Studies of lithiumization and boronization of ATJ graphite PFCs in NSTX-U

Theory: *F. J. Dominguez[1] and P. S. Krstic[1]*
Experiment: *F. Bedoya[2], J. P. Allain[2], A. L. Neff[2], and K. Luitjohan[3]*
[1]*Institute for Advanced Computational Science, Stony Brook University, New York, USA.*
[2]*Departament of Nuclear, Plasma and Radiological Engineering, University of Illinois, Urbana, IL, 61801.*
[3]*School of Material Engineering, Purdue University, West Lafayette, IN 47907 .*

Motivation:

In the newly upgraded National Spherical Tokamak Experiment (NSTX-U), wall conditioning using lithium and boron provide one method for fuel density control. Prior computational modeling coupled with in-situ surface characterization of lithiated graphite have elucidated critical mechanisms that drive deuterium retention at the plasma- facing surface. This work examines the role of lithiumization and boron conditioning on ATJ graphite surface and its effect on deuterium retention.

Approach:

*In-situ studies include x-ray photoelectron spectroscopy (XPS) and used to examine B treatment of lithiated and non- lithiated ATJ graphite for irradiation energies between 100-1000 eV/amu for moderate fluences up to $10^{19}cm^{-2}$.The Materials Analysis Particle Probe (MAPP) is an in situ characterization device for diagnosing samples exposed to fusion reactors.

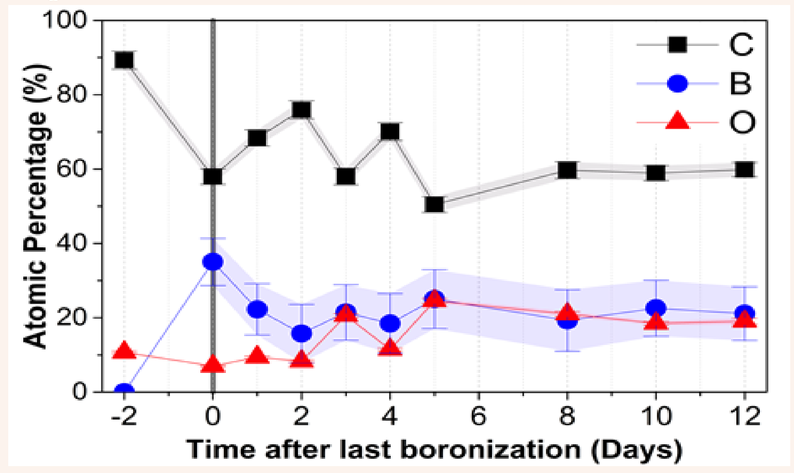
*MD simulation of the B-C-O surfaces bombarded by D to elucidate role of boron, oxygen and deuterium concentrations in the B-C-O-D chemistry. We use CMD with LAMMPS-ReaxFF and QCMD based on SCC-DFTB

Theoretical Method

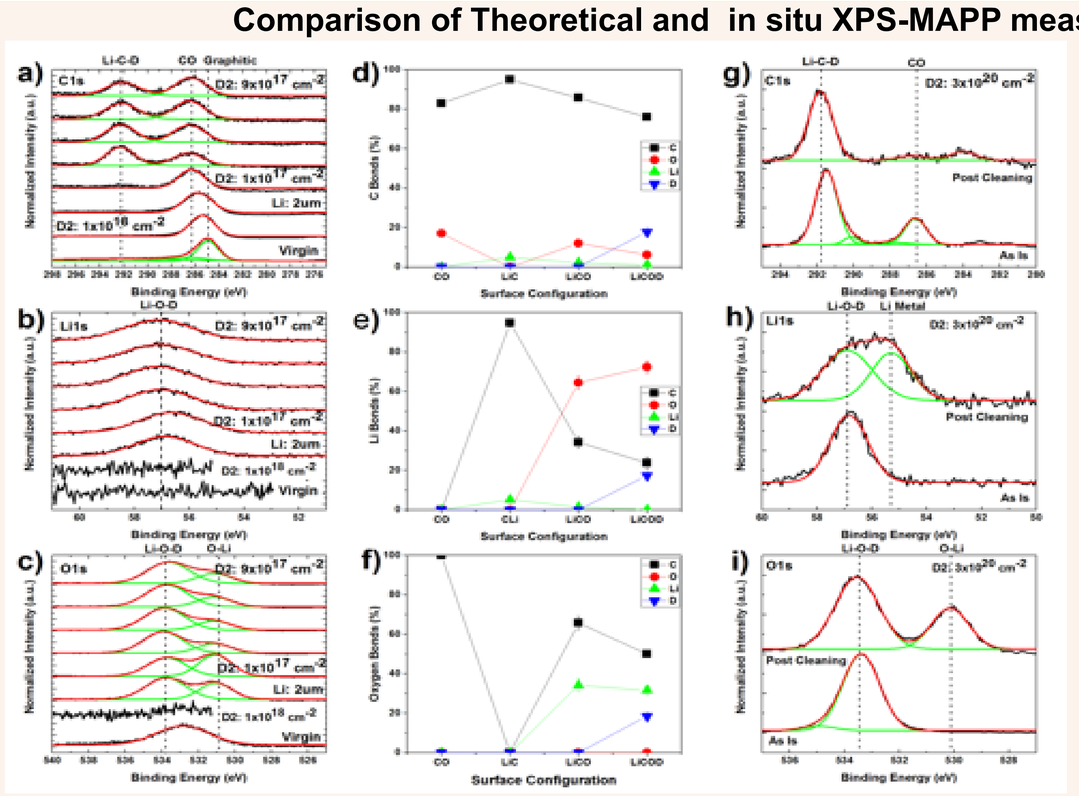
C, CO, (Li)BC, and (Li)BCO mixed surfaces with over 400 atoms are energy-optimized and thermalized to 300 K, prepared by cumulative irradiation of D when needed. The surface is then bombarded by more than 3000 D atoms of 5 eV energy, homogeneously varying its impact localization over the surface cell.

