

Surface chemistry and physics of D-retention in lithiated graphite*

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Fusion devices such as TFTR, CDX-U, FTU, T-11M, TJ-II and NSTX have found improvements in plasma performance through the implementation of Li wall conditioning. Improvements include edge localized mode (ELM) reduction, reduction in lower divertor C and O luminosity, and deuterium particle control [1,2]. Previous work has shown that pure liquid Li allows for full uptake of incident deuterium ions to form lithium deuteride [3]. Post-mortem NSTX tiles and control studies show that lithiated graphite reacts readily with oxygen to form additional chemical bonds, including lithium-peroxide and lithium carbonate [4]. Recent experiments at Purdue University examine the affect of D irradiation of lithiated graphite. X-ray photoelectron spectroscopy (XPS) results show that the surface chemistry of a Li conditioned graphite sample after D ion bombardment is fundamentally different from that of non-Li conditioned graphite with hydrogenization followed by sp, sp² and sp³ hybridizations [5]. Instead of simple LiD bonding as seen in pure liquid Li, graphite introduces additional complexities with XPS measuring bonding functionalities between Li-O-D (manifest at 533.0 ± 0.5 eV in the photoelectron spectra) and Li-C-D (manifest at 291.2 ± 0.5 eV).

XPS spectra show Li-O-D and Li-C-D peaks become “saturated” with D at a fluence between 3.8 and 5.2×10^{17} cm⁻². Controlled experiments presented in this work demonstrate that D binds to O and C in the presence of Li by means of dipole interactions between Li atoms and the graphite matrix. XPS analysis indicates that deuterium has at least two bonding states in lithiated graphite: 1) weak bonding due to dipole interaction and 2) covalent bonds to C and O, which correlate with prompt thermal desorption spectroscopy (TDS) analysis from in-vacuo plasma material interface (PMI) probe analysis in NSTX presented in a separate paper [6]. Experimental results are complemented by atomistic simulation of the surface chemistry. Using molecular dynamics simulation we theoretically study the nature of the Li-C-D chemistry, showing few energetically different bonding substrates.

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