TEXAS TECH UNIVERSITY
Department of Mechanical Engineering

Ph.D. Defense Announcement

Molecular Dynamics Simulations of Atomic Material Behaviors at the Head-Disk Interface in Hard Disk Drives

By

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Abstract

In hard disk drive (HDD), diamond-like carbon (DLC) is used on the head and disk surfaces as an ultra-thin protective coating due to its high mechanical strength, wear resistance, thermal stability, chemical inertness, and low friction. Also, on the disk DLC surface, perfluoropolyether (PFPE) lubricant is applied to reduce friction and protect the disk surface. However, during the HDD operation, it is found that the intermittent contact occurs between the head and disk surfaces, which may result in surface damage and eventually read/write errors of the HDD. Also, after the HDD operation, it is observed that liquid droplets form on the head surface, which may cause the change of head dynamics and instability of the flying height during its operation. After analyzing the droplets, it is concluded that the droplets contain both PFPE lubricant and hydrocarbon contaminant that is from the drive components due to the outgassing during the HDD operation in elevated temperature. Therefore, it is important to understand the DLC material properties and behaviors during the sliding contact. It is also crucial to understand the material properties and behaviors of PFPE lubricant and hydrocarbon on DLC surface. In this research work, molecular dynamics (MD) simulations were used to study the DLC sliding contact. Both hydrogen free and hydrogenated DLCs were included in the sliding contact MD simulations. The forces and temperatures at the contact interface were obtained during the sliding contact. It indicated that the hydrogen content in DLC increased the mechanical strength of DLC and the temperature rise on the DLC surface due to higher friction heat generation. Also, the graphitization of DLC was slowed down by the hydrogen content. Next, the interactions between hydrocarbon, PFPE lubricant and DLC were investigated. The attractive forces and surface energies between hydrocarbon, PFPE lubricant and DLC were obtained, and the bonding preference of hydrocarbon to PFPE lubricant and DLC was studied. The results indicated that hydrocarbon had higher bonding preference to DLC surface than PFPE lubricant. And within the PFPE lubricant, hydrocarbon tended to bond to the backbone first. Last, the PFPE lubricant material properties and behaviors on the DLC surface were studied using MD simulations. Different types of PFPE lubricant were used in the MD simulations. Their droplets were created and equilibrated on the DLC surface. The stabilized droplet contact radii and heights were calculated from the simulations, and the lubricant transfer behaviors were analyzed. The results showed that the contact radius decreased as the percentage of functional end group increased, and the droplet height was not significantly affected by the percentage and polar strength of the functional end group. Also, the shear movement of PFPE lubricant decreased as both the percentage and polar strength of functional end group increased. Finally, the lubricant transfer was reduced as the percentage and polar strength of functional end group increased. These findings can be used to improve the design and reliability of HDD and increase the lifetime of the products.