



Deposited via The University of Leeds.

White Rose Research Online URL for this paper:

<https://eprints.whiterose.ac.uk/id/eprint/91834/>

Version: Accepted Version

Proceedings Paper:

Mangolini, F, McClimon, JB, Hilbert, J et al. (2014) In situ XPS and NEXAFS investigation of the thermally-induced structural evolution of advanced amorphous carbonbased surfaces. In: Abstracts of Papers of the American Chemical Society. 248th ACS National Meeting and Exposition, 10-14 Aug 2014, San Francisco, CA, USA. American Chemical Society. Article no: 118-COLL. ISSN: 0065-7727.

Reuse

Items deposited in White Rose Research Online are protected by copyright, with all rights reserved unless indicated otherwise. They may be downloaded and/or printed for private study, or other acts as permitted by national copyright laws. The publisher or other rights holders may allow further reproduction and re-use of the full text version. This is indicated by the licence information on the White Rose Research Online record for the item.

Takedown

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing eprints@whiterose.ac.uk including the URL of the record and the reason for the withdrawal request.

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

Filippo Mangolini¹, J. Brandon McClimon¹, James Hilbert², Jennifer R. Lukes², Robert W. Carpick²

¹ *Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA*

² *Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA*

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 sp³ bonds to sp². 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 500°C. 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 450°C. 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.