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Modeling of plasma/lithium-surface interactions in NSTX: Status and key issues☆

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ABSTRACT

We are studying lithium sputtering, evaporation, transport, material mixing, and surface evolution for the National Spherical Torus Experiment (NSTX) for various surfaces and plasma conditions. Lithium modeling is complex, particularly for NSTX short pulse, multiple material, variable plasma conditions. Cases examined include: (1) liquid lithium divertor (LLD) with planned high heating power/low-D-recycle plasma, (2) non-pumping/high-recycle solid or liquid divertor surface, (3) Li and C impingement on a molybdenum surface. An impurity erosion/redeposition code package is the overall integration tool, with sputter yield and velocity distributions from binary collision mixed-material codes, sheath code input for NSTX boundary conditions, and inputs of plasma edge solutions from external data-calibrated plasma fluid codes. Analysis predictions are generally favorable, showing non-runaway lithium self-sputtering, acceptable net erosion (~5 nm/s), and moderate edge (~10%) and core plasma (~0.1–1%) Li contamination, for the cases studied. A Mo divertor surface is significantly affected by C and Li impingement but with low core plasma contamination predicted for a high-recycle edge plasma.

1. Introduction

The National Spherical Torus Experiment (NSTX) has made major use of lithium containing plasma facing surfaces, e.g., as discussed in [1], and this will apparently continue. Both evaporated/deposited and static liquid surfaces have been used. Lithium can control particle recycling via deuterium trapping, and at least in liquid form, can be used for high heat removal. *Flowing* liquid lithium is a promising surface material for future fusion devices such as a fusion nuclear science facility or DEMO. Accordingly, we have been analyzing lithium plasma surface interactions in NSTX; to understand the basic science, to aid the NSTX mission, and to improve predictive modeling for future applications.

A detailed surface interaction analysis has recently been done [2] for the NSTX static liquid lithium divertor (LLD) with planned high core plasma heating power, and using a high D trapping "low recycle" edge plasma solution [3]; this follows earlier work [4]. We have now analyzed the important case of a non-D trapping Li surface with resulting high-recycle edge plasma, and we compare this to the LLD results.

We report here also on initial erosion/redeposition and material-mixing analysis for the planned molybdenum inner divertor surface subject to carbon and lithium impingement.

2. General issues for NSTX lithium surface interaction analysis

Lithium surface response and near-surface transport is highly complex, second only to carbon with chemical sputtering. Key issues include high ion sputter fraction (~2/3 ions) with sputtered ion sheath-caused redeposition and subsequent surface re-emission, high vapor pressure, complex chemistry with D and C, and strong temperature dependent sputtering including self-sputtering. Our understanding and present models for some of these issues is discussed in [2,4].

Paradoxically, modeling of Li in NSTX is more complicated than for future tokamak application, due to NSTX having a solid surface or static liquid surface with likely major difference in surface performance/evolution between static and flowing liquid states, short plasma pulses with variable heating, high surface to volume ratio, possibly different sheath structure, and use of multiple surface materials (Li, C, Mo).

NSTX has large carbon plasma facing surfaces, e.g., first wall, with typically observed 1–2% core plasma carbon content; C effect on Li surfaces is thus a major consideration. It appears, however, that a ~2% C flux to a liquid Li surface would not significantly affect the LLD response, for planned 1 s high power shots [2]. We are continuing analysis of C effects on Li, including for very high C fluence, with both binary collision and molecular dynamic codes, and will report on this in the future.

An overriding issue for NSTX is D/Li pumping. A carbon surface intercalated with Li may or may not have significant D pumping, and likewise for a static liquid Li surface depending on C, D fluence,

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Table 1
WBC NSTX lithium divertor sputter erosion/redeposition analysis summary for two edge plasma regimes (100,000 histories/simulation).

Parameter	Low-recycle plasma case[a]	High-recycle plasma case
Location/surface-condition	Outer divertor/LLD; with high D pumping	Inboard divertor/HIBD; nominally C and/or Mo, but with assumed low-D-pumping Li coverage[b]
Plasma solution/D^+ reflection coefficient	UEDGE $R = 0.65$ [Stotler et al.]	SOLPS $R \sim 1$ [Canik]
Peak electron temp. at divertor, eV	247	57
Peak electron density at divertor, m^{-3}	5×10^{17}	3×10^{20}
Sheath structure/width	Debye-only (~1 mm)	Magnetic + Debye (~2 mm)
Ionization mean free path[c], mm	64	0.77
Transit time[d], μs	36	1.4
Charge state[d]	1.06	1.00
Incidence (elevation) angle[d], ° from normal	19	15
Energy[d], eV	406	38
Sputtered Li current (atoms, effective)[e], /D^+ ion current to divertor, s^{-1}	$1.43 \times 10^{20}/1.98 \times 10^{21}$	$6.12 \times 10^{21}/4.31 \times 10^{22}$
Fraction from self-sputtering	.10	.07
Fraction redeposited on divertor	.55	.99
Fraction to core plasma[f]	.09	<.005
Core plasma Li contamination potential	~1%	<0.1%