We use the reactive force field (REAXFF) of Van Duin in the CMD LAMMPS code with embarrassing parallelization. Periodic surface boundary conditions are applied. The CMD results are verified with QCMD (based on SCC-DFTB), obtaining full qualitative agreement.

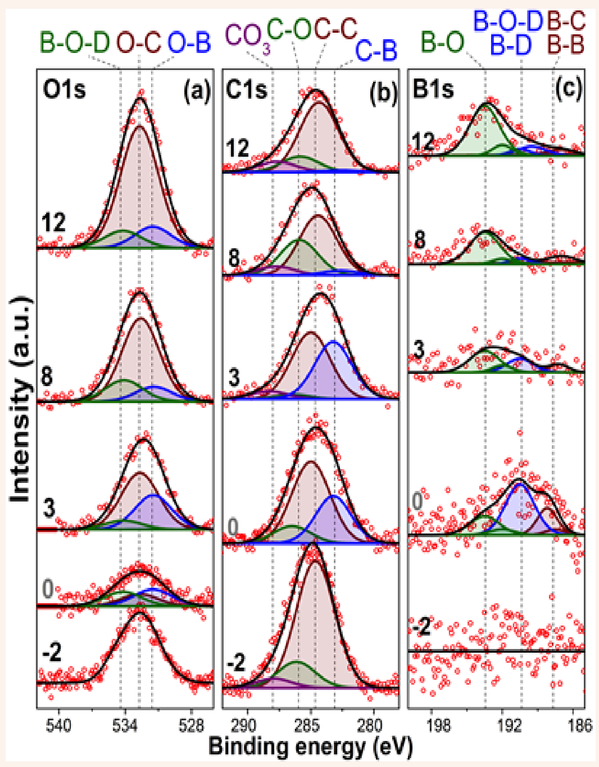
In calculations above we used 20%B, 20%O, and 60% of C: Agree well with the measured concentrations



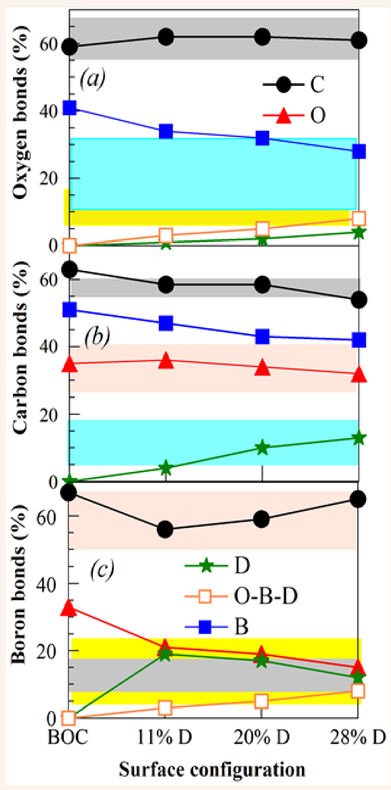
Comparison of Theoretical and in situ XPS-MAPP measurements: (Li-)B-C-O Surface.



a)-c) *In situ* XPS results from controlled D irradiation for the C 1s, Li 1s, and O 1s regions. g)-i) *post mortem* XPS of samples exposed at DIFFER of the same regions. d)-f) The simulation results of the oxygen, carbon and lithium chemistry for various configurations, CO, LiC, LiCO, LiCO, and LiCOD

