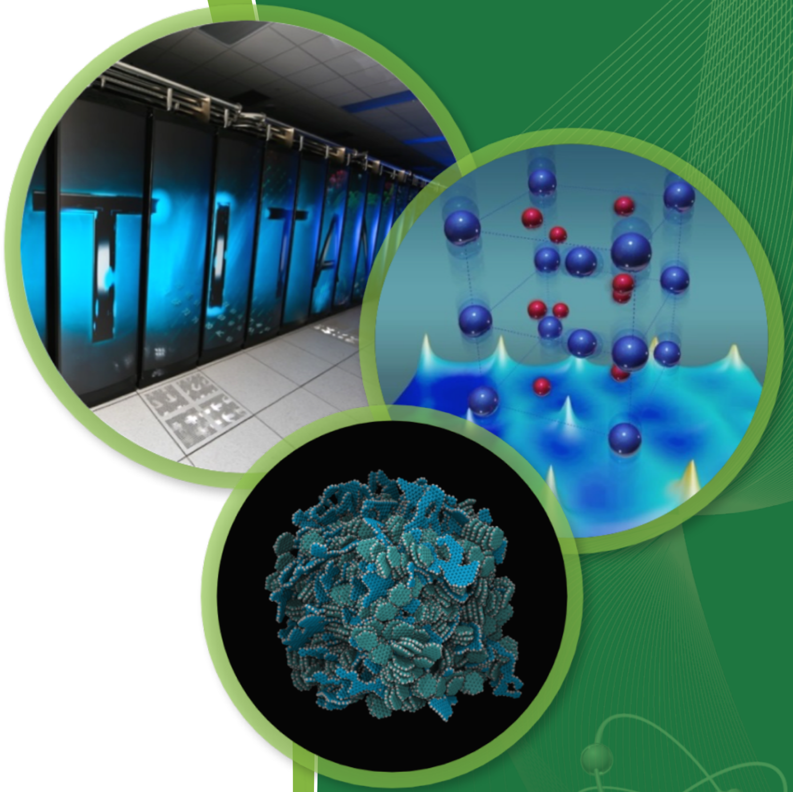
Multi-physics modeling of the long-term evolution of surfaces exposed to steady-state plasmas



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T. Younkin, S. Blondel, B.D. Wirth (UTK)

J. Drobny, D. Curreli (UIUC)

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APS-DPP, Milwaukee, WI, Oct. 26th 2017

ORNL is managed by UT-Battelle
for the US Department of Energy

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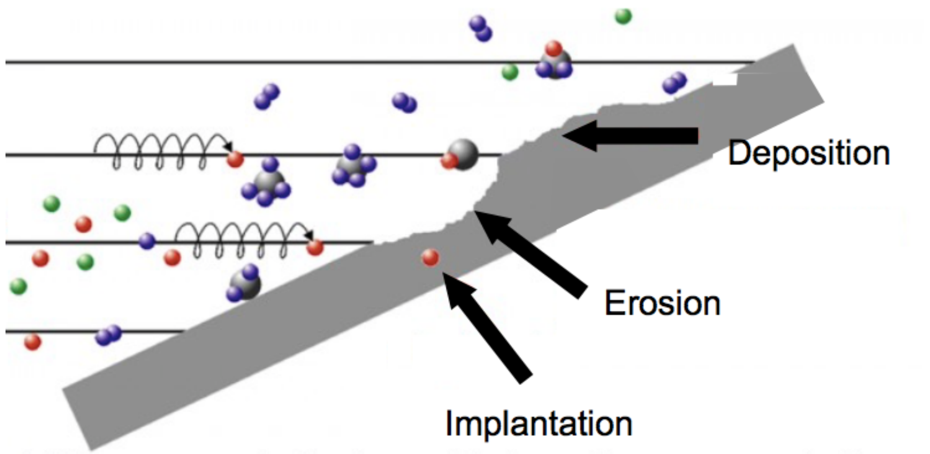
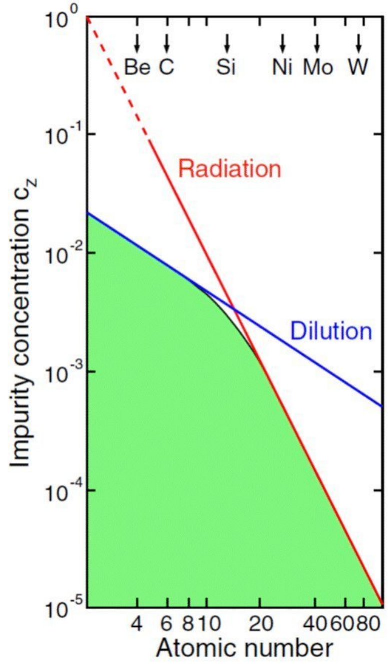
Plasma-Material Interactions can cause a wide range of plasma and material degrading effects

