Erosion/redeposition analysis of lithium-based liquid surface divertors

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Abstract
A sputtering erosion/redeposition analysis was performed for three candidate tokamak fusion reactor liquid divertor surfaces—lithium, tin–lithium (Sn80Li20), and flibe (LiF + BeF2 salt). The analysis uses coupled edge-plasma, impurity-transport, and sputtering codes (UEDGE/WBC/VFTRIM), and available sputtering data. A pure-lithium surface strongly absorbs impinging D–T ions—this results in a high temperature, low density, (≈200 eV, ≈1 × 1019 m⁻³) low-recycle plasma edge regime. Lithium appears to perform well in this regime. Although overall sputtering is high, self-sputtering is finite. Most (≈95%) of the sputtered lithium is confined to the near-surface region and redeposited on the divertor with the remainder (≈5%) also being redeposited after transport in the scrape-off layer. Lithium core plasma contamination is low (≈10⁻⁵ Li/D–T). Tin–lithium and flibe would likely operate in a high-recycle regime (e.g., 30 eV, 3 × 10²⁰ m⁻³). Erosion/redeposition performance of these materials is also good, with finite self-sputtering and negligible core plasma contamination predicted, but with some concern about changing surface composition due to different constituent element redeposition distances. © 2001 Published by Elsevier Science B.V.

Keywords: Erosion; Redeposition; Lithium

1. Introduction
Flowing liquid surfaces for fusion reactors mitigate sputtering and disruption lifetime concerns, but there are remaining concerns about self-sputtering runaway, plasma contamination, tritium codeposition in far-transported solidifying material, and overall edge-plasma/surface compatibility. As part of the US ALPS project [1] we are assessing these issues for several materials. In this study we report on initial analysis for three lithium based liquids. This analysis covers sputtering erosion issues; follow-up studies using detailed engineering designs and including MHD issues, thermal issues, etc., are planned.

2. Pure lithium surface
2.1. Method
The UEDGE fluid plasma code [2] is used to compute an edge plasma solution for an ITER-type reactor with a vertical divertor [3] flowing liquid lithium surface and strongly absorbing D–T boundary conditions. The UEDGE calculation for the outer half of the scrape-off layer (SOL) is done with 100 MW power input from the core, core/SOL boundary D–T density of 4 × 10¹⁹ m⁻³, and particle and energy diffusion coefficients of D = 0.33 m²/s, D_e = D_i = 0.5 m²/s. We use a D–T ion recycling coefficient at the lithium divertor, R = 0.5, representing an initial rough estimate based on high hydrogen solubility in lithium and high removal capacity due to constant replenishment of the surface by flow. (The plasma solution is not strongly dependent on R for roughly R ≤ 0.75.)

Next, the WBC kinetic impurity transport code [4] is run using the UEDGE plasma solution, with angular
and energy dependent $D^+$ and $Li^+$ on D-saturated liquid Li sputtering coefficients, and sputtered velocity distributions, from VFTRIM code [5] calculations calibrated to available data [6]. (For this study, $T_+^+$ sputtering of pure lithium was taken equal to $D^+$ sputtering). We use a two-layer (Li, D-saturated Li) smooth-surface (fractal dimension = 2.00) model, with empirically adjusted binding and bond energies. Lithium atoms are launched in WBC with an energy distribution based on a binding energy of 1.1 eV, as best fits the data of Ref. [6], and well matches PISCES physical sputtering data [7]. Also used for lithium are ADAS [8] density-dependent collisional radiative electron impact ionization rate coefficients. Both UEDGE and WBC were run with magnetic field $B = 5$ T at 33° poloidal angle to the divertor plate. (There are differences in total angle and sheath heat transmission models between UEDGE, WBC, and other work e.g., [3], and these need further resolution. Limited tests with UEDGE and WBC for low recycling show that changes in the poloidal angle results primarily in the plate peak heat flux varying inversely with the wetted area, while the amount of impurities escaping upstream is relatively insensitive to this angle.)

WBC computes the self-consistent, near-surface (0–5 cm from the plate) transport of D–T sputtered and self-sputtered lithium. The computed lithium flux escaping the near-surface region is then used as a lithium source for a further run with UEDGE, to compute lithium transport over the whole SOL.