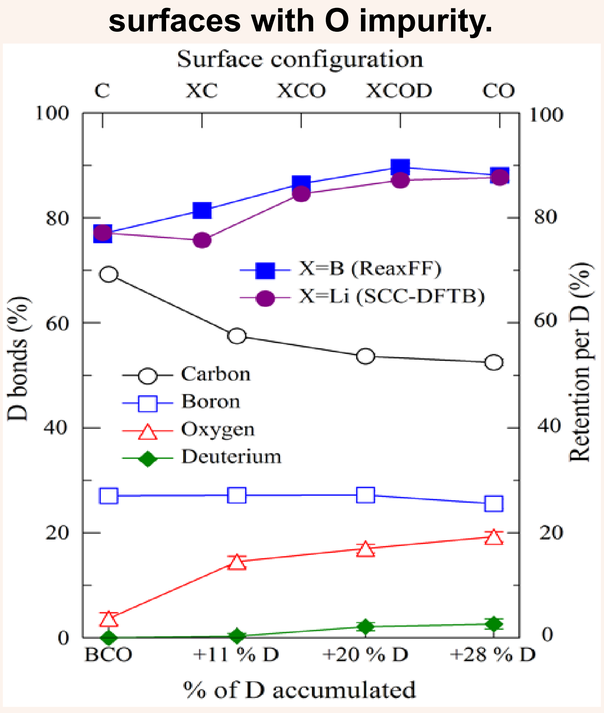


(*a*) O1s, (b) C1s, and (*c*) B1s XPS spectra from boronized ATJ graphite for various days of deuterium plasma exposure.



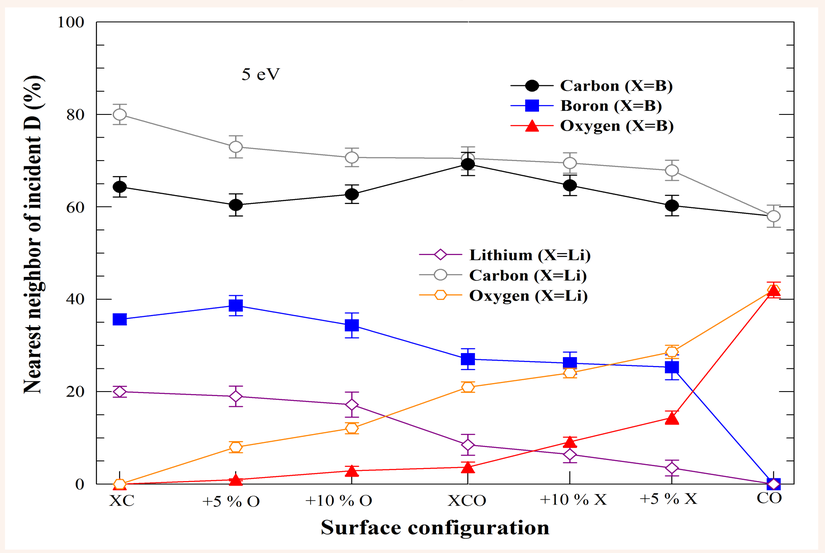
Bonds of (a) O, (b) C, and (c) B to other constituents in the BCOD as a function of D concentration in the upper sample 0.75 nm .

D Retention predictions for boronized surfaces with O impurity.

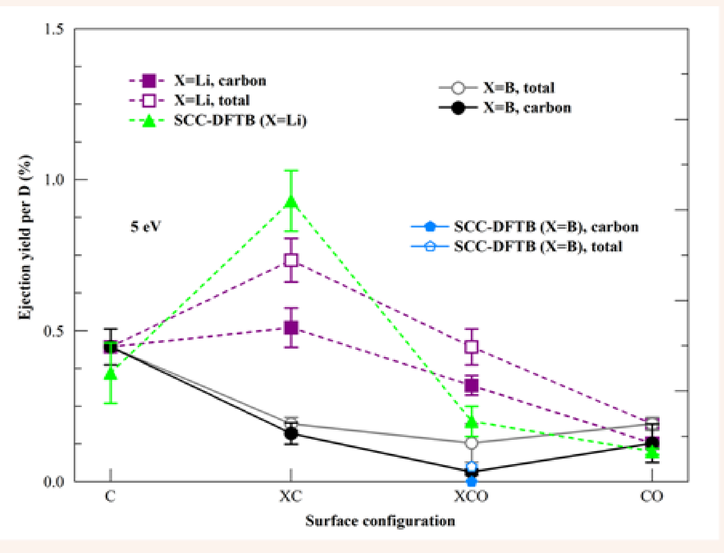


Percentage of D bonds with constituents of the deuterated BCO surface as function of D accumulated concentration (left axis). Total retention per impact of D (%) on BCOD and LiCOD (right axis).