[a] Values from Ref. [2] analysis.
[b] 300 °C surface assumed for D and Li on Li sputter yields.
[c] Normal-to-surface; for sputtered Li atoms ionized in divertor region.
[d] Average for redeposited Li ions on respective divertor.
[e] Includes sputtered atoms, and sheath-reflected sputtered ions re-emitted as atoms from surface.
[f] At ~20 cm from the LLD surface and within the UEDGE or SOLPS grid.

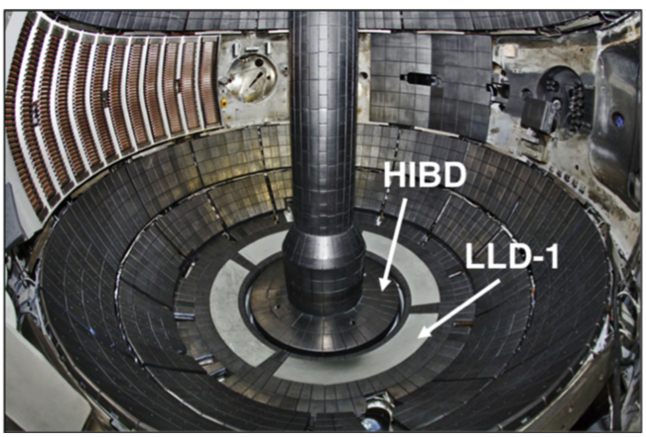

Fig. 1. NSTX lower boundaries showing liquid lithium divertor (LLD) and Horizontal Inboard Divertor (HIBD) locations. Li, Mo, and C surfaces are analyzed for HIBD.

Li thickness, and other factors. It is thus important to examine Li surfaces for a range of plasma conditions.

3. Lithium divertor surface with high D-recycle plasma

3.1. Geometry and plasma

The NSTX Horizontal Inboard Divertor (HIBD) is shown in Fig. 1, along with the LLD. The HIBD surface is currently carbon, but a replacement (~outer half) with molybdenum is planned. With either base material, a Li surface layer could be created e.g., by pre-shot Li evaporation, and/or by in-shot Li transport from the LLD. We examine a presumed non-pumping Li surface on the HIBD, and also C and Mo surfaces. A plasma solution with outer strike point located on the HIBD, for a typical magnetic field configuration and with high-recycling boundary condition, was furnished by Canik [5] using the SOLPS fluid code and EIRENE Monte Carlo neutrals code. In contrast to the LLD low-recycle solution the predicted edge plasma temperatures are much lower ($T_e \sim 60$ vs. 250 eV at the strike point), with much higher plasma density (~×100). We use the REDEP/WBC code package, with sputter yields/distributions from TRIM-SP and ITMC binary collision codes, to compute sputter erosion/redeposition, and with SOLPS 2D scrapeoff layer (SOL) plasma parameters (density, ion and electron temperature, electric field, plasma flow velocity), such computational method described more fully in [2] and references therein.

A fixed surface temperature of 300 °C is used for the present HIBD Li calculations. Sputter enhancement is small at this temperature and evaporation is negligible.

3.2. Sheath structure

The plasma sheath affects impurity transport. Boundary conditions at the LLD are somewhat non-standard, with lower B-field (~0.5 T), and less tangential angle (~5–10° to the surface) than most tokamaks. A Debye-only sheath was predicted [2] for these conditions, as opposed to the usual dual structure (Magnetic + Debye) sheath (both however with similar sheath potential $e\Phi/kT_e \sim 3$). For the inner divertor the typical plasma discharge has a higher and more tangential B-field (~1 T @ 3°), and with smaller Debye length and D^+ gyroradius. The BPHI code [6] was run for these conditions. It was found that the dual structure sheath obtains, and this model is used for WBC-HIBD calculations. (A caveat is that while an ad hoc Bohm type ion particle diffusion model, with 1 m^2/s diffusion coefficient, is included in the BPHI calculation, it is not clear how a *rigorous* turbulence treatment would affect the analysis. Turbulence distorts in-sheath ion gyro-rotation, and thus ion transport to the surface. This may be important due to the NSTX low field/large D^+ gyroradius—it is not a significant concern, e.g., for ITER with ~5 T field. This issue is beyond the scope of this paper but needs analysis.)

