ENGINEERING

A Validated Multi-Physics Modeling Approach to Predicting impurity Erosion, Re-deposition & Gas Retention in Tokamak Divertors

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A Validated Multi-Physics Modeling Approach to Predicting impurity Erosion, Re-deposition & Gas Retention in Tokamak Divertors

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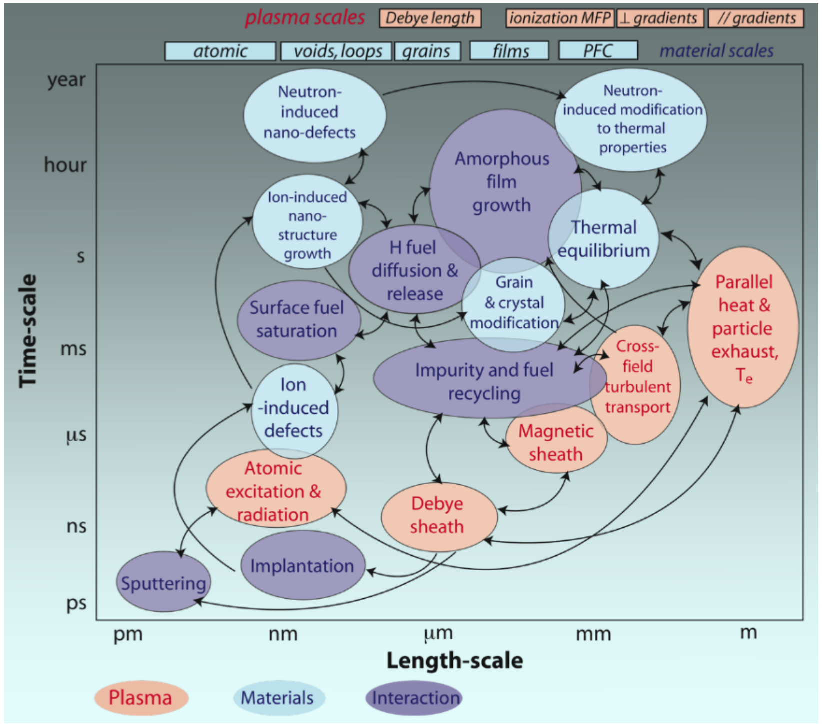
Plasma-material interactions (PMI) impact plasma and material's performance

- PMI compromise both material and plasma performance
  - Mutually degrade
  - Erosion, fuel trapping, morphology changes, etc.
- Critical for future fusion reactors, their wall design and material choice

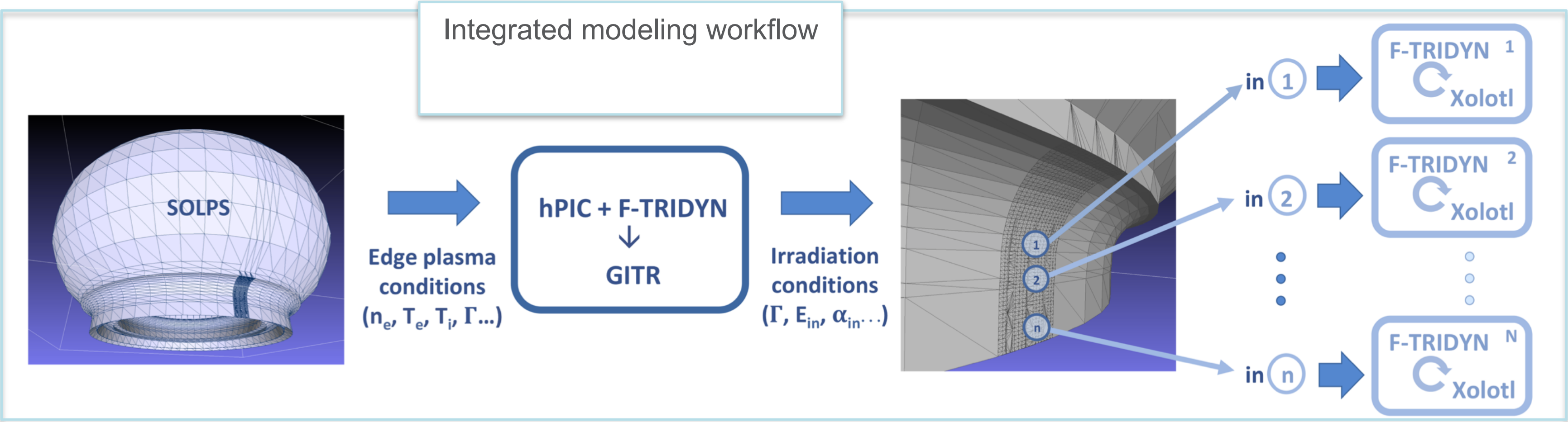
Plasma-material interactions (PMI) are multi-physics and multi-scale in nature

- PMI compromise both material and plasma performance
  - Mutually degrade
  - Erosion, fuel trapping, morphology changes, etc.
- Critical for future fusion reactors, their wall design and material choice
- It's a multi-scale physics problem
  - We address it by integrating multiple, high-fidelity models



Wirth et al., *MRS Bulletin* **36** (2011)

The resulting integrated model is applied to simulate PISCES & ITER plasma exposures



OUTLINE

- The model was benchmarked against PISCES experiments
- We applied it to predict the evolution of the ITER divertor under He operation and burning D-T plasmas
- Take a deeper look at the effect of He on hydrogenic retention

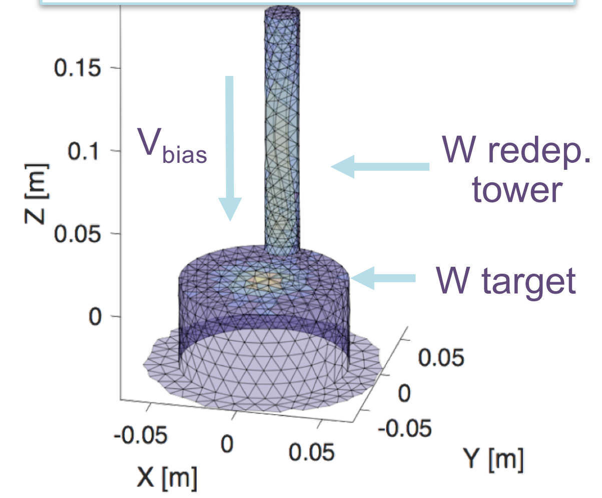
Model validation

Benchmark against PISCES experiments

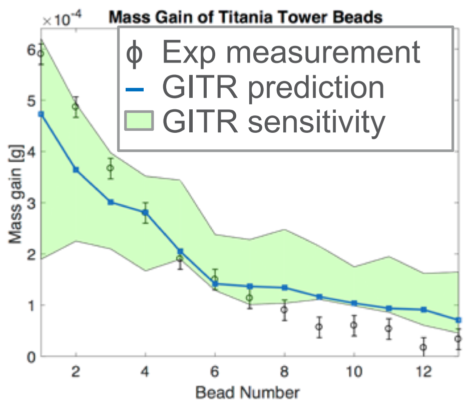
The integrated model was benchmarked against PISCES experiments

