passivated with OH/H by reacting with H₂O₂ leads to a very low friction coefficients (down to 0.01). These results suggest that the origin of the superlubricity observed in the DLC system arises from the smooth OH-terminated surface, which is consistent with experiment (the Martin group in Lyon). We also investigated the relationship between the friction and interfacial adhesion. The MD simulations suggest that friction is determined by variations in the adhesion during sliding, rather than the absolute value of the adhesion between interfaces. Larger variations (energy barrier) induce larger deformations of the sliding objects, leading to higher friction.