2.2. Results

The reference UEDGE plasma solution is shown over the SOL in Fig. 1 and at the ~40 cm wide divertor plate in Fig. 2. Peak electron temperature at the plate is 185 eV – in striking contrast to much colder high-recycle regimes. The plasma density and temperature profiles in the entire SOL are fairly constant along poloidal flux surfaces, and thus the high temperature/lower density extends upwards to the SOL/edge plasma boundary. This

Fig. 1. Electron temperature contours in the outer scrape-off layer for the UEDGE plasma solution with low-recycle liquid lithium divertor.
The WBC/UEdge lithium erosion/redeposition results are summarized in Figs. 4 and 5, and Table 1. In spite of high redeposited Li⁺ energies and generally oblique incidence, self-sputtering is limited, comprising some 25% of the total. Of the total sputtered lithium current, ~95% is locally redeposited via near-surface impurity/plasma transport processes, ~5% leaves the near-surface region but returns to be redeposited after SOL transport, and ~0.2% enters the private flux region or hits the first wall. Lithium is thus mostly confined to

![Fig. 2. Plasma density and temperature profiles at the lithium divertor plate.](image)

![Fig. 3. Sputtering data [6] and VFTRIM-3D code calculations for oblique incidence D⁺ and Li⁺ on D-saturated lithium.](image)

![Fig. 4. Gross and instantaneous (before liquid flow) net erosion rates from the WBC analysis of the lithium divertor. (Net erosion rate with flow is zero.)](image)

![Fig. 5. WBC/UEdge computed lithium density along a poloidal field line midway in the scrape-off layer (~15 cm from the separatrix on the plate).](image)
the near surface region. A liquid surface has, of course, zero net erosion on the time scale of the liquid flow, however, gross and instantaneous (i.e., before liquid flow) net erosion rates are shown (Fig. 4) for comparison to previous solid-material studies. These rates are high, but due to the continuous replenishment, of apparently limited significance.

Fig. 5 shows the combined WBC/UEEDGE computed lithium density along one poloidal field line in the SOL. As mentioned, the codes are coupled at 5 cm perpendicular to the plate or 8 cm along the poloidal field line. The trends seen in Fig. 5 are similar for other field lines. The lithium concentration is about 0.2 Li/D–T near the surface but falls off very rapidly away from the plate, reaching a very low value at the top of the tokamak and along the entire edge/SOL boundary. This implies low core plasma contamination by sputtered lithium.

An additional UEDGE/WBC run (not shown) made with a 50% lower core density boundary condition-possibly needed to mitigate D–T refueling concerns shows similar acceptable low sputtered lithium transport to the core but significantly higher transport to the private flux region. Such higher transport might require keeping all surface temperatures above the lithium melting point (181°C) to prevent tritium from codepositing in solidifying lithium regions. This should not be difficult.

3. Flibe and tin–lithium

3.1. Method

Flibe (Li₂BeF₄) and tin–lithium (Sn₆₀Li₄₀), even though containing lithium, should not significantly pump D–T, due to very low hydrogen solubility. They will typically operate in a ‘conventional’ high recycle regime with recycling coefficient R close to unity. Analysis of these materials is complicated due to their multi-component nature. We use at present a simpler plasma model in WBC, namely a uniform plasma with typical high recycle plasma parameters of $T_e = 30$ eV, $N_e = 3 \times 10^{20}$ m⁻³. (Future plans are to do a more sophisticated coupled WBC/UEEDGE analysis.)

The complete sputtering coefficient matrix for flibe, i.e., with all partial yields of F, Be, Li, for incident bombardment by D⁺, T⁺, Li⁺, Be⁺, and F⁻, is computed with VFTRIM-3D for molten salt flibe. A bond energy of 6.0 eV is used for both LiF and BeF₂ [9,10]. This is justified based on the chemical state of molten salt flibe as consisting of LiF and BeF₂ components.

The analogous sputtering matrix for tin–lithium is supplied from TRYDIN (self-sputtering) and TRIM.SP (D–T sputtering) calculations [11]. Tin–lithium is assumed to be non-segregated, i.e., with no Li overlayer. Experiments [11] do show segregation at a low surface temperature (200°C) but not at high temperature (800°C), with data needed at intermediate temperatures. (Also, data are needed to assess possible thermally enhanced emission, e.g., due to macroscopic emission – the present calculations are for non surface temperature dependent physical sputtering only.)

Ionization rate coefficients from ADPAK (Sn) [12], Bell et al. and Lennon et al. (Be, F) [13,14] were used in WBC. WBC computed the near-surface transport of all sputtered elements of the respective materials, with self-consistent sputtering based on the angular and energy dependent sputter yield matrices, and the redeposited ion velocities.

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**Table 1**

Selected erosion/redemption parameters from WBC analysis of three liquid divertor surfaces