3.3. Lithium erosion

Table 1 compares selected lithium sputter erosion/redeposition results for the low and high plasma recycle cases. Although the cases differ in divertor location, this is secondary compared to the plasma differences.

Sputtered Li transport is closely confined to the near-surface region for the high-recycle case, due to much higher plasma electron density, faster ionization of Li atoms, and stronger collisions with the inflowing plasma. Divertor redeposition is accordingly higher and transport to other regions is lower. For both cases sputtered Li current is of order 10% of the impinging D^+ current—this

Table 2
Erosion/redeposition performance comparison of three surface materials. NSTX inner divertor, high-recycle plasma regime.

Parameter	Carbon	Molybdenum	Lithium
Ionization mean free path[a], mm	5.3	0.72	0.77
Gross erosion rate, typical, nm/s	20	15	200
Net erosion rate, typical, nm/s	2	0.5	5
Core plasma contamination potential[b]	$<2\times10^{-3}$	$<5\times10^{-5}$	$<1\times10^{-3}$

[a] Normal-to-surface; for sputtered atoms ionized in divertor region.
[b] Numerical bound.

yields a moderate Li/D ion density ratio of like order 10% in the near-surface plasma. Self sputtering comprises about 10% of the total sputtering. (We note that Li sputtering would increase substantially for design conditions with higher surface temperatures, particularly 400 °C or higher.)

A key issue for any surface material is core plasma contamination due to divertor sputtering. This depends on the sputtered current reaching the edge/core plasma boundary and on subsequent core plasma transport. The contamination *potential* is given by the ratio of edge/core boundary impurity current from the divertor to D^+ current from the core, and is a good estimator of core impurity fraction for many core transport cases. Such Li contamination is seen to be very low for the high-D case, and higher but still tolerable for the LLD case.

4. Material erosion comparison

Table 2 compares sputtering performance of lithium with molybdenum or carbon HIBD surfaces. In addition to a D^+ flux the Mo calculations use data and model-derived characteristic NSTX impinging ion fluxes of 1% C^{+3} and 1% Li^{+2}—these species actually do most of the Mo sputtering, with self-sputtering also occurring. The Mo results are for the pure metal; initial material mixing/evolution analysis is discussed in the next section.

Both Li and Mo sputtered atoms are ionized close to the surface—for Li and Mo due to high electron impact ionization rate coefficients, and also for Mo, the high mass/low sputtered atom speed. As per Table 2 results, carbon and molybdenum have similar gross erosion rates, with Mo net erosion lower than C due to a higher redeposition fraction. For Li the gross erosion rate is high but with net erosion a factor of ∼50 lower due to high redeposition.

Due to some numerical and model-coupling issues (e.g., re. use of the fluid plasma solution with the kinetic WBC calculations), the present calculations can reliably define upper bounds only, for the contamination potential, for very low values of the latter. As per Table 2, carbon contamination is similar to lithium and is an order of magnitude less than the ∼1–2% observed core carbon fraction typical of NSTX shots. This suggests, but is not conclusive, of major carbon contamination arising from non-inner-divertor surfaces (e.g., inner first wall). For Mo the bound seen here is an order of magnitude less than C or Li.

5. Dynamic surface evolution during NSTX discharge

Surface erosion due to sputtering and resulting dynamic surface composition is modeled using the ITMC-DYN code, a new dynamic version of the HEIGHTS-ITMC [7] package. ITMC-DYN is a binary collision approximation (BCA) code which considers elastic and inelastic interactions of ions and atoms in compounds. The dynamic part of the code takes into account changes in target composition as result of various time-dependent processes occurring simultaneously during ion beams deposition and interaction with target materials. The code is being developed for detailed investigation of plasma material interaction in a multiple/mixed materials environment. Code models consider processes of multiple and simultaneous ion penetration and mixing, scattering, reflection, physical and chemical sputtering of composite materials, dynamic surface evolution, thermal diffusion, hydrogen isotope molecular recombination, and surface segregation. The package allows tracking of time-dependent dynamic changes in surface erosion/growth rate, material composition and structure, and temperature dependent effects.