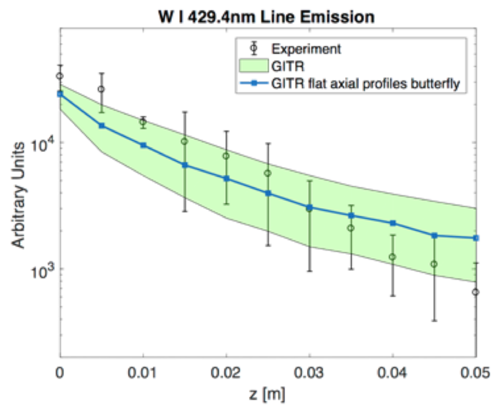
- We performed an extensive comparison of impurity transport (GITR+ F-TRIDYN) and sub-surface evolution (F-TRIDYN+Xolotl) predictions to experiments, across a range in
  - Flux: 0.5-5.4·10^{22} /m^2s
  - Biasing voltage: 75V, 250V
  - Plasma composition: 100% He,10%He-90%D
- Langmuir probe measurements provided the background plasma n_e, T_e
- Two sets of experiments
  - W I spectroscopy, target mass loss, tower mass gain to measure erosion and transport (GITR)
  - Removable W targets to analyze with LIBS and LAMS (Xolotl)

impurity transport experiment

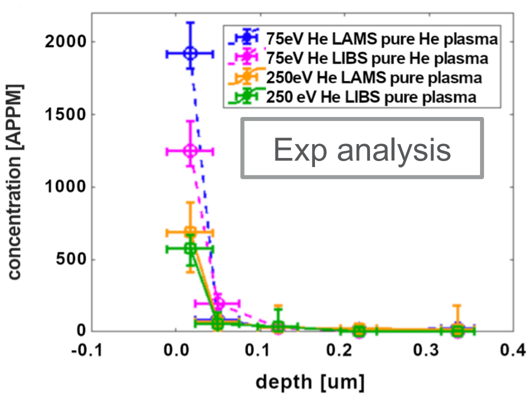


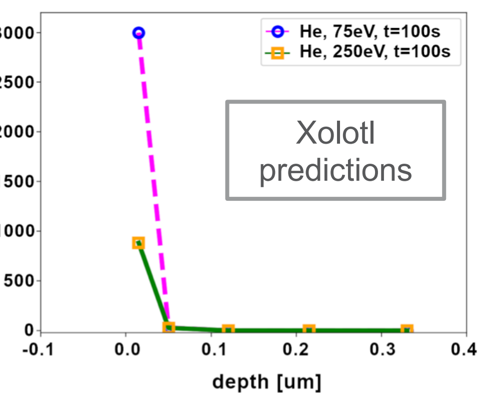
Xolotl and GITR show good agreement with experimental measurements





	Mass Loss [g]	%Eroded Material Returned to Target
Experiment	0.079533	-
GITR flat profiles	0.0563 - 0.0737	70 - 77
GITR +/- Te	0.0475 - 0.0888	65 - 81
GITR +/- ne	0.0475 - 0.0888	65 - 81





- GITR reproduces experimentally measured mass loss, W I lines and tower mass gains
- Experimentally measured He & D concentrations are fairly reproduced by Xolotl

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Model application

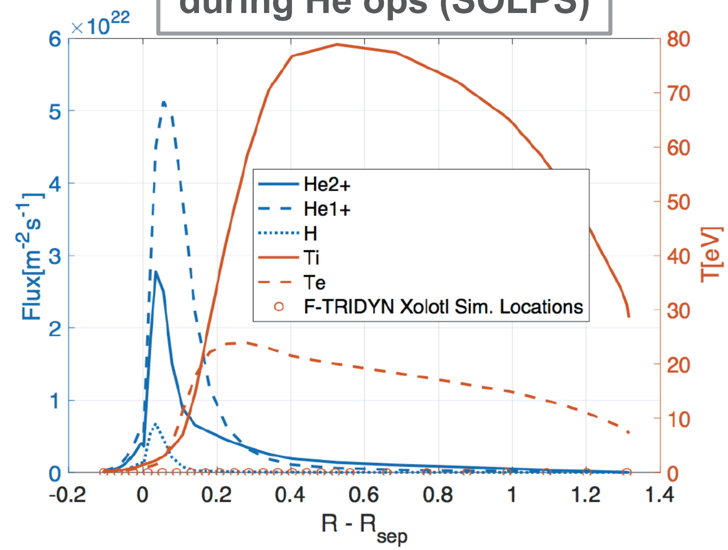
Predicting the evolution of the ITER divertor under He plasma and burning plasma operations

SOLPS predicts a partially detached divertor during He and burning plasma ops

- These are standard strongly radiating, partially-detached scenarios
  - Very low temperature (~1 eV), high flux near separatrix strike point
  - Higher temperature, lower density and flux away from strike point

- During BPO, nearly 75% of power is radiated, mainly by Ne in the divertor; peak heat flux of ~7 MW/m^2

plasma parameters during He ops (SOLPS)

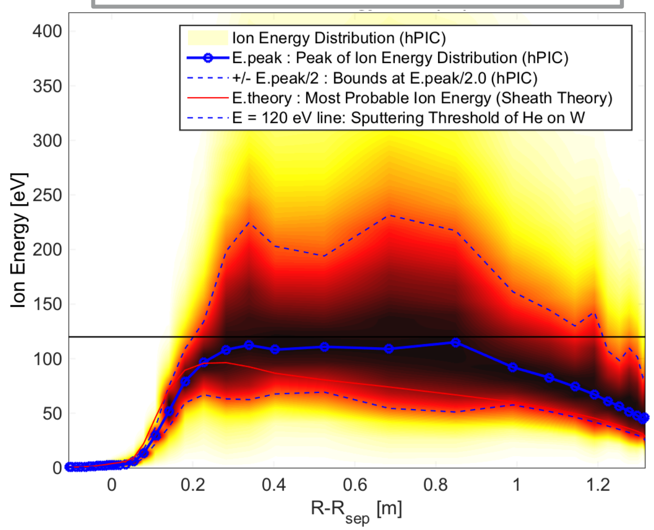


Heavy impurities dominate sputtering when present, with contributions from the high-energy tail of light species