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Lithium (pure)</th>
<th>Tin–lithium</th>
<th>Flibe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plasma conditions at divertor; Te</td>
<td>Variable 185⁺</td>
<td>30/3</td>
<td>30/3</td>
</tr>
<tr>
<td>(eV)/Ne (10⁻³ m⁻³)</td>
<td>0.1 at separatrix</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Binding energy (eV)</td>
<td>1.12</td>
<td>2.40</td>
<td>2.40</td>
</tr>
<tr>
<td>Neutral ionization distancea (mm)</td>
<td>4.6</td>
<td>0.29c</td>
<td>0.15</td>
</tr>
<tr>
<td>Charge state</td>
<td>1.1</td>
<td>1.0</td>
<td>1.5</td>
</tr>
<tr>
<td>Transit time (µs)</td>
<td>15</td>
<td>0.33</td>
<td>0.17</td>
</tr>
<tr>
<td>Elevation angle (°)</td>
<td>53</td>
<td>32</td>
<td>15</td>
</tr>
<tr>
<td>Energy (eV)</td>
<td>238</td>
<td>96</td>
<td>110</td>
</tr>
<tr>
<td>Poloidal distance from launch point (standard deviation) (mm)</td>
<td>70</td>
<td>2.0</td>
<td>1.1</td>
</tr>
<tr>
<td>Redeposition fraction (for 5 cm near-surface-cutoff)</td>
<td>0.950d</td>
<td>1.000</td>
<td>1.000</td>
</tr>
</tbody>
</table>

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a Except where noted denotes average value for redeposited ions.

b Normal to surface.

c Includes effect of high reflected Li component.

d Total redeposition (with SOL transport) = 0.998.
3.2. Results

Non-runaway self-sputtering is calculated for both materials, with very high local redeposition. For flibe, the highest predicted average sputter yield is the F-yielding-F yield of ~0.4-0.6 short of the necessary-condition value of 1.0 for self-sputter runaway. For tin–lithium, the average Li-yielding-Li yield is ~0.75, due in part to a high reflection of lithium from the more massive tin component, but this is also below unity. Figs. 6, and 7 show sputtered ion densities near the divertor surface. These densities are all low compared to the D–T density and fall off rapidly away from the surface. Essentially zero core plasma contamination by sputtering is predicted. There is also negligible transport to the first wall/private flux area. Full-profile plasma effects might be somewhat different.

Table 1 summarizes various redeposition parameters for the flibe and tin–lithium components, and also as mentioned previously, for pure lithium. The sputtered tin–lithium atoms have short mean free paths for ionization, due to a combination of low binding energy (lower sputtered energies), high electron density, and high ionization cross-sections. Much ionization occurs in the magnetic sheath, for these high-recycling plasma conditions. Lithium from flibe behaves similarly. The beryllium and fluorine components travel longer but still fairly short distances. After ionization, subsequent strong collisional friction with the incoming plasma – and particularly for Sn and Li, sheath field acceleration – gives rise to the high local redeposition. The redeposited ion angle and energy parameters suggest data needed from sputtering experiments. For tin–lithium it is significant that redeposited Sn impacts at near-normal incidence, in contrast to the F and Be components of flibe which redeposit at more oblique incidence.

Although short, there are significant differences in component redeposition distances, e.g., for flibe, fluorine travels poloidally about four times as far as lithium. This is due to mass and ionization rate differences. This would definitely affect properties of the redeposited surface for a solid material. The effect, if any, on flowing liquid surface properties will need evaluation.

3.3. Discussion and conclusions

A liquid surface divertor can potentially last the lifetime of a fusion reactor. This study has examined several key plasma surface interaction issues for three candidate liquids. For a hydrogen absorbing pure lithium surface, plasma SOL temperatures are an order of magnitude higher than the usually studied solid material regimes. This may have implications for fusion reactor performance, over and above effects on the divertor itself – an issue being studied for the ALPS project. Lithium sputtering rates are high, but the sputtered lithium is well confined close to the divertor surface with resulting low core plasma contamination. The high confinement is due to high electron-impact ionization rate coefficients, low binding energy/sputtered-velocities, and reasonably high impurity/plasma collision frequencies. Based on WBC code results for redeposited lithium ion energies and impingement angles, and on available data, we predict that lithium self-sputtering is well short of runaway. Helping in this regard is the high hydrogen isotope content expected in the lithium surface [15] which reduces self-sputtering, and the high sputtered ion fraction. Further evaluation is needed for lower density/
higher temperature plasma regimes. Other critical psi issues not examined here but needing analysis for pure lithium are: effect of high tritium removal rates on plasma refueling requirements and helium removal by trapping in the lithium.

An important related psi/engineering issue is the maximum allowable surface temperature. The lithium calculations here are based on code/data results for 200°C. Evaporation/sheath analysis sets an upper limit for lithium of order 500°C [16,17]. A lower limit, however, could be set by thermally-enhanced sputtering rates as possibly seen in PISCES [7] and preliminarily in IIAX, and depending also on the spectrum (e.g., thermal) and form (atom, ion, macroscopic) of the emitted material.

For flipe and tin–lithium we analyzed basic erosion/redeposition performance for a typical high recycle fusion edge plasma, and assuming stoichiometric surface composition. As with pure lithium, the analysis shows high confinement of impurities in the near-surface region with low potential for core plasma contamination, and no runaway self-sputtering. These results are encouraging but more work is needed on, for instance, full plasma profile effects, performance for different plasma edge temperatures/densities, surface temperature effects, surface segregation properties and properties of redeposited material. Sputtering data are also needed.

Acknowledgements

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References

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