Theoretical analysis and experimental validation in DIII-D of predictive modeling for tungsten erosion and redeposition in tokamak divertors

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GENERAL ATOMICS

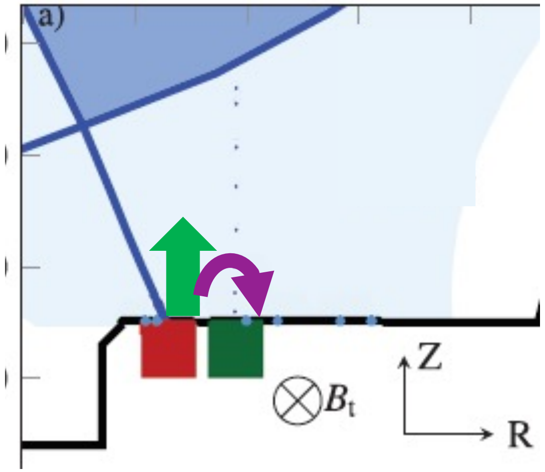
W net erosion from divertor PFCs largely determined by W prompt redeposition but no direct measurement available in tokamak divertors

W net erosion in divertor ≈ **gross erosion** x **(1- prompt redeposition)** x **(1 – non-prompt local redeposition)**

Impurity fluxes + sputtering physics + ionization physics + sheath physics + parallel impurity transport physics + cross-field impurity transport physics

- **In-situ exp. measurements of W gross erosion (WI 400.9 nm +SXB)** [1,2]
  - BCA models (TRIM,SRIM,…)

- **No in-situ measurements of W deposition/transport**
  - Post-mortem analysis of W deposition on PFCs
  - Kinetic models (ERO,GITR,…)



[1] J. Guterl Nuclear Fusion 2019

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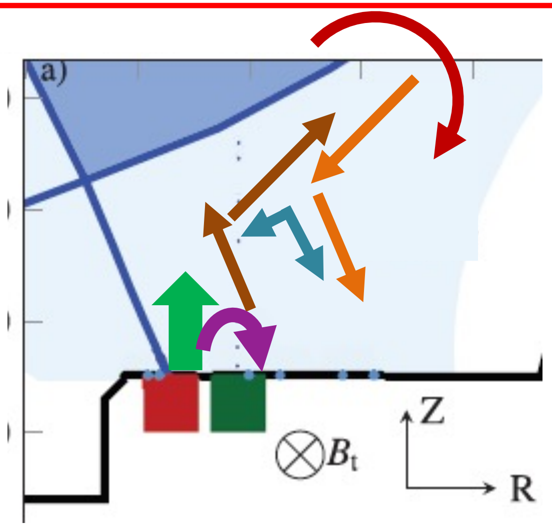

- For impurity in trace approximation (concentration ≲1%) like W, non-prompt local redeposition driven by balance between:
  1. *Friction with plasma particles (push particles toward divertor)*
  2. *Thermal forces (asymmetry in collisions due to temperature gradient take particles away from divertor)*
  3. *// electric field (ExB radial and poloidal drifts)*

  => Recirculation of impurity in divertor[1]

[1] J. Guterl Nuclear Fusion 2019

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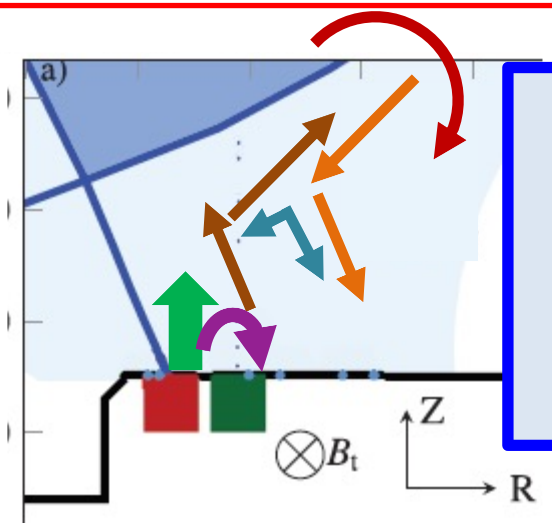