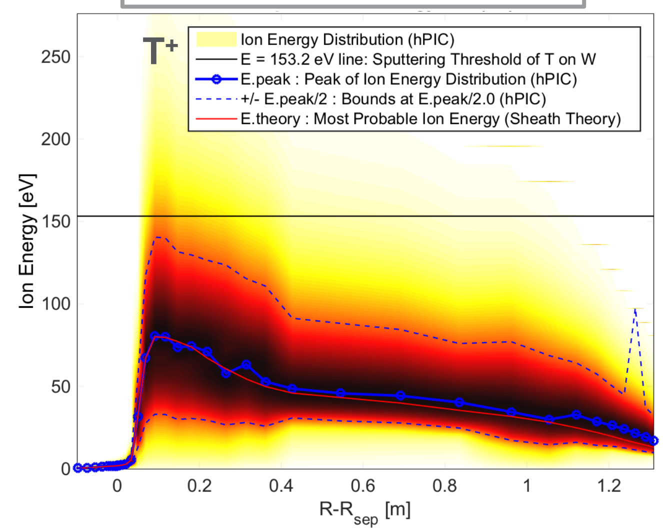
hPIC shows that

- while much of the impact energy-angle distribution (IEAD) for light ions is below energy threshold for W sputtering,
- the high-energy tail extends well above sputtering threshold

IEADs for He^+ (hPIC), He ops



IEADs for T^+ (hPIC), BPO



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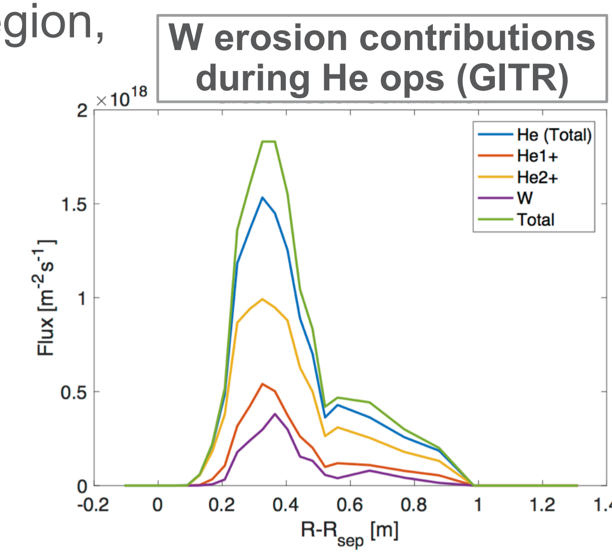
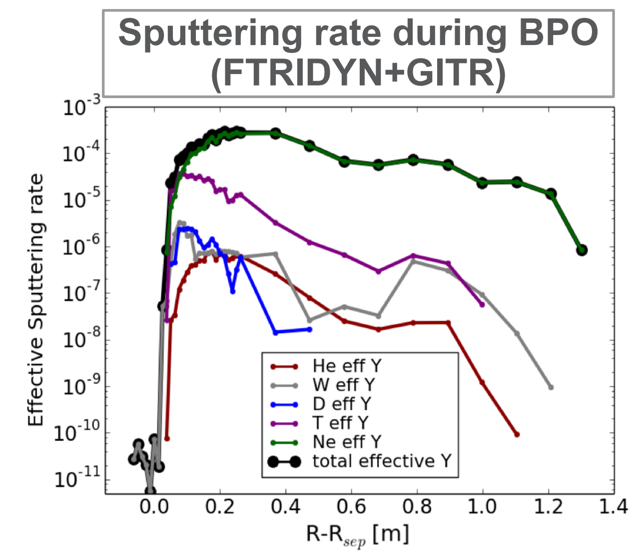
Heavy impurities dominate sputtering when present, with contributions from the high-energy tail of light species

Accounting for sputtering and reflection rates provided by F-TRIDYN, integrated impurity transport calculations predict

- He^{2+} is the main impurity source during He plasma operations
- heavy impurities dominate sputtering during BPO
  - W in the private flux region,
  - Ne elsewhere



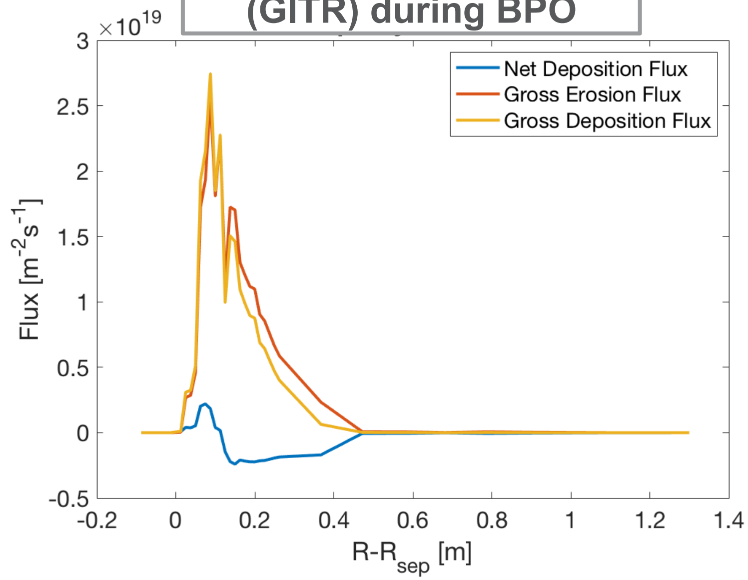


GITR predicts strong local re-deposition, with net deposition around the strike point

