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In Situ XPS and NEXAFS Investigation of the Thermally-Induced Structural Evolution of Advanced Amorphous Carbon-Based Surfaces

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Silicon oxide-doped diamond-like carbon (SiO_x-DLC) coatings are fully amorphous thin-film materials consisting of two interpenetrating networks, one being a hydrogenated amorphous carbon (a-C:H) network and the other a silica glass (SiO_x) network. At temperatures above 150°C, pure a-C:H films undergo a rapid degradation that starts with the evolution of hydrogen and is followed by the conversion of sp^3 bonds to sp^2. However, SiO_x-DLC exhibits much lower susceptibility to oxidative degradation, and much higher thermal stability compared to a-C:H. This makes SiO_x-DLC an attractive material for many applications, including for the development of next generation hard disk drives, which require novel overcoat materials that are thermally stable up to temperatures above 500ºC. Even though it is well-established that SiO_x-DLC possesses superior thermal stability and oxidation resistance relative to a-C:H, the scientific basis for this behavior is not understood. To investigate this, a combined *in situ* XPS and NEXAFS study was performed. Changes in the surface chemistry and bonding configuration of SiO_x-DLC (*e.g.*, silicon oxidation state, carbon hybridization state) could be accessed *in situ* at temperatures up to 450ºC. A novel methodology for processing NEXAFS spectra, which makes it possible to account for the presence of a carbonaceous contamination layer on an air-exposed material, was developed. This allowed quantitative evaluation of the carbon hybridization state in the film as a function of the annealing temperature. These experimental results could be well fit with a thermally activation-based model that describes the structural transformations occurring in vacuum in SiO_x-DLC as a function of time and temperature. To determine the environmental dependence of the surface structural evolution of SiO_x-DLC, the results of the *in situ* XPS/NEXAFS investigation were compared to those for SiO_x-DLC samples heated in air, showing a strong effect of atmospheric oxygen.