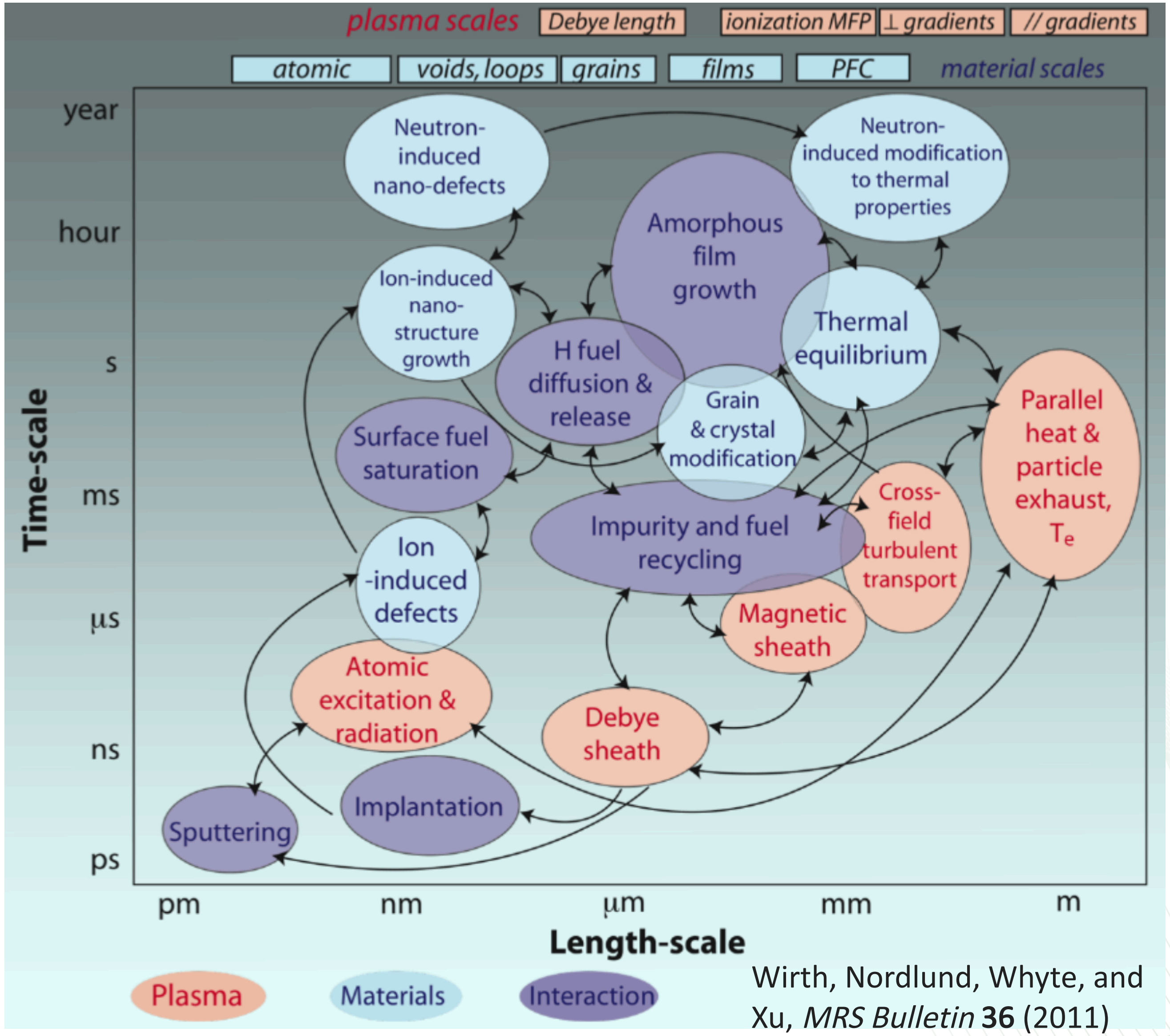
- 1st and 4th state of matter do not peacefully co-exist
- Their interaction compromises both material and plasma performance
  - Erosion, heat loads, n-irradiation… reduce PFC lifetime, increase retention
  - Sputtering + inward migration → core contamination, impurity accumulation
  - Impurity co- and re-deposition → Underperforming mixed materials, enhanced fuel retention





[K. Krieger, IPP]