Impurity transport calculations of GITR predict

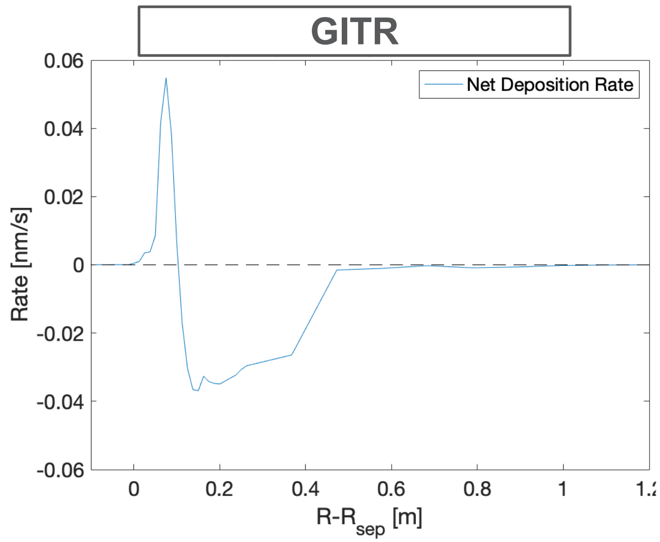
- strong (>95%) prompt or local re-deposition of the eroded W
  - strong drag forces that push impurities back to the surface
- net deposition around the strike point
  - transport by local E fields
  - higher deposition rate at lower T_i
- net erosion further along the target

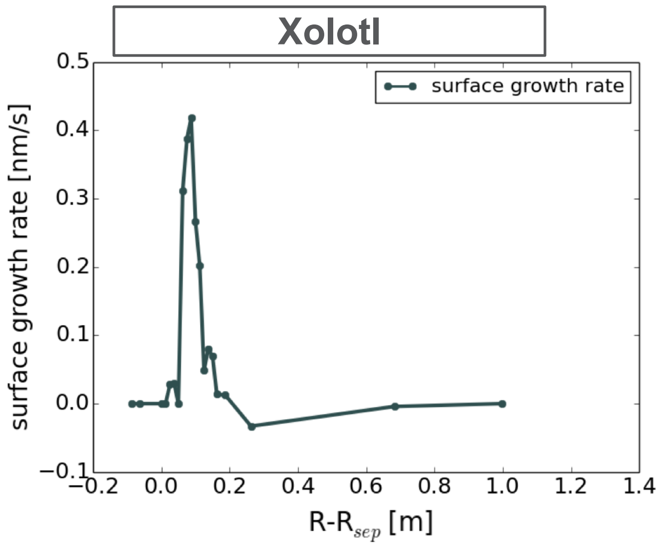
Gross & net erosion (GITR) during BPO



Surface height in Xolotl is similar to GITR, with enhanced, He-induced surface growth

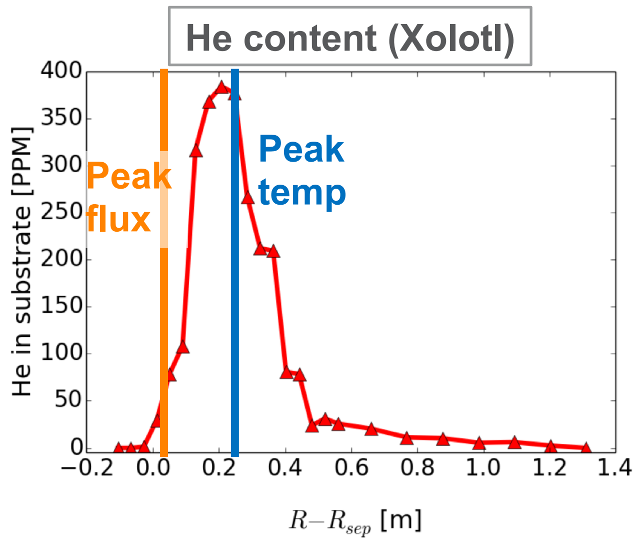
- The same surface height pattern is predicted by GITR and Xolotl
- Differences arise around the strike point (T_i~eV) from shallow gas implantation, He-induced trap mutation and surface growth
- These processes affect less the locations with high impact energies (T_i~40eV, further up the target)

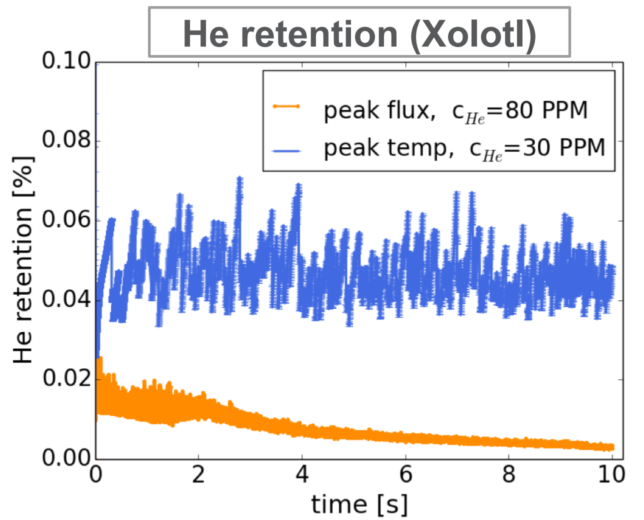




During He ops, He accumulation & retention are a balance between implantation rate & energy

- He accumulation largely follows the flux profile, with larger retention where T_i is high, even though flux is ~10x less than at its peak value
  - Shallow implantation at low T_i leads to higher outgassing rates and more frequent, small bursts; thus lower He retention
  - Deeper implantation at high T_i leads to less outgassing and larger, less frequent bursts; thus higher He retention



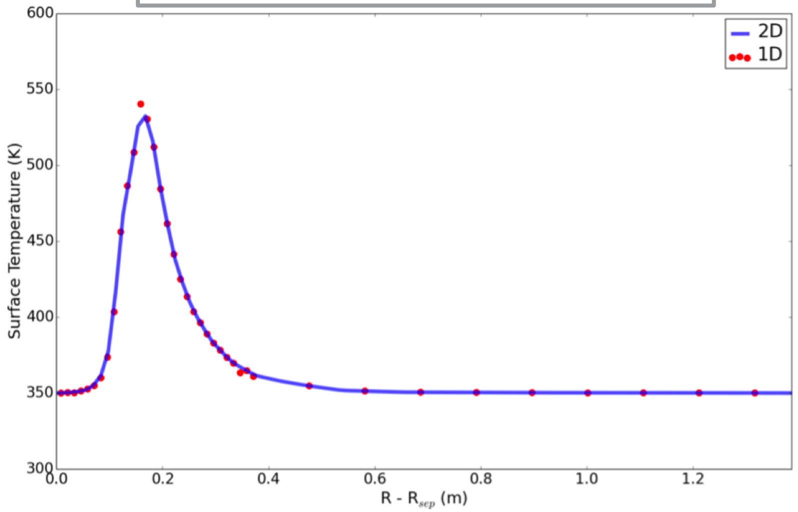


During BPO, heat fluxes increase the surface temperature by up to ~200K

- For $P_{in, SOL}$= 100 MW discharge, T_{surf} increases up to ~200K
  - While this is no threat of melting or recrystallization (no transients included)
  - It does affect gas dynamics

