Multi-physics modeling of the long-term evolution of surfaces exposed to steady-state plasmas

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Plasma-Material Interactions can cause a wide range of plasma and material degrading effects

- 1\textsuperscript{st} and 4\textsuperscript{th} state of matter do not peacefully co-exist
- Their interaction compromises both material and plasma performance
  - Erosion, heat loads, n-irradiation… reduce PFC lifetime, increase retention
  - Sputtering + inward migration $\rightarrow$ core contamination, impurity accumulation
  - Impurity co- and re-deposition $\rightarrow$ Underperforming mixed materials, enhanced fuel retention
PSI processes involve multiple physics that extend over orders of magnitude in time and length scales.
Multi-physics description is needed to capture the wide range of processes occurring in PSI

- We aim to model
  - long term evolution,
  - surfaces exposed to steady-state plasmas,
  - incl. erosion & sub-surface driven changes
Code integration allows to incorporate multi-physics models needed to describe PSI

- We integrate high fidelity codes targeting multiple physics
  - edge plasma, sheath, impurity transport, irradiation effects, surface thermodynamics…

   to model different scenarios
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• Linear devices experiments of W exposed to
  i. Pure (He) plasma
  ii. Mixed (D-He) plasma

• The ITER W divertor (across several tiles) exposed to
  iii. Pure (He) plasma
  iv. Mixed (D-T-He) plasma
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Focus of the current example
Dedicated experiments exposing W targets to He plasma have been performed in PISCES

- W target exposed to He plasma
  - Biased target ~ 250V
  - 2 pulses: similar $T_e$, different $n_e$
  - Flux $0.25 - 4 \times 10^{22} \text{ m}^{-2}\text{s}^{-1}$
  - $t_{\text{pulse}}$ ~ 5000 – 10000 s
  - ‘low’ substrate temp. (no fuzz)
We use the IPS framework to integrate plasma edge and materials modeling codes

• It’s a HPC interface, supported by the ATOM SciDAC
• Sequentially run codes, file-based integration
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**COMPONENTS**

- EDGE PLASMA
- IMPURITY MIGRATION
- MATERIAL’s MODELING
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![Diagram showing the integration of edge plasma, impurity migration, and material's modeling.

**Components**
- **Edge Plasma**
  - Ne, Te, ...
  - Outgas

- **Impurity Migration**
  - Ne, sheath...
  - Imp. Flux, Ein, Ain...

- **Material's Modeling**
  - Composition, outgas...
  - Ein, Ain, flux ...

**Info flow**
- Ne, Te, sheath...
- Outgas, surf. composition...
- Implantaion profile, Ysp...

**Driver**
- Ne, Te, sheath...
- Ein, Ain, Eout, Aout...
A simplified code integration strategy is sufficient for modeling the PISCES experiment

• Linear machine
  – Only the material evolves (plasma in steady state) → 'one-way' coupling

experimental values for the background plasma

\( n_e, T_e, \text{He flux} \ldots \)
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• Linear machine
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• B-field perpendicular to target
  – Standard sheath models (no coupling with PIC/sheath code)

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GITR
Impurity migration and re-deposition

T. Younkin, 2nd talk this session
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![Diagram showing the integration of FTriDyn, GITR, and Xolotl codes for materials evolution]

**Experimental values for the background plasma**

(ne, Te, He flux...)

**GITR**

Impurity migration and re-deposition

**T. Younkin, 2nd talk this session**

**Materials' Evolution**

- FTriDyn
  - Implantation profile

- Xolotl
  - Material composition
Coupling of materials models is necessary for a complete description of materials’ evolution.

**MATERIALS’ EVOLUTION**

- **FTriDyn**
  - Ion implantation & sputtering
  - *J. Drobný, 3rd talk this session*

- **Xolotl**
  - Evolution of surface height & implanted species
  - *S. Blondel, 4th talk this session*

**Implantation profile**

**Substrate composition**
Flux varies significantly across the surface and is known to impact fuel retention

- Plasma flux ($\Gamma$) can impact the W sputtering yield ($Y_{\text{sp}}$) and He retention
- We used $\Gamma_{\text{max}}$ and $\Gamma_{\text{min}}$ from the PISCES experiment

- Expected output
  - the radial profile of He retention
  - $Y_{\text{sp}}(r)$ → use **average or radial profile of $Y_{\text{sp}}$**
He retention is greatly affected by flux and vacancies are essential to model low fluxes.

- Impact of plasma flux on W sputtering is negligible.

![Evolution of W sputtering yield (by FTridyn)](image)
He retention is greatly affected by flux and vacancies are essential to model low fluxes

- Impact of plasma flux on W sputtering is negligible.

- Large effect on retention

→ introduce vacancies to induce He nucleation at low fluxes

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**He retention, low flux (0.25e4 nm\(^{-2}\)s\(^{-1}\))**

- Initial trapping by He+V → HeV
- Growth of He clusters (until trap mutation)

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**He retention, high flux (4.0e4 nm\(^{-2}\)s\(^{-1}\))**

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Including W re-deposition is an intermediate step in coupling F-Tridyn and Xolotl to GITR

- W re-deposition modeled by GITR
  \[ E_{in}, \alpha_{in}, W \text{ fraction} \]
  \[ T. \text{ Younkin, 2}^{nd} \text{ talk} \]

- F-Tridyn: implantation profile and \( Y_{sp} \) for each \( (\alpha_{in}, f(E_{in})) \)
  \[ J. \text{ Drobny, 3}^{rd} \text{ talk} \]

- Xolotl: implant W as interstitials
  \[ S. \text{ Blondel, 4}^{th} \text{ talk} \]
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- At first glance, little effect on retention
  - Slight increase in surface growth
  - possibly a cumulative effect

\[ \begin{array}{c}
\text{Time [s]} \\
\text{Surface growth [nm]}
\end{array} \]
Need to optimize Xolotl simulations to reach experimental time-scales

• Longer (exp. time-scale, $O(10^4 s)$) simulations are needed to draw conclusions with confidence
  – Cumulative effects will only manifest in long time-scales
  – Effect of (initially important) parameters may be dampened over time

• Xolotl has been run for $10^2$-$10^3$  
  S. Blondel, 4th talk

• Optimization options in Xolotl need to be tested
  – Currently the maximum time-step ($dt_{\text{max}}$) used is $10^{-5}$ s
  – Need to explore solver options: e.g., increase $dt_{\text{max}}$ with fluence (cluster size)
Upcoming code integration steps for modeling more complex (and relevant) scenarios

- To start simulating some interesting physics

Beyond…

- Couple to GITR

- Run to experimental time-scales → introduce roughness  
  J. Drobný, 3rd talk
Upcoming code integration steps for modeling more complex (and relevant) scenarios

- To start simulating some interesting physics
  - Couple to GITR
  - Implement ITER’s geometry, handing mixed (H+He) plasma…
  - Run to experimental time-scales → introduce roughness
  - Introduce H, bubble bursting, simultaneous runs… in Xolotl
  - Comparison to experiment

J. Drobny, 3rd talk
S. Blondel, 4th talk
T. Younkin, 2nd talk
Thank you for your attention!

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