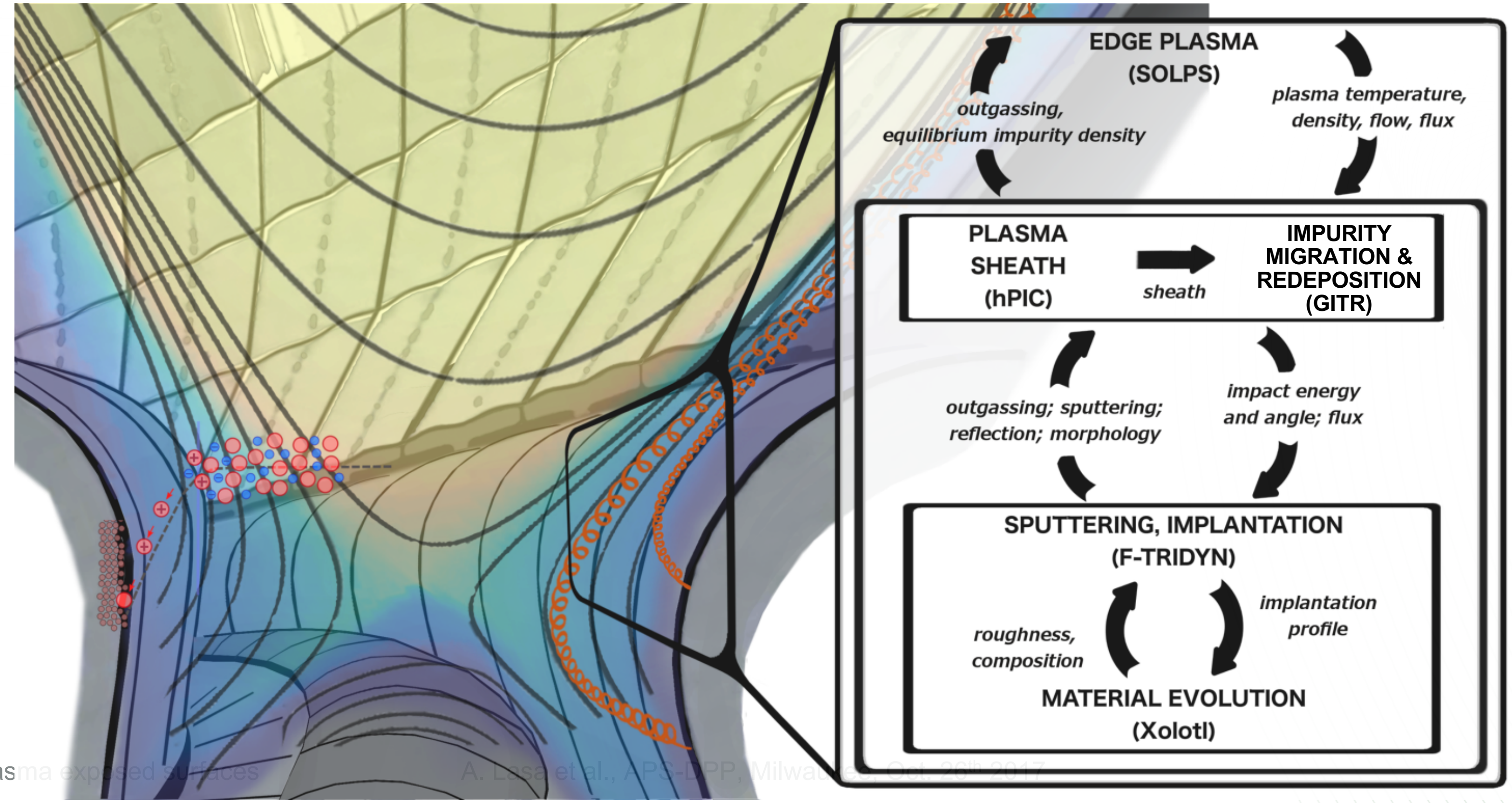
PSI processes involve multiple physics that extend over orders of magnitude in time and length scales



Wirth, Nordlund, Whyte, and Xu, *MRS Bulletin* **36** (2011)

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



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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

COMPLEXITY

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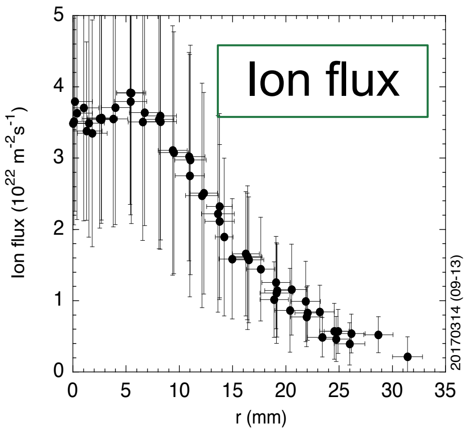
Focus of the current example

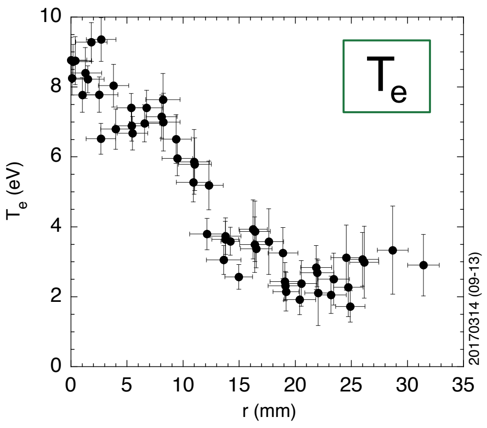
- The ITER W divertor (across several tiles) exposed to
  iii. Pure (He) plasma
  iv. Mixed (D-T-He) plasma