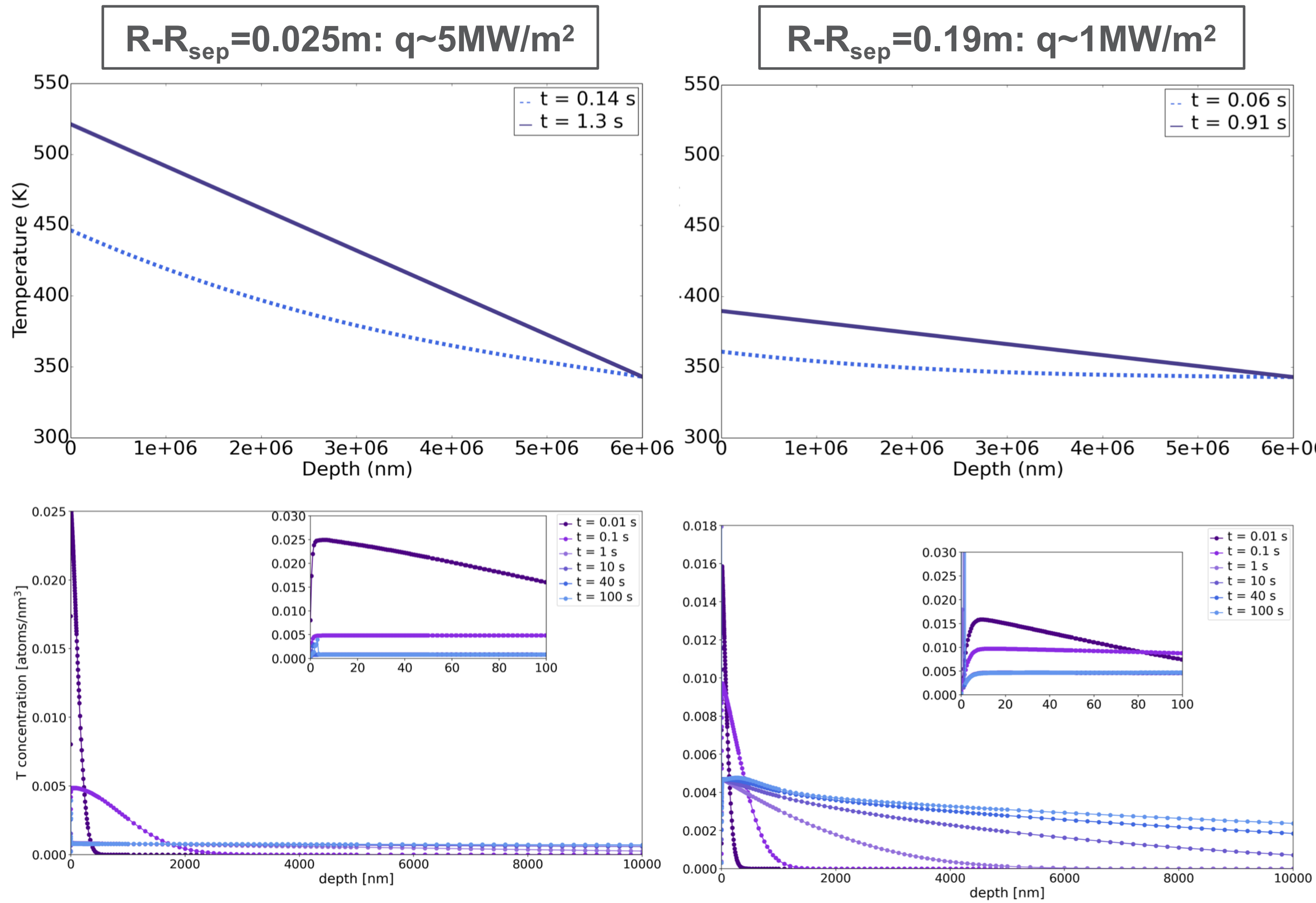
- The thermal coupling between locations is negligible
  - We model multiple, independent 1D locations

Surface temperature (Xolotl)



Differences in gas diffusion correlated with the local heat flux

- Tritium diffuses faster with increasing surface temperature (T_{surf}), mainly outgassing
- The peak in hydrogen concentration takes the value expected for $T_{surf}=T_{surf}(t)$



Gaining insight into the effect of He on hydrogenic retention

How pre-existing damage drives D&T content, as well as their depth-distribution

We now evaluate sequential exposure to He plasmas & ITER Burning Plasma Ops

- For each of the 3 substrate compositions (He-V clusters), resulting from exposure to:
  - 100s of He plasma in PISCES, at V_{bias} ~ 75 V
  - 100s of He plasma in PISCES, at V_{bias} ~250 V
  - 10s of early ITER He ops

Higher He fluence (first two items)

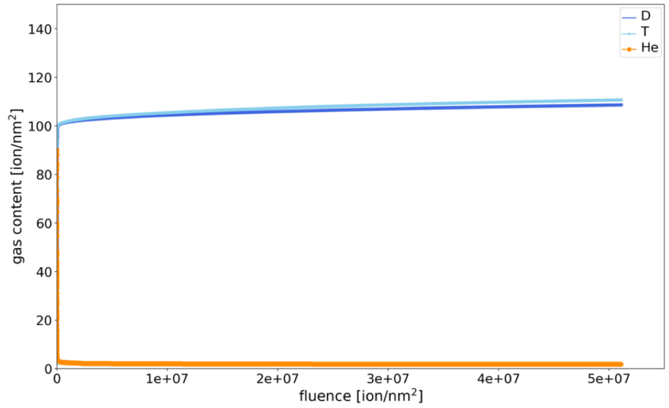
Realistic He spectrum (third item)

- We use Xolotl to model the subsequent exposure to 100s of full power BPO, in 5 locations:
  - Peak in particle flux ($R-R_{sep}$~0.025m)
  - Peak in heat flux ($R-R_{sep}$~ 0.05m)
  - Peak in plasma temperature ($R-R_{sep}$~ 0.1m)
  - 2^{nd} peak in He flux ($R-R_{sep}$~0.2m)
  - Further upstream ($R-R_{sep}$~ 1m)