Comparison between lithiated and boronized CO surfaces

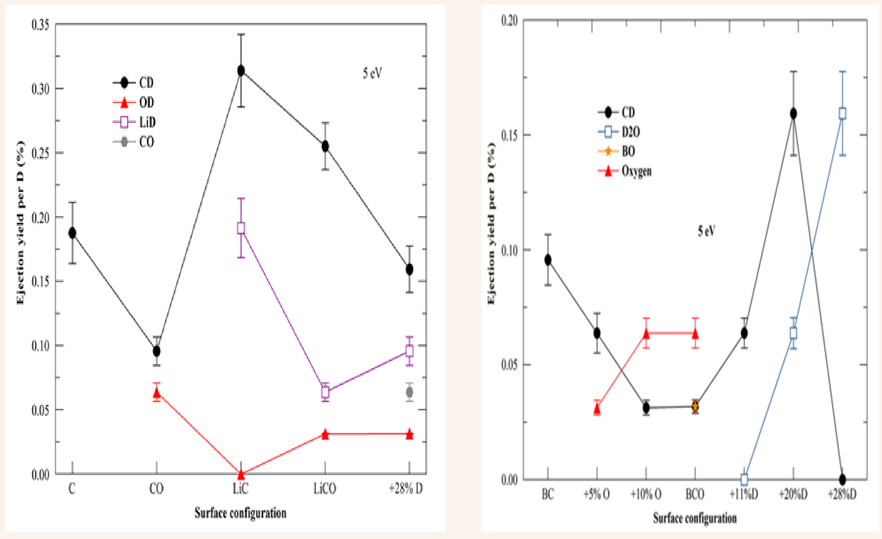


Nearest neighbor distance (%NN) to the final rest location of incident D as function of the surface configuration. Considering non-cumulative case for the LiCO and BCO configurations at 5 eV.



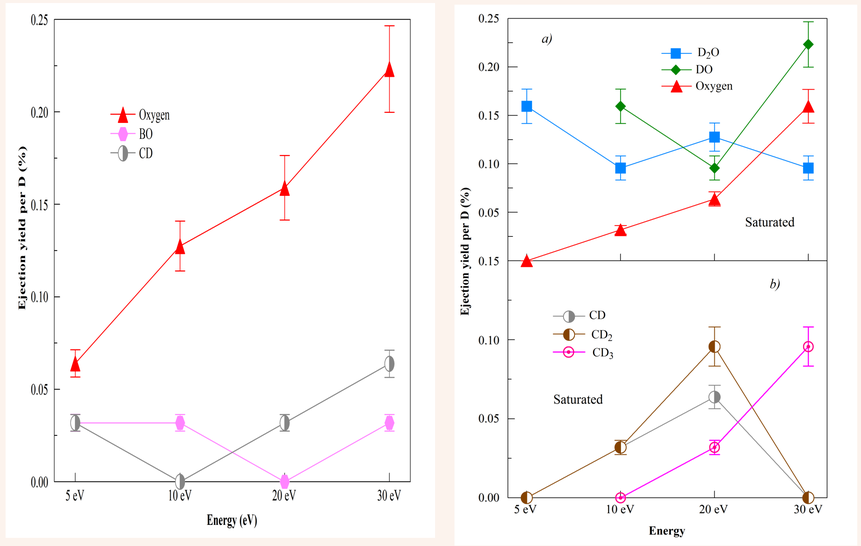
Total and C ejection yield per D for various surfaces configurations and comparing different methods of calculation (CMD with ReaxFF and QCMD with SCC-DFTB).

Analysis of sputtering process for different surfaces



Ejection yield per D (%) for different molecules

Sputtering process in BCO at different energies



Non-cumulative system

Cumulative system

Conclusions

- Retention of D by O in BCO surface significant only after accumulated D, because D binds to O binding partners (often B) and destroy their bond to O, making room for O-D.
- Bonding of D to carbon decreases somewhat with D fluence, since C is more flexible in its coordination number.
- Boron in general is more reactive than carbon because of octet rule (coord. number 4 preferred). Also electron withdrawing ligands ro B such as O further increase D uptake on B. Boron sometimes has coord. number 5.
- Sputtering yield per D significantly smaller in BC than in LiC surfaces

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References: [1] P. S. Krstic et al, Phys. Rev. Lett. 110, 105001 (2013).[2] C. N. Taylor et al. Phys Plasma 21, 057101 (2014). [3] A.C.T. Van Duin et al, J. Phys. Chem. A 114, 5485 (2010). [4] J. Winter, Plasma physics and controlled fusion 38, 1503 (1996). [5] F. J. Dominguez et al. J. Nucl. Mat and Ener. (submitted) (2016).