

Abstract Submitted  
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**Carbon Hybridization Dynamics Inside the Bombarded Carbon Surface**<sup>1</sup> STEVEN J. STUART, Clemson University, PREDRAG S. KRSTIC, CARLOS O. REINHOLD, Oak Ridge National Laboratory — We study the density and hybridization depth profiles of amorphous carbon and graphite, bombarded by D and D<sub>2</sub>. Cumulative impacts produce modifications in the substrate structure and the sputter yields. For graphite samples, the surface continues to evolve up to the highest fluences studied, of  $1.9 \times 10^{21}$  m<sup>-2</sup>, while for the deuterated amorphous carbon surface, however, the sample reaches a steady state at fluences of less than  $3 \times 10^{20}$  m<sup>-2</sup>. At this point the structure of the surface and sputtering properties of lighter hydrocarbons change slowly within statistical fluctuations. The steady-state surface structure is examined in detail and is found to be very different from the initial surface: It is highly supersaturated with deuterium, with enrichment in sp<sup>3</sup> bonds. The yields of the light hydrocarbons sputtered from these surfaces are found to be directly related to the hybridization structural properties and the depth profiles. Our simulations indicate that it is necessary to perform sputtering simulations on surfaces that have been dynamically created by impacts, rather than equilibrium surfaces, to obtain a good agreement with experiments.

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