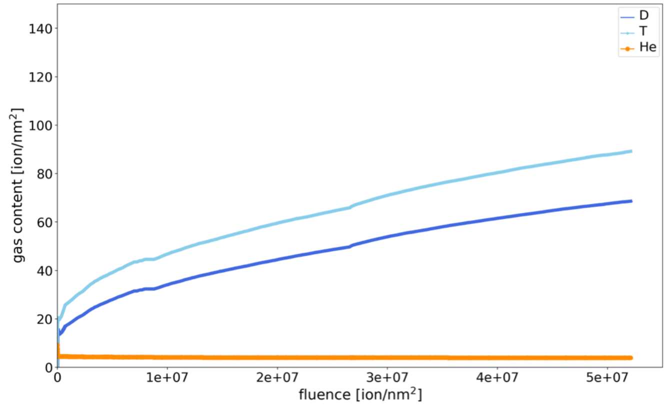
Gas content saturation depends on both vacancy content & their depth distribution

- In substrates pre-exposed in PISCES, T content stabilizes quickly, within fluences $O(10^{22}$ ion/m$^2)$
  - quick increase in D-T content due to localized near-surface V content
- Continues to grow in substrates pre-exposed to ITER He ops or initially undamaged
  - ITER He+BPO: larger increase in H on the long scale because of higher V concentration between 100 and 1000 nm

Pre-exposed in PISCES, at 75 V



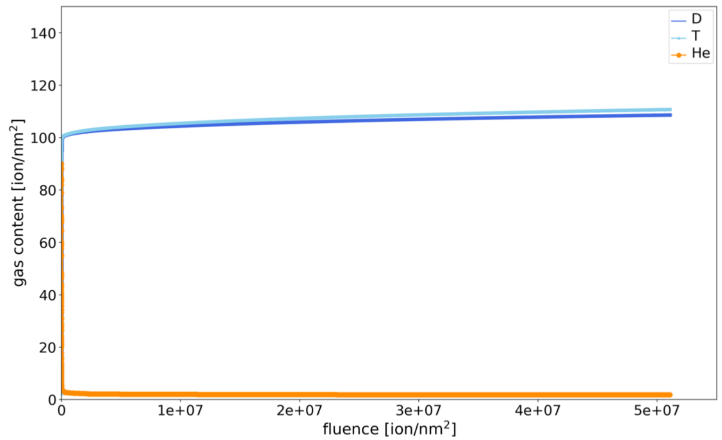
Pre-exposed to ITER He plasma



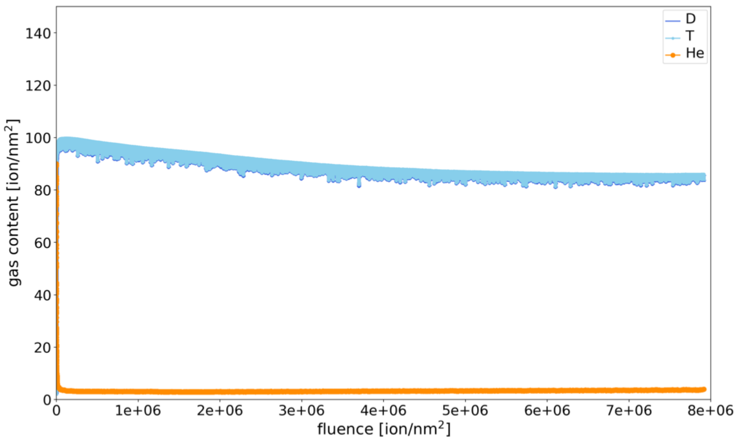
Pre-existing damage sets the saturation level of hydrogenic retention

- The amount of T contained in the PISCES pre-exposed material stabilizes at a fixed value for each V_{bias}
  - $1.4 \cdot 10^{20}$ at/m^2 at 250 V, $1 \cdot 10^{20}$ at/m^2 at 75 V
- These values are maintained over a wide range of parameters, although can be slightly altered e.g., by large presence of bursting

Exposed to peak particle flux during BPO



Exposed to peak in T_i during BPO

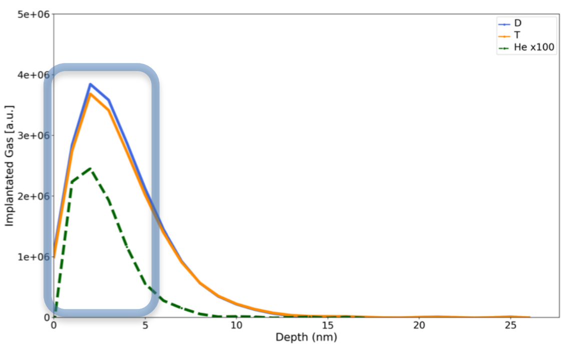


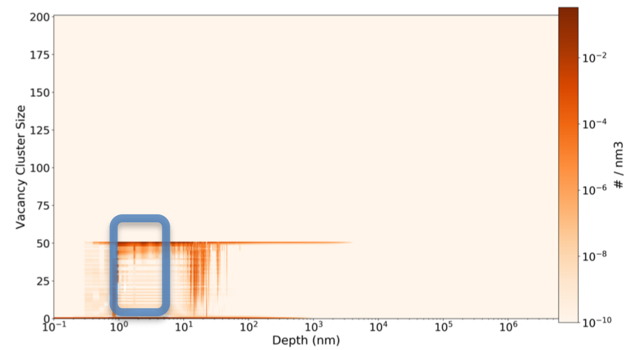
He implantation in pre-existing vacancies leads to bursting