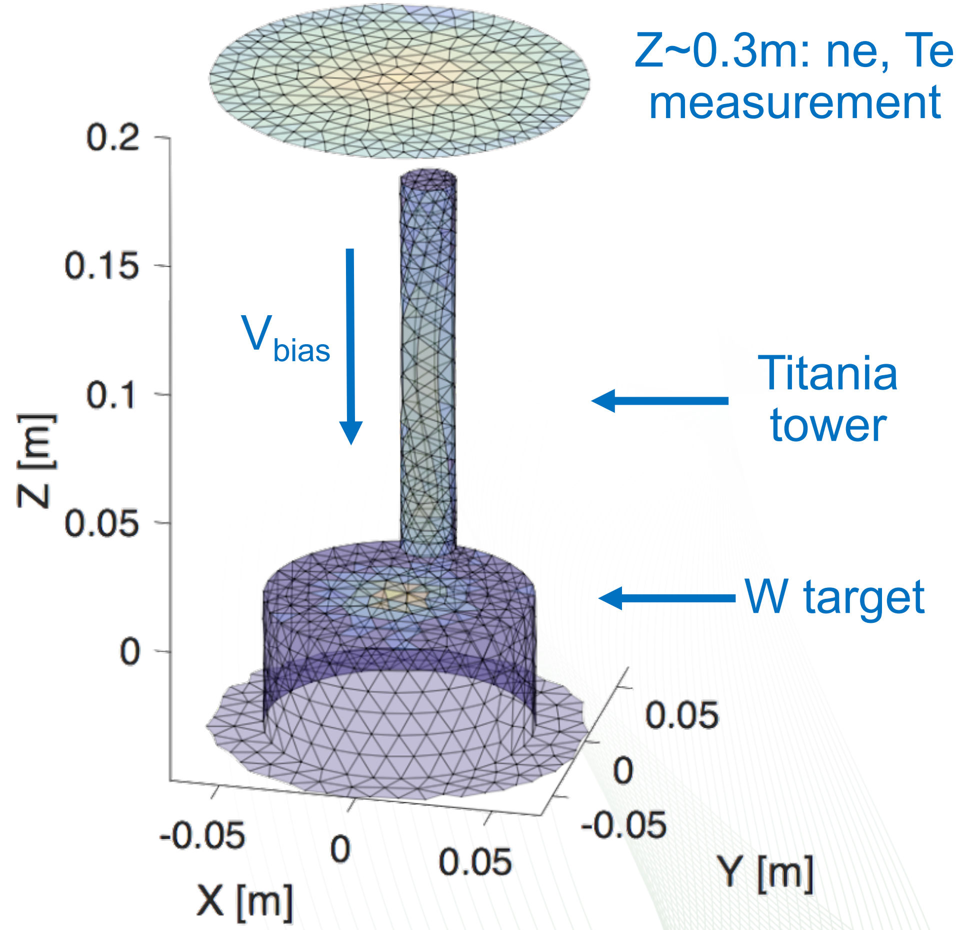
C O M P L E X I T Y

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 10^{22} $m^{-2}s^{-1}$
  - t_{pulse} ~ 5000 – 10000 s
  - ‘low’ substrate temp. (no fuzz)







T. Younkin, 2nd talk this session

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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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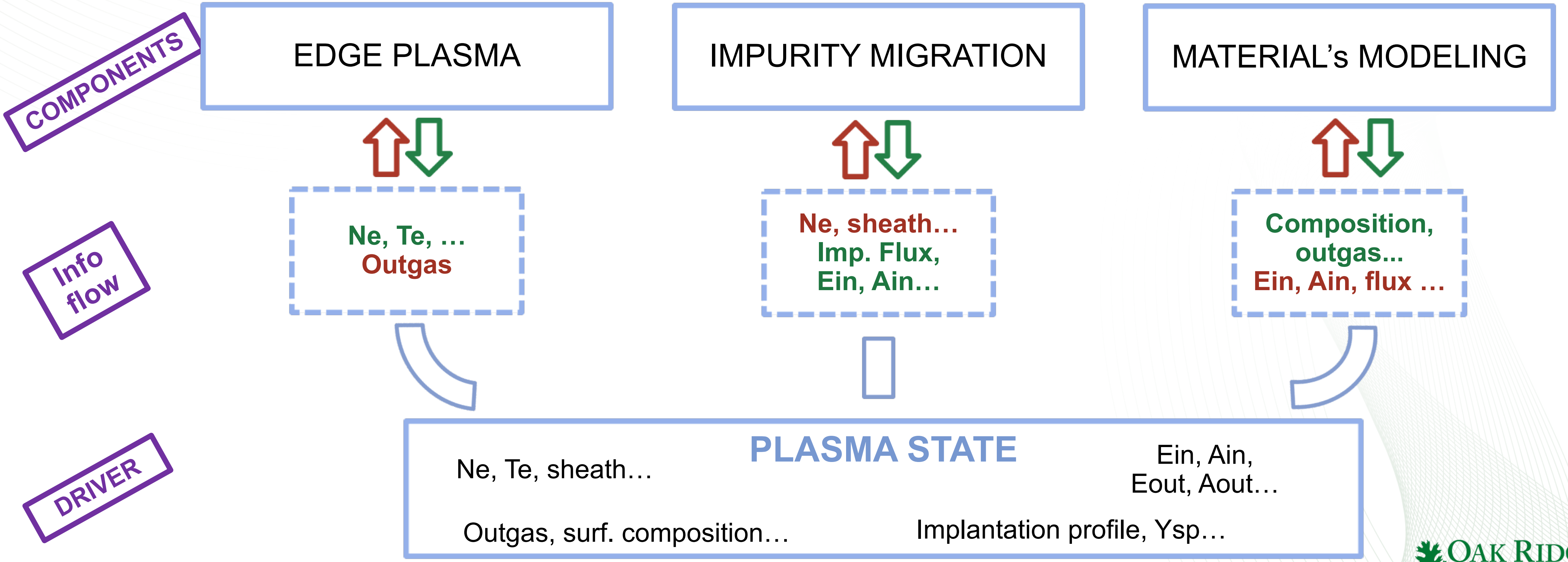

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A simplified code integration strategy is sufficient for modeling the PISCES experiment

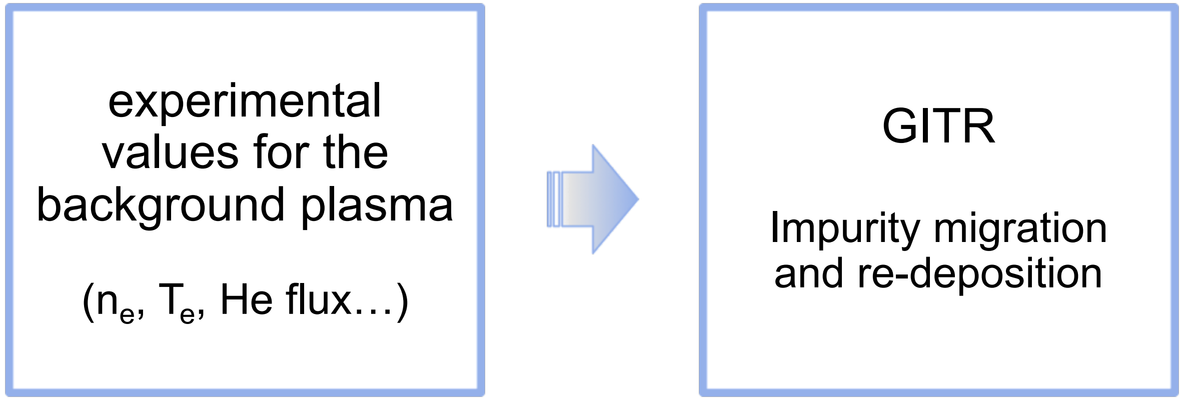
- Linear machine
  - Only the material evolves (plasma in steady state)→ 'one-way' coupling

experimental values for the background plasma

(n_e, T_e, He flux…)