Worst case scenario:
All W non-promptly redeposited transported upstream
=
W influx in SOL
W net erosion in divertor ≤ gross erosion x (1- prompt redeposition)

[1] J. Guterl Nuclear Fusion 2019

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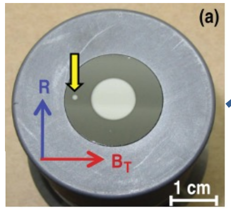
- **W prompt redeposition is usually large in attached plasma conditions and determines the overall W net erosion (prompt redeposition~1)**
- **Developing predictive models for W prompt redeposition in divertors requires to:**
  - → ***understand fundamental physics processes governing W prompt redeposition***
  - → ***validate predictive models of W prompt redeposition against experiments***

Predictive model benchmarking

DIII-D experiments

Metal ring experiment [2]

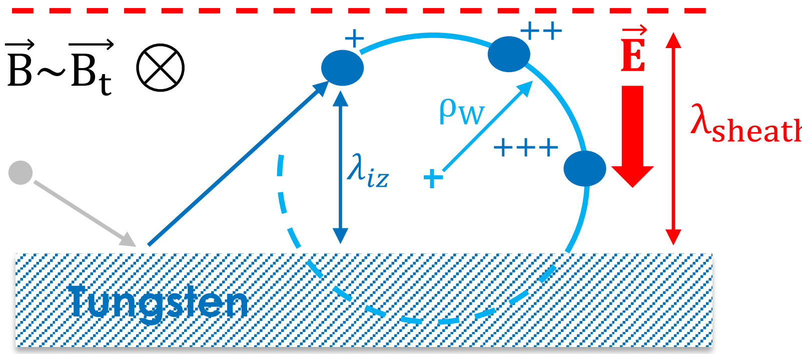


small/large dots experiment [1]

[1] D. Rudakov *Physica Scripta* 2014
[2] J. Guterl *Nuclear Fusion* 2019

Modeling of W prompt redeposition in presence of grazing magnetic field must include sheath effects and multiple ionizations of W

- Ionization of sputtered W near divertor surface due to collisions with electrons*
- **W prompt redeposition (redeposition of charged W impurities during their first gyration) affected by multiple ionizations of W impurities & electric sheath**



* *could also be induced by CX (see David Tskhakaya's talk)*

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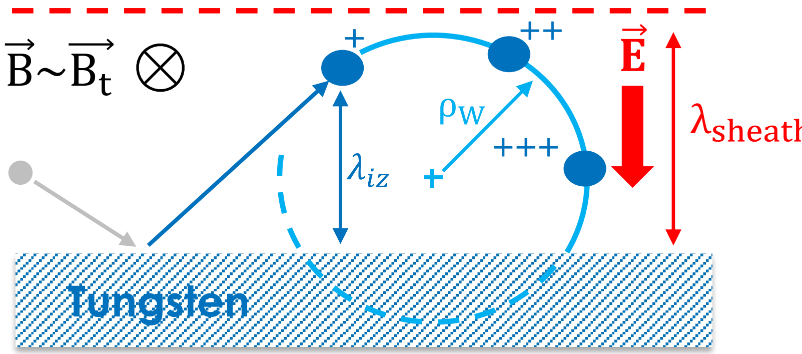

- 3D trajectory of W impurities modeled by Monte-Carlo particle pusher with E and B fields embedded in ERO-D3D (HPC version of ERO[1])
  - Collisions of W impurities with plasma ion and neutral species negligible for W prompt redeposition in attached plasma conditions* $(\tau_{collision}\omega_c \gg 1)$
- **Effects of electric sheath and multiple W ionizations on W prompt redeposition qualitatively described by Brooks[2] and Fussmann[3] in 90's …**
- **…but quantitative modeling of W prompt redeposition now required for ITER W divertor and beyond!**