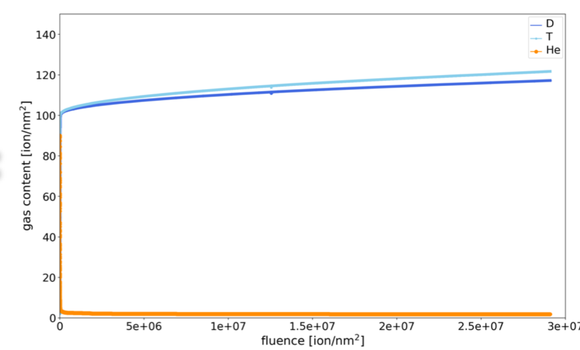
Implantation profile

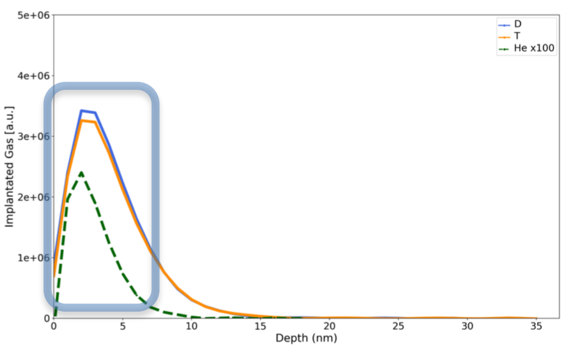
Initial V size-depth distribution

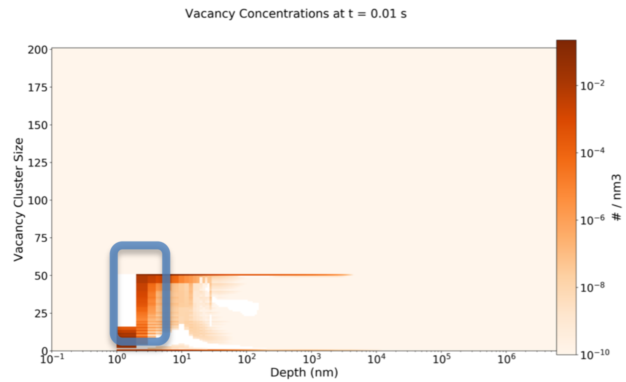
Evolution of gas content

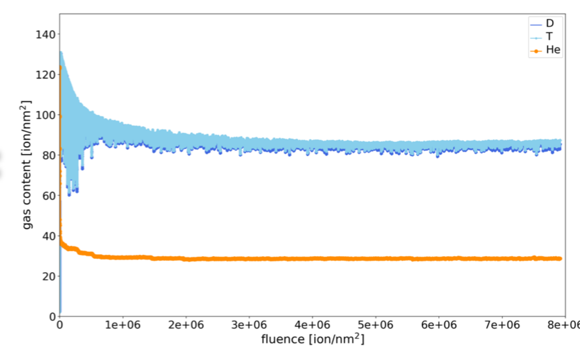












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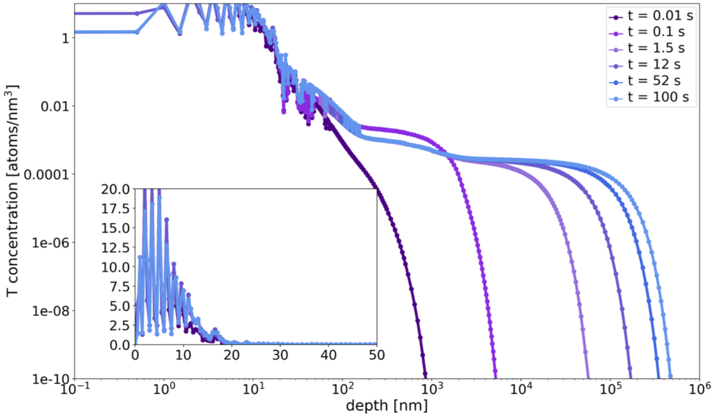
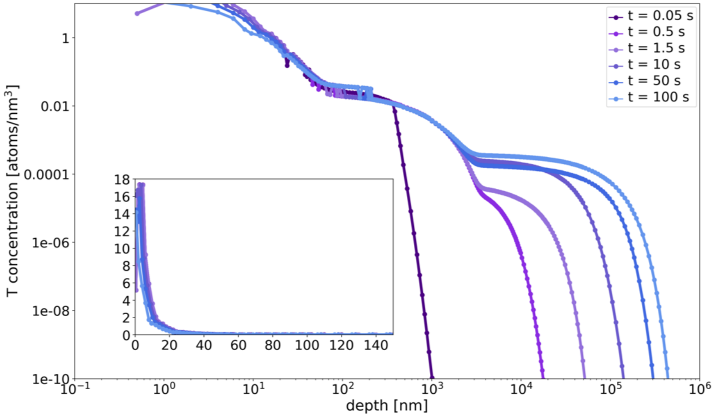
Substrates with pre-existing damage show a reduced temperature sensitivity

- Heat-flux induced temperature variations (<200K) are insufficient to de-trap T from He-V clusters (present in all pre-damaged substrates)

T concentration, PISCES 75V



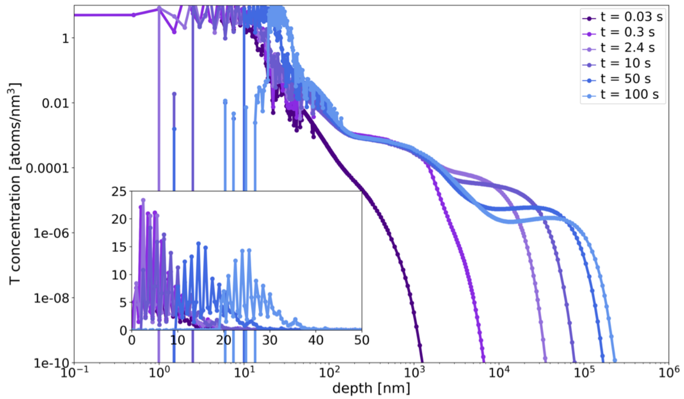
T concentration, PISCES 250V



He-induced damage modifies the depth-distribution of hydrogen species

- We observe 3 depth-ranges for gas accumulation:
  a) near-surface, present in all pre-exposed substrates & driven by He damage

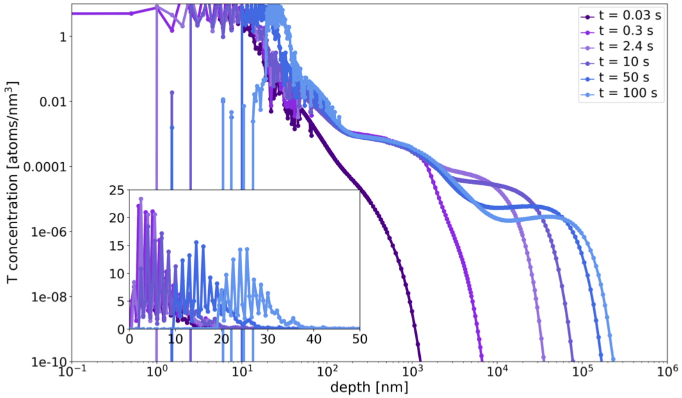
a) **T concentration, PISCES 75V**



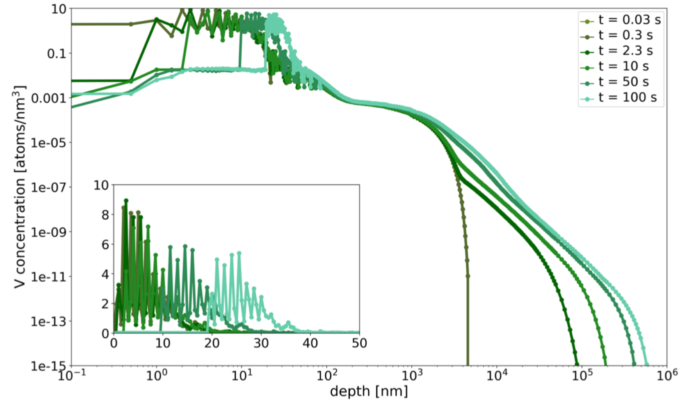
T remains closer to the surface in pre-damaged substrates