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
- B-field perpendicular to target
  - Standard sheath models (no coupling with PIC/sheath code)



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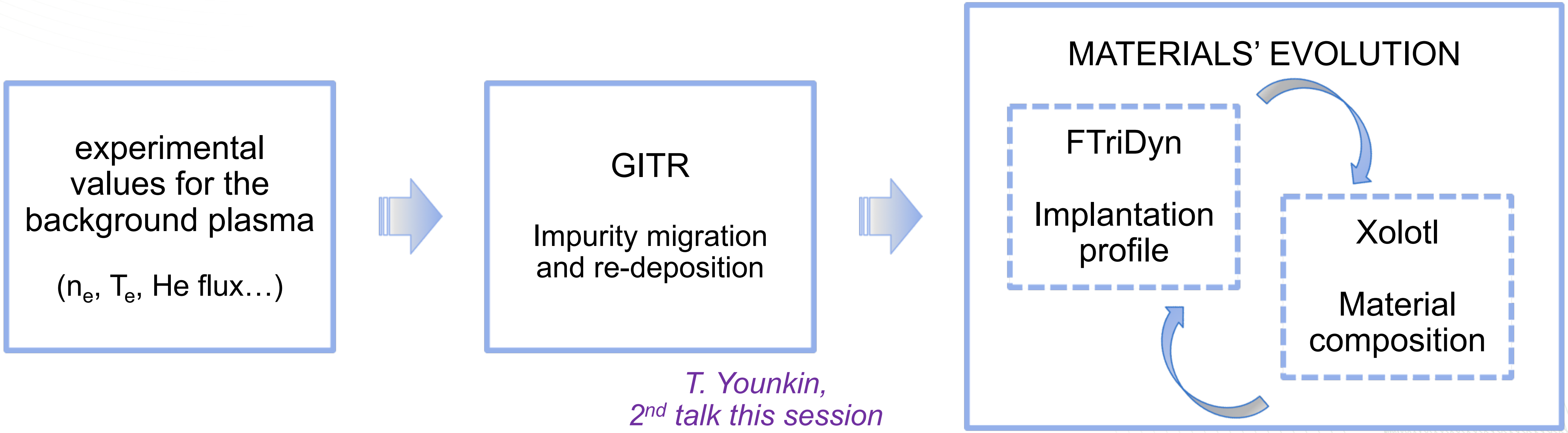


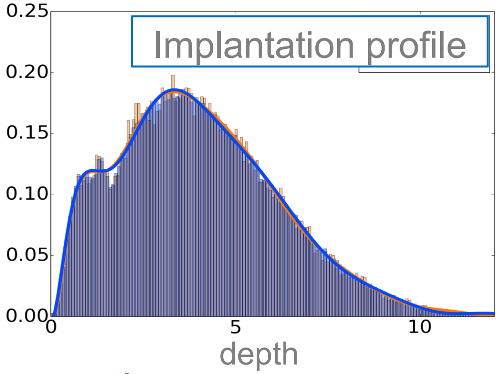
T. Younkin, 2nd talk this session

Coupling of materials models is necessary for a complete description of materials’ evolution

