Deuterium retention enhancement in lithiated graphite plasma-facing surfaces in fusion devices

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Lithium conditioning has been adopted in a number of magnetic confinement devices resulting in significant effects on plasma performance. In NSTX for example effects include: reduction of ELMs, reduced edge neutral density, increased pedestal electron and ion temperature, and improved energy confinement [1]. The main assumption conjectured for the effects observed in NSTX plasmas is the retention of hydrogen by coatings of lithium on ATJ graphite tile surfaces. The main binding channel understood to be the ionic lithium hydride bond. However, the likelihood that the dominant retention mechanism is governed by lithium-hydride bonding seems less probable based on well-known intercalation effects of lithium in graphite. The observed effects on plasma behavior in NSTX, despite the strong chemical interaction of D, Li, O and carbon, indicate an enhanced mechanism for retaining hydrogen in addition to Li-D binding. This paper summarizes the key mechanisms understood today of enhanced hydrogen retention in lithium-treated ATJ graphite surfaces. The mechanisms are elucidated by four major efforts: 1) controlled in-situ off-line experiments at Purdue [2,3], 2) post-mortem NSTX tile analysis, 3) in-vacuo PMI probe data in NSTX, and 4) computational quantum-based atomistic simulations. Results show that a saturation limit of D pumping by lithium conditioning of ATJ graphite surfaces is reached in a few number of shots. Computational modeling using semi-empirical quantum mechanics of electrons and classical mechanics of nuclei elucidate on the polar-covalent interactions that emerge between lithium and the C-D-O system.