

Surface Chemistry, Retention and Sputtering of Solid Li, Li-O and C-Li-O surfaces, irradiated by D and D₂

P. S. Krstic¹, B.E. Koel², and F. J. Dominguez-Gutierrez³

¹*Institute for Advanced Computational Science, Stony Brook University, Stony Brook, NY 11794-5250, USA*

²*Department of Chemical and Biological Engineering, Princeton University, Princeton, New Jersey 08544, USA*

³*Max-Planck Institute for Plasma Physics, Boltzmannstrasse 2, 85748 Garching, Germany*

Lithium coatings evaporated on a variety of metallic and graphitic surfaces in over ten tokamak fusion machines around the world, has provided evidence of the sensitive dependence of plasma behavior on lithiated plasma facing surfaces [1]. Thus, in NSTX, Li evaporation decreased the H-mode access power threshold, increased the stored energy and allowed longer plasma discharges than for the plasma-facing walls with no Li conditioning [4]. These improvements have been associated with the reduction of impurities and with the reduction of fuel recycling with the formation of Li-O-D complexes.

Our computational studies, a combination of molecular dynamics, quantum physics and computational chemistry modeling [2], extend in spatio-temporal scales not accessible by empirical means and therefore opens the opportunity for a systematic approach at irradiation surface science studies of the plasma-material interface for NSTX and LTX fusion machines. We present our recent theoretical and validating experimental results on the complex surface chemistry processes that evolve from lithium conditioning on plasma-facing materials [3,4,5]. We discuss in details the effects of the lithium coatings at oxidized carbon surfaces to the retention of deuterium and sputtering of the plasma-facing surfaces. The critical role of oxygen in the surface chemistry during hydrogen-fuel irradiation is found to drive the kinetics and dynamics of these surfaces as they interact with fusion edge plasma that ultimately could have critical effects on fusion plasma confinement behavior. The effects of the surface temperature to the retention of deuterium of lithium and lithium-oxide surfaces is also studied [6]. Finally, we report novel data for sputtering, retention and reflection when solid lithium surfaces are irradiated with deuterium atoms and molecules in a wide range of impact energies.

1. M Lucia, R. Kaita, R. Majeski et al., *J. Nucl. Mater.* **463**, 907 (2015).
2. P. S. Krstic, J.P. Allain, C.N. Taylor, et al., *Phys. Rev. Lett.* **110**, 105001 (2013).
3. C.N. Taylor, et al., *Journal of Applied Physics* **114**, 223301 (2013).
4. F. J. Domínguez-Gutiérrez and P. S. Krstić. *J. Nucl. Mater.* **492**, 56 (2017).
5. P.S. Krstic, et al., *Mater and Radiation Under extremes* **2**, 165 (2018).
6. L. Buzi et al, *J. Nucl. Mater.*, **502**, 161 (2018).

PSK and BEK acknowledge support for this work of the U.S. Department of Energy, Office of Science/Fusion Energy Sciences under Award Numbers DE-SC0019308, and DE-SC0013752 (PSK). FJDG acknowledges funding from the A. von Humboldt Foundation for a research fellowship. Calculations were done using the SeaWulf cluster of the IACS/SBU.