MATERIALS’ EVOLUTION

FTriDyn

Ion implantation & sputtering

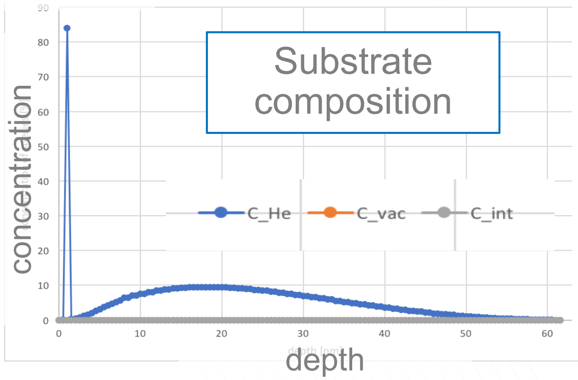


J. Drobny, 3rd talk this session

S. Blondel, 4th talk this session

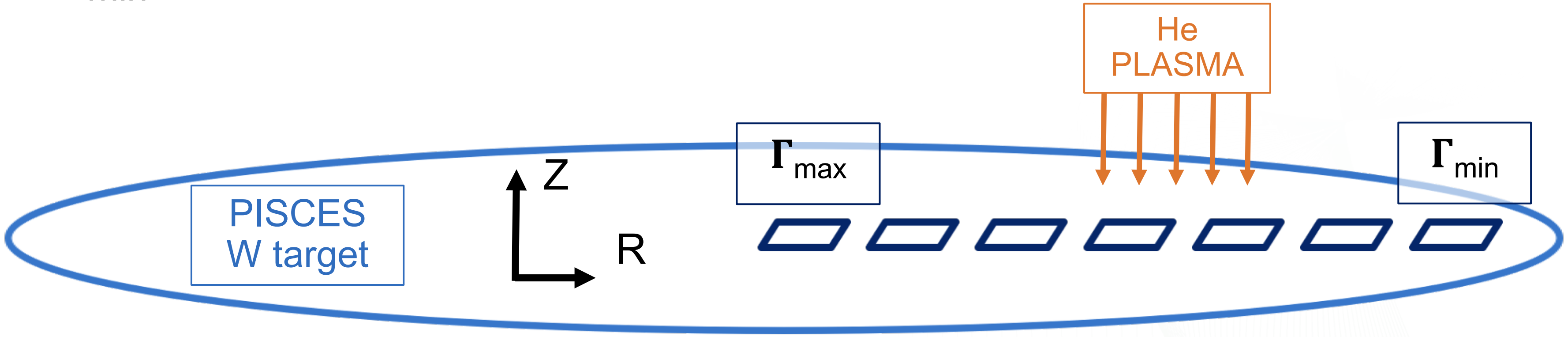
Xolotl

Evolution of surface height & implanted species



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

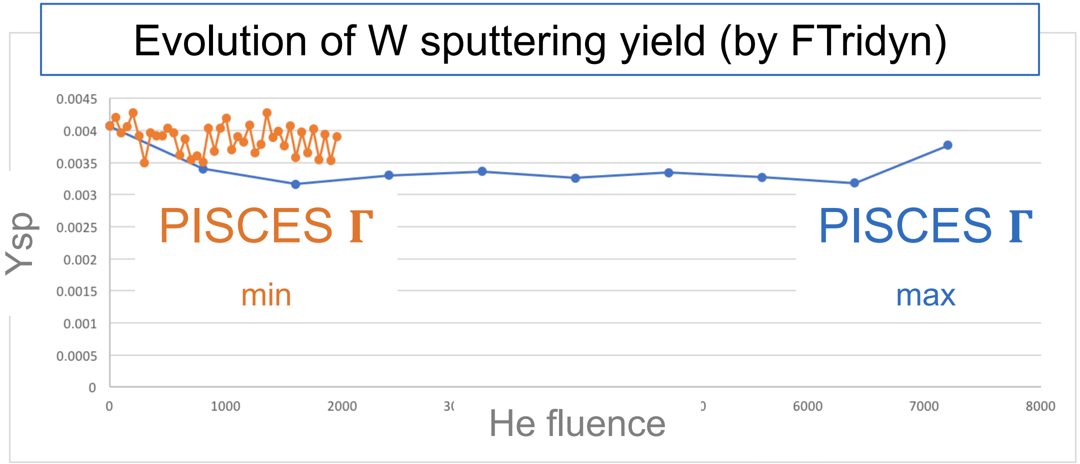
- Plasma flux (Γ) can impact the W sputtering yield (Y_{sput}) and He retention
- We used Γ_{max} and Γ_{min} from the PISCES experiment



- Expected output
  - the radial profile of He retention
  - **Y_{sput}(r)** → use **average or radial profile of Y_{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.



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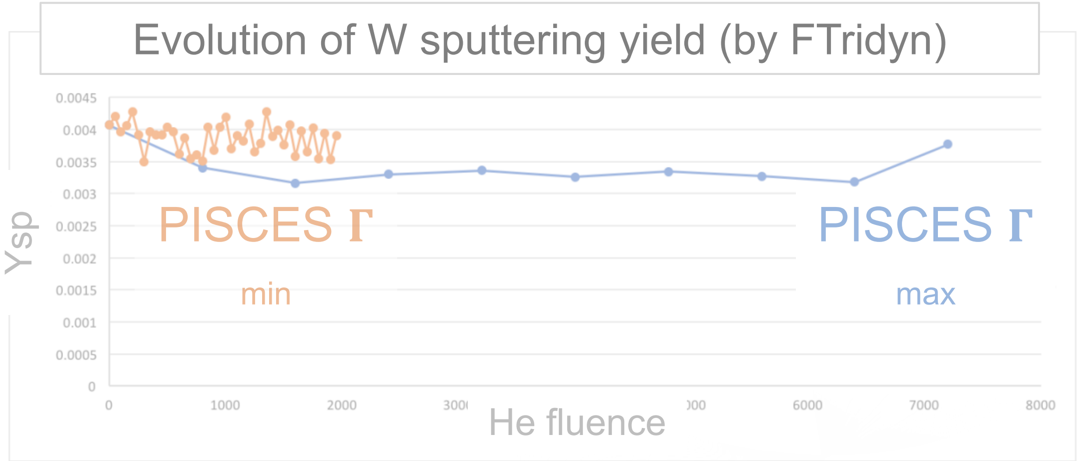
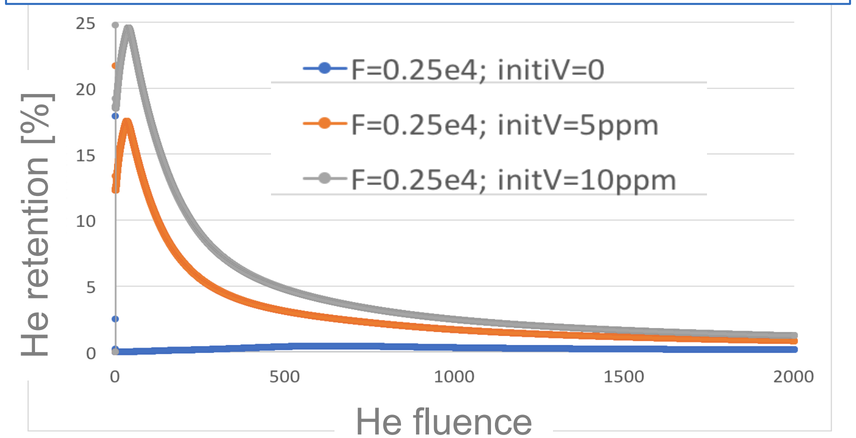


