NSTX Advanced Lithium etc. Plasma/Surface Interaction (PSI) Modeling: Supercomputing and Code/Data Integration Needs/Ideas

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NSTX-U Theory & Computation Brainstorming
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Some Past NSTX Li etc. PSI Modeling

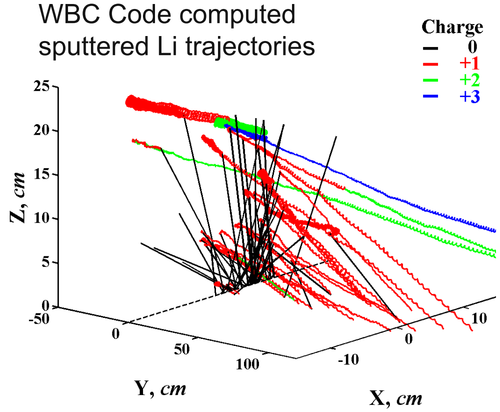
- Liquid Lithium Divertor (LLD) plasma/surface interaction analysis

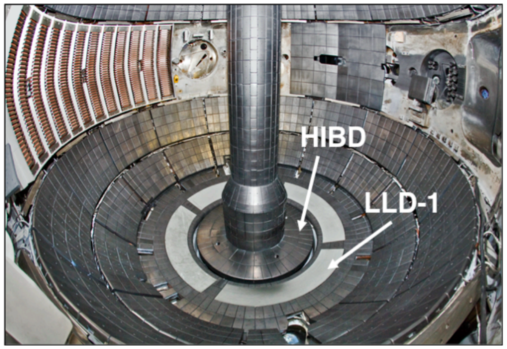
[J.N. Brooks, J.P. Allain, T.D. Rognlien, R. Maingi., J. Nuc. Mat. 337-339(2005)1053]

[J.P. Allain, J.N. Brooks, Nuclear Fusion 51(2011)023002]

  - *static liquid lithium response, low-D recycle (UEDGE/Stotler et al.) plasma*

WBC Code computed sputtered Li trajectories





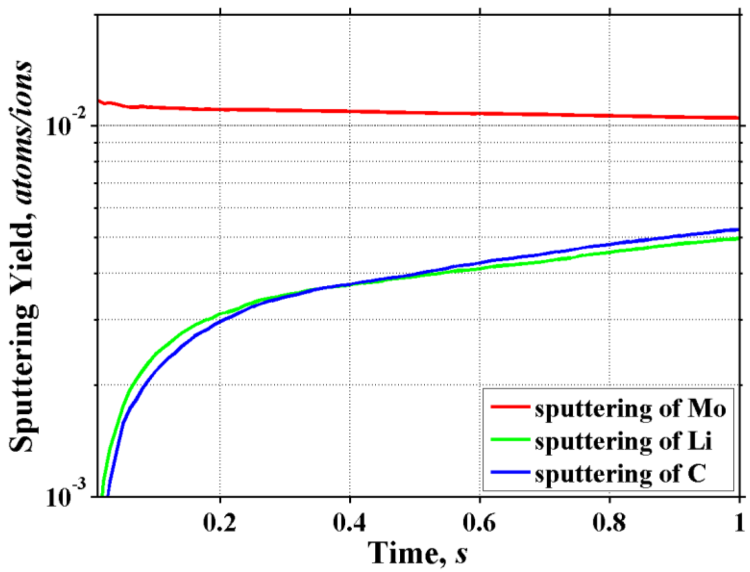
- **Lithium Inner Divertor (HIBD)**
  - *static (pure) liquid Li or solid Li surface, high D-recycle plasma (SOLPS/B2-IRENE, Canik et al.)*

[J.N. Brooks, A. Hassanein, T. Sizyuk, J.P. Allain, 2nd Inter. Symposium on Li applications for Fusion Devices, PPPL, 4/11, Fus. Tech. t.b.p.]

