ABSTRACT

Structural and Chemical Investigations of Nanotribology Using *In Situ* Transmission Electron Microscopy and Defect Based Analytical Modeling

Ariel M'ndange-Pfupfu

A combination of structural and chemical investigations into nanoscale tribological processes were carried out both experimentally and theoretically. Using *in situ* transmission electron microscopy (TEM) techniques, imaging and spectroscopy were performed in real time on a sliding contact. Uniquely, this approach allows for direct, comprehensive observations of tribological phenomena and an unprecedented amount of quantification. Sliding-induced changes in the carbon bonding structure were observed in amorphous hydrogenated "N3FC" diamond-like carbon films. Taking into account the effects of the electron beam, the rate of the transformation from sp^3- to sp^2-hybridized bonding was quantified as between 0.009% and 0.018% of the sampled film volume per sliding pass, and discovered not to be limited to the surface. Further investigations of these samples using an environmental TEM to apply various pressures of N_2 and H_2 gas showed that the same bonding phase transformation occured more rapidly than the vacuum experiments. In addition, in 0.15 torr N_2, significant amounts of sliding-induced tribochemical wear were observed in regions of the surface highly localized to where the sliding contact was made, totaling approximately 1.2×10^6 nm^3 of lost material over 100 sliding passes. The same experiments in H_2 showed little discernible wear, and the differences in surface chemical activity are discussed.

Separately, traditionally bulk defect theory was used to examine the role of dislocations in crystalline nanotribology. A model was developed to calculate the shear and plowing components of friction in a model system: the shear component being due to the drag of misfit dislocations and the plowing component due to creep-mediated deformation around the asperity. Asperity velocity, shape, and normal load dependence are discussed in addition to thermal effects. Furthermore, the role of mobile arrays of dislocations is examined with regards to the shielding effects such arrays would experience from directional phonon drag. For the relevant range of scattering angles and cross-sections, the adjustment due to shielding is calculated to be 6-25%, small enough that the widely used single dislocation approximation can be considered valid. These sorts of multifaceted approaches to tribology are necessary if we want to continue developing our understanding at a fundamental level.