- Large effect on retention

→ introduce vacancies to induce He nucleation at low fluxes

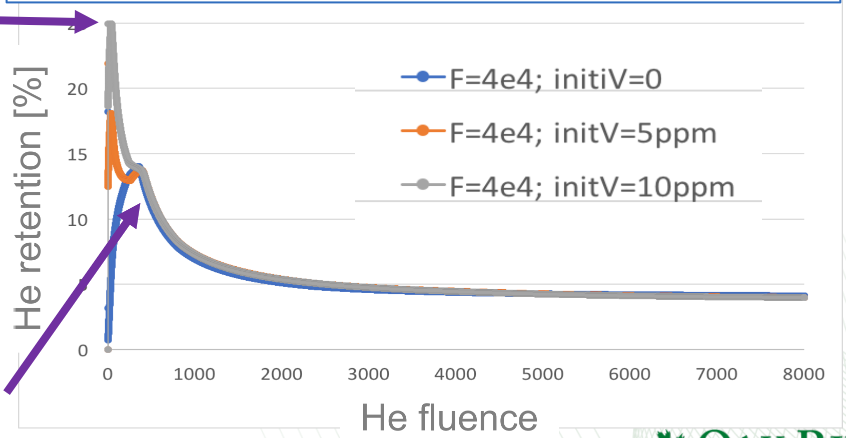
He retention, low flux (0.25e4 $nm^{-2}s^{-1}$)



initial trapping by He+V → HeV

growth of He clusters (until trap mutation)

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}, α_{in}, W fraction

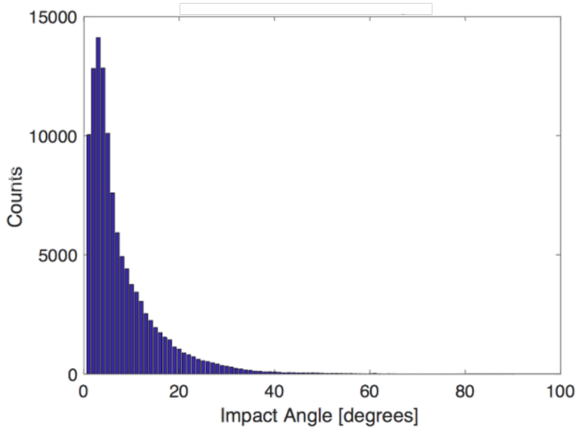
T. Younkin, 2nd talk

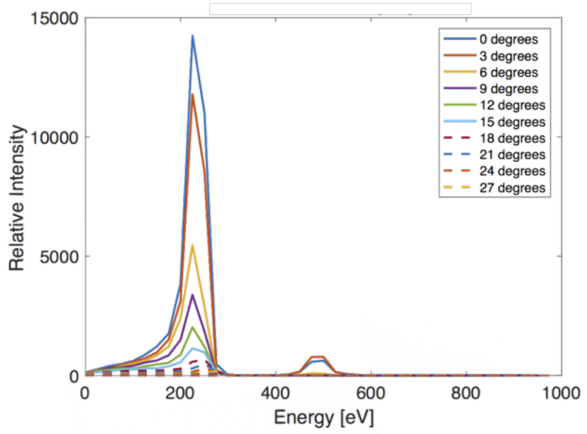
- F-Tridyn: implantation profile and Y_{sp} for each (α_{in}, f(E_{in}))

J. Drobny, 3rd talk

- Xolotl: implant W as interstitials

S. Blondel, 4th talk





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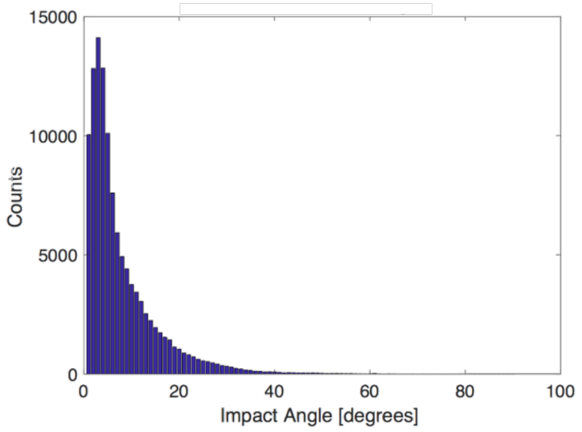