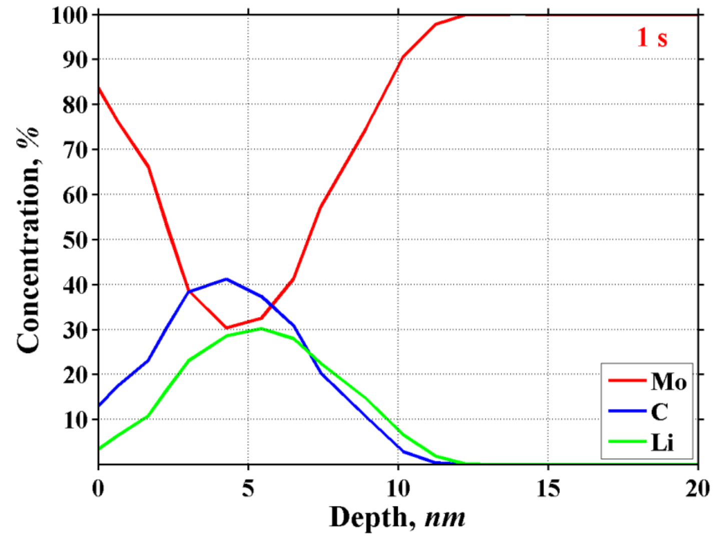
- **Molybdenum Inner Divertor and mixed material analysis**:
  - Li + C on Mo inner divertor, high-D-recycle plasma
    surface evolution: composition and sputtering

(ibid. and continuing)

ITMC-DYN analysis (ibid): Time dependent sputtering of NSTX Mo inner divertor (at strike point); with D, 1% C, 1% Li impingement



Time dependent sputtering



Spatial distribution of the deposited C and Li impurities in Mo substrate; at 1 second.

- Substantial carbon and lithium sputtering occurs by end-of-shot
- C and Li surface contamination extend to ~10 nm, by end of shot
- C and Li concentrations peak at ~ 5 nm depth and about equal the Mo concentration

Why do we need advanced modeling? #1

Lithium is the 2nd most complex surface material we have modeled (carbon is first due to chemical sputtering):

- D trapping/pumping—highly dependent on surface content/structure
- High vapor pressure
- Temperature dependent sputtering & evaporation
- Material-mixing issues: e.g. Li intercalation in carbon
- Liquid vs. solid issues
- Most (~2/3) sputtering is Li^+ ions
- Li^+ ion redeposition in sheath and re-emission at surface

Why do we need advanced modeling? #2

Specific Concerns for NSTX analysis: *Much more difficult to model than future devices*

--- Transient conditions: ~1 second pulse

--- Small device–edge/boundary effects dominate

--- Lithium is not a flowing liquid (i.e., is static liquid or solid)

--- Many materials present (C, Mo, etc.)

--- Non-standard boundary conditions

Major need for ***code/data validation***; in particular with advanced near-surface plasma diagnostics for background plasma parameters and sputtered Li atom/ion density.

Idea

- **Integrated Petascale Simulation of Plasma Facing Materials Response to Normal and Transient Fusion Plasmas** (SCIDAC proposal, Purdue, LLNL, LBL, ORNL, PPPL, ANL)

- Implement and couple 7 major codes/packages on Petascale machine to create and use two integrated advanced simulation packages for predicting the 1) *normal plasma response* (SUPER-REDEP) and 2) *transient plasma response* (SUPER-HEIGHTS), of candidate PFC materials and components.

- REDEP/WBC material erosion/redeposition package
- ITMC-DYN dynamic material response code
- QCMD-MC molecular dynamics codes
- UEDGE-BOUT plasma edge solution codes
- DEGAS2 plasma neutrals code
- HEIGHTS transient plasma material response package
- ALE-AMR transient bulk material response code

SUPER-REDEP Application to NSTX-U

- Predict D retention/recycling, Li contamination, and plasma evolution, for a lithium surface that is evolving with surface impurities and "slag" during NSTX shot operation. Use massive increase in computing speed (~10^5 cores), with coupled codes, and with advanced binary-collision and molecular dynamics material response codes. Assess wide range of plasma solutions via multi-dimensional, coupled, self-consistent simulations.

- A SUPER-REDEP simulation for NSTX would typically involve ~100 spatial points @ 10,000 sputtered particle histories per point, totaling ~10^6 histories for one time step. For order of 1000 time steps and 10 plasma conditions (e.g. with variable D recycling coefficient, plasma heating power, and magnetic field topology) an NSTX material assessment will involve some 10^{10} particle histories.

- Code/data validation is a vital need—to be performed as NSTX-U data becomes available.