- We observe 3 depth-ranges for gas accumulation:
  a) near-surface, present in all pre-exposed substrates & driven by He damage
  b) mid-range, where the deepest post-PISCES exposure vacancies existed

a) **T concentration, PISCES 75V**



b) **V concentration, PISCES 75 V**



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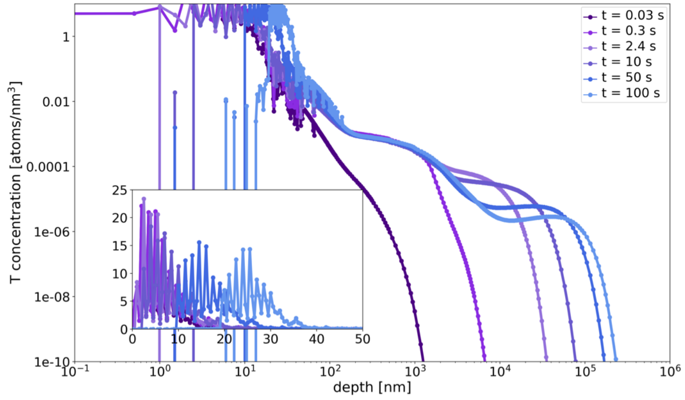
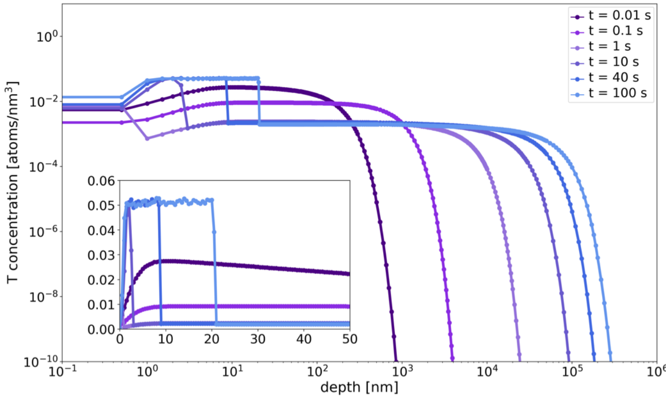
T remains closer to the surface in pre-damaged substrates, while bulk content is higher for initially pristine ones

- We observe 3 depth-ranges for gas accumulation:
  a) near-surface, present in all pre-exposed substrates & driven by He damage, & mid-range, where the deepest post-PISCES exposure vacancies existed
  c) deeper in the bulk (diffusion); consistently higher in initially pristine substrates

a) **T concentration, PISCES 75V**

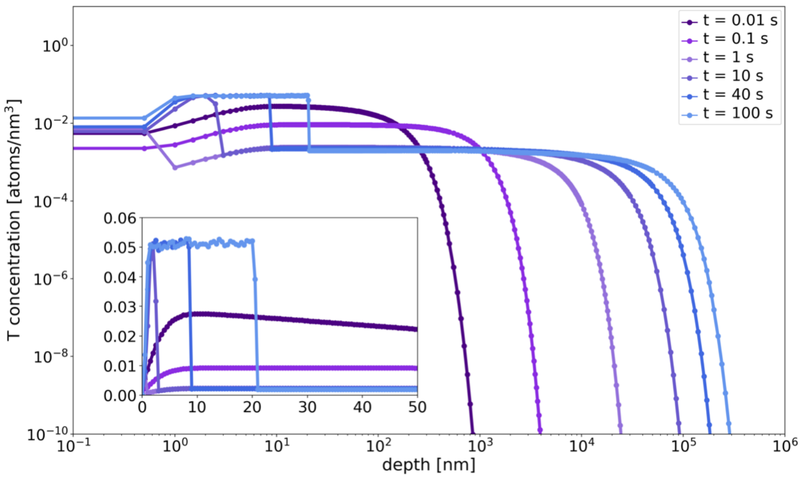


c) **T concentration, pristine W**



Even small concentrations of He can induce near-surface T trapping in the long term

- the surface grows because of net W re-deposition (x3 the sputtering rate)
- modified trap mutation (TM) creates He-V clusters near the surface, which move as the surface grows
- when the surface moves up, the He gets implanted where the HeV had been created (implantation at 1-5 nm), trapping directly with the HeV clusters and generating bubbles large enough to burst
- after bursting, the He outgasses and V's remain; the cavity is refilled with D-T, the main plasma species, which saturate the bubble



Summary

- We've integrated and successfully validated our multi-physics PMI model
- Our predictions of ITER simulations reveal that:
  - The edge plasmas are representative of partially detached divertors
  - Heavy impurities dominate erosion when present, with contributions from light ions due to the high-energy tail of IEADs
  - 80-90% of eroded W is locally or promptly re-deposited
  - sub-surface gas dynamics leads to additional surface growth in areas of low T_i
  - High heat flux decreases near surface T concentration
- Subsequent exposures to He plasmas and BPO reveal that D-T interact & bind with He-V clusters, modifying retention & permeation
  - Gas content stabilizes in substrates pre-exposed in PISCES, at levels set by pre-existing V's, while continues to grow in substrates initially pristine or pre-exposed ITER He plasmas
  - Bursting occurs when gases implanted in pre-existing vacancies
  - T remains closer to the surface in pre-damage substrates, while the bulk content is higher for initially pristine cases

Outlook

- Experimentally verify hydrogenic retention in growing W layers
- Evaluate the impact of pre-damage beyond plasma ops, e.g. in maintenance phases (baking temperature and duration)
  - Need for further parametrization of the H-He-V system for mainly hydrogenic, non-over-pressurized bubbles

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- We are **experimentally validating** our PMI model in all-metal devices (WEST), and expanding usage of our models to understand erosion-redeposition experiments (DIII-D)
- Extend the models to self-consistently treat **seeded impurities** (e.g., neon), the effects of **mixed materials** (W-Be) and evolving **thermo-mechanical properties**
- Transition into dynamic simulations; e.g., to model ELMs