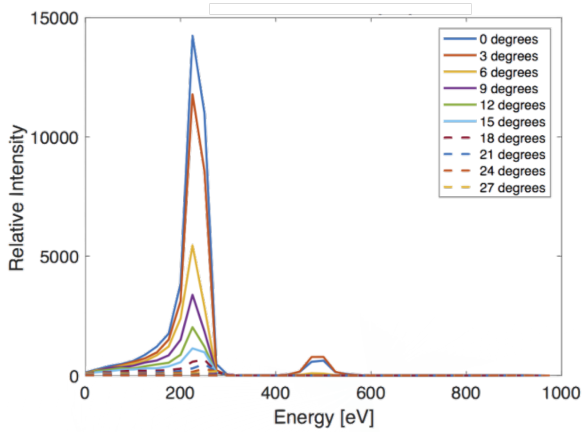

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  J. Drobny, 3rd talk

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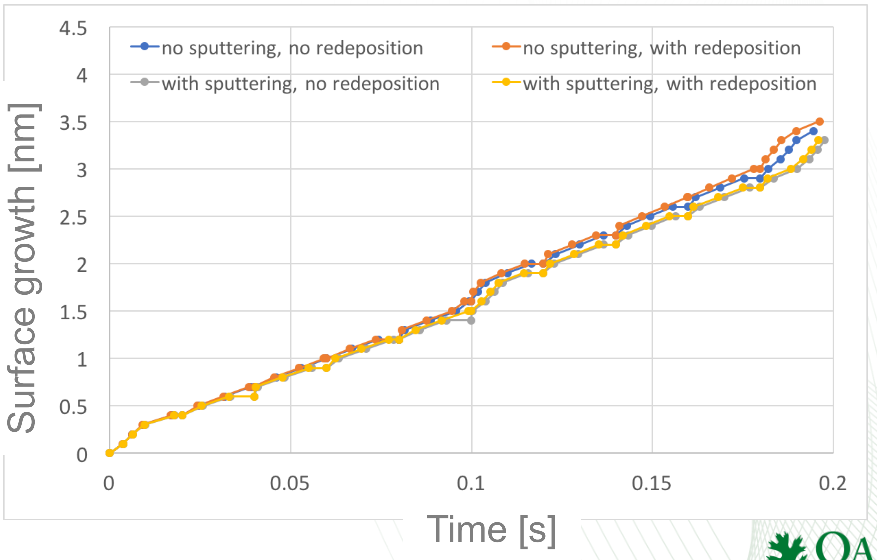
  S. Blondel, 4th talk

- At first glance, little effect on retention
  - Slight increase in surface growth
  - possibly a cumulative effect



Need to optimize Xolotl simulations to reach experimental time-scales

- Longer (exp. time-scale, *O(10⁴s)*) 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_{max}) used is 10^{-5} s
  - Need to explore solver options: e.g., increase dt_{max} with fluence (cluster size)

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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. Drobny, 3rd talk*

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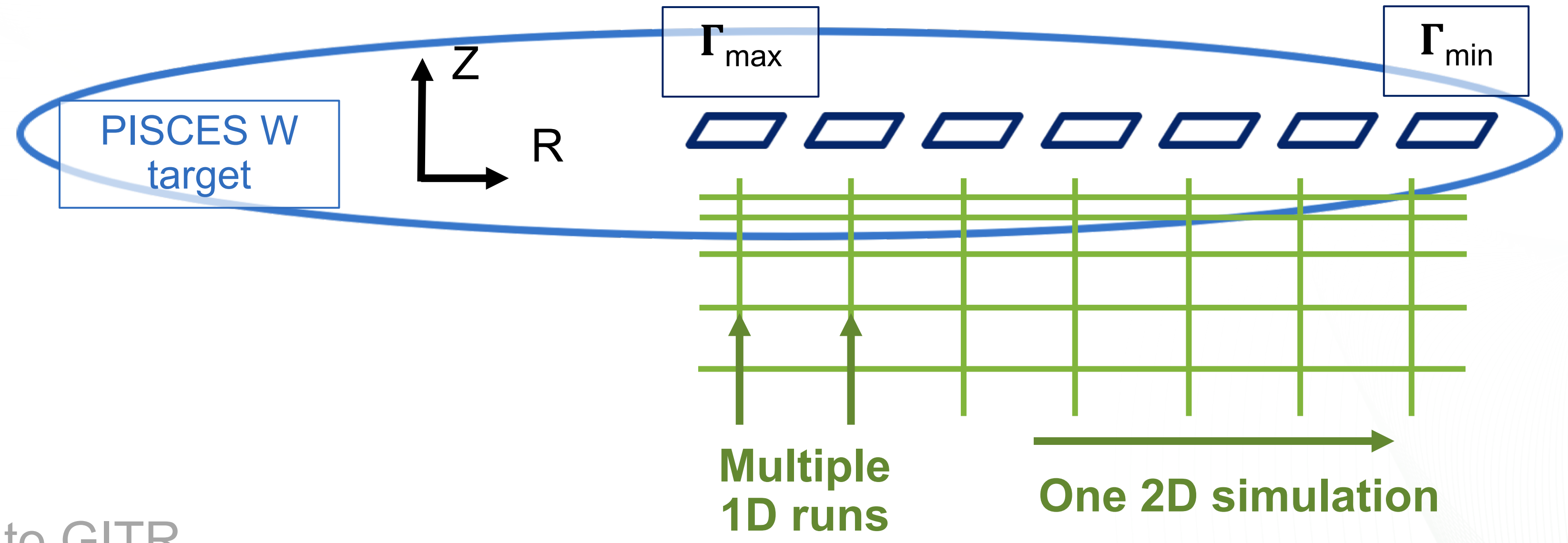

  - Couple to GITR
  - Implement ITER's geometry, handing mixed (H+He) plasma…
  - Run to experimental time-scales → introduce roughness *J. Drobny, 3rd talk*
  - Introduce H, bubble bursting, simultaneous runs… in Xolotl *S. Blondel, 4th talk*
  - Comparison to experiment *T. Younkin, 2nd talk*

Thank you for your attention!

This work is supported by the US DOE under contract DE-AC05-00OR22725