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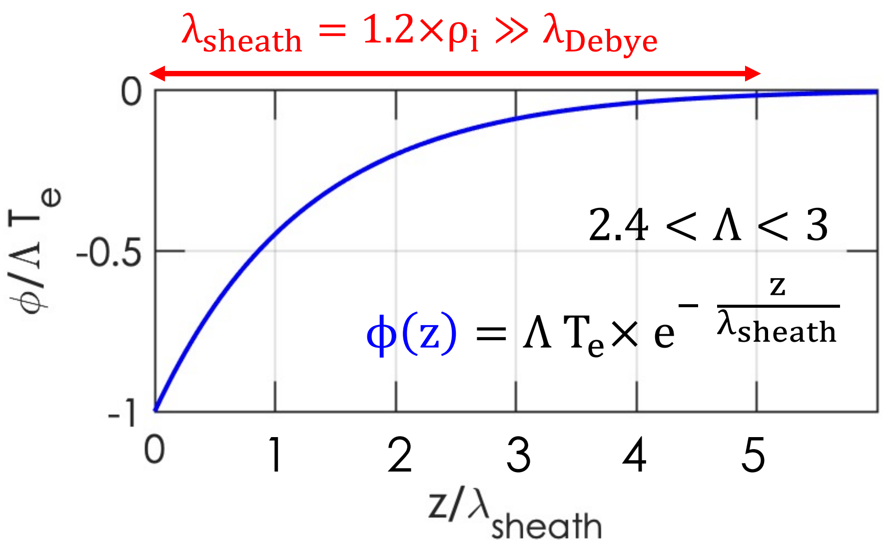
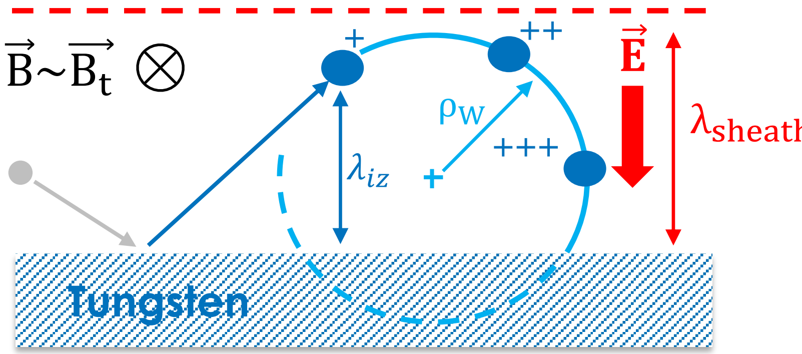
W impurities ionized within the sheath because of the large sheath width due to magnetic field lines intersecting divertor targets at grazing incidence

- **Wide electric sheath (Chodura sheath) due to grazing magnetic field ($< 5°$) in divertor[1]:** $\lambda_{sheath} \sim \rho_i$
- Sheath "frozen" for tungsten impurities (trace approximation)
- Sheath electric potential profile provided by kinetic simulations [2,3]





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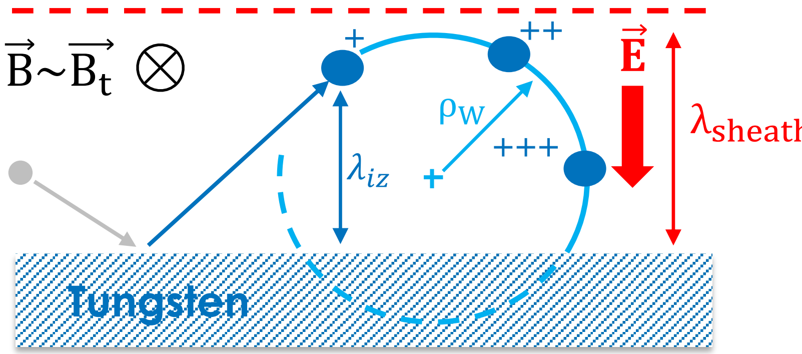

