The role of oxygen in retaining deuterium on lithiated graphite surfaces*

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Lithium wall coatings have improved plasma performance on a number of fusion devices including TFTR, CDX-U, FTU, TJ-II, MAST, and NSTX [1, 2]. These improvements have come via a reduction in deuterium recycling and in some cases, a reduction in oxygen and carbon impurities. Based on the basis of LiD formation in solid and liquid lithium, the initial conjecture of deuterium retention in lithiated graphite was primarily by LiD binding channels. Our initial X-ray photoelectron spectroscopy (XPS) analyses showed that the binding chemistry included more complicated Li-O-D and Li-C-D interactions that were manifest in the photoelectron spectrum energy range at ~532.9 eV and 291.2 eV, respectively [3].

Recent atomistic simulations have corroborated the above experimental observations and show that several mechanisms contribute to deuterium retention in a graphite (carbon) matrix with oxygen and lithium present. In particular, oxygen-deuterium bonding is the dominant mechanism when the oxygen content is comparable to that of lithium, with lithium playing a catalytic role of attracting oxygen to the surface. The experiments show that the surface oxygen content increases from ~5% on virgin graphite to >10% after lithium deposition, and >40% following deuterium irradiation in ultra-high vacuum. This dramatic increase in surface oxygen is due to two ion-induced mechanisms: surface mixing to liberate reactive lithium for molecular oxygen gettering, and ion-enhanced bulk-to-surface oxygen segregation. *In-situ* D-irradiation experiments are conducted in the PRIHSM facility at Purdue University capable of measuring the surface composition and chemistry evolution as a function of deuterium fluence and lithium content. Systematic studies will also be presented that connect these laboratory experiments to explain observed plasma behavior in fusion devices.

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