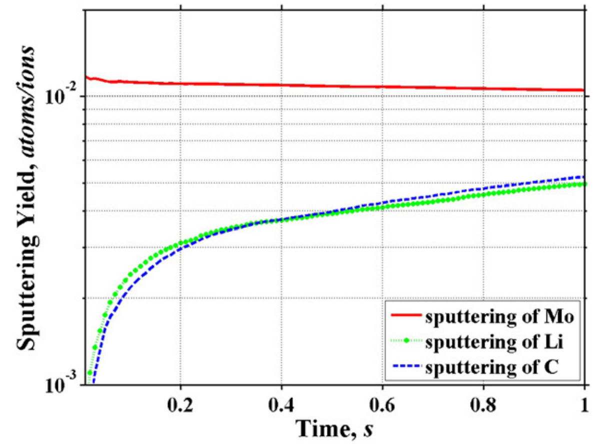

Fig. 2. ITMC-DYN computed time dependence of sputtering (due to D, 1% Li, and 1% C) yields of Mo and the deposited C and Li.

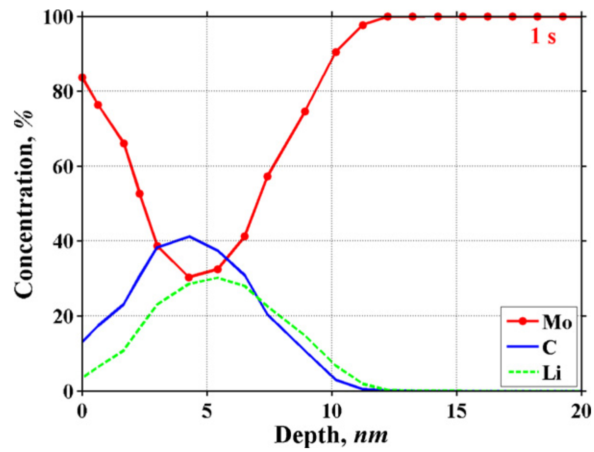

Fig. 3. ITMC-DYN computed spatial distribution of the deposited C and Li impurities in Mo substrate after 1 s.

ITMC-DYN calculations are made for the NSTX HIBD Mo surface. Typical input parameters at the high-recycle plasma inner divertor strike point are used, using SOLPS and WBC-derived parameters, with *D* flux of 10^{23} m^{-2} s^{-1} at incident energy of 200 eV, containing carbon impurities of 1% with incident ion energy of 700 eV, and 1% of 450 eV lithium ions. (These energies result from pre-sheath thermal and plasma flow kinetic energy plus sheath acceleration). The NSTX discharge time is taken as 1 s. Surface temperature is assumed to be 900 K (operating temperatures are not fully known but can be higher for Mo than for Li). The diffusion coefficient of D in pure Mo for such temperature is $\sim10^{-8}$ m^2/s [8]. For more accurate future analysis the diffusion of D in a *mixed* Li/C/Mo component should be taken into account.

Fig. 2 shows the time dependence of the sputtering yield of Mo and the deposited C and Li over the 1 s discharge time. Initially, the surface is pure Mo and then continues to be enriched in C and Li.

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This results in a decrease in Mo sputtering yield and an increase in the sputtering yield of C and Li. A steady state surface concentration of Mo, C, and Li is not yet reached at the end of the discharge. Fig. 3 shows the spatial distribution of the deposited C and Li impurities in Mo at the end of the discharge. The surface contamination from C and Li extends up to 10 nm and the C concentration peaks at about 5 nm beneath the surface and exceeds that of the Mo concentration.

A next obvious but major step would be coupled, self-consistent, computations of material evolution from the ITMC-DYN code with WBC calculations of sputtered impurity transport, and for the entire divertor surface.

6. Conclusions

Analysis of lithium erosion/transport in NSTX is important but highly complicated. We have analyzed this subject with code packages for full-kinetic sputtered lithium transport and mixed-material sputtering, and using characteristic plasma SOL solutions for low and high D recycling. We note the uncertain nature of all results due to the stated complexity of lithium/NSTX modeling and general issues in plasma predictive modeling.

The above qualification notwithstanding, an NSTX high-recycle inner divertor lithium surface is predicted to work well—from the sputtering and evaporation standpoint, as is the LLD system with characteristic low-recycle plasma solution. In general, a Li surface (solid or liquid) has high erosion but low core plasma contamination potential.

A molybdenum surface can be substantially changed, in 1 s, by C and Li impingement. Mo core plasma contamination potential appears to be low, due to low sputter yields and high local redeposition for the high-recycle plasma regime.

Desirable future analysis would involve: (1) additional plasma cases—such as effect of a low-recycle LLD plasma on inner divertor plasma/surface interactions, (2) self-consistent material-mixing/erosion–redeposition calculations (via supercomputing), and (3) various data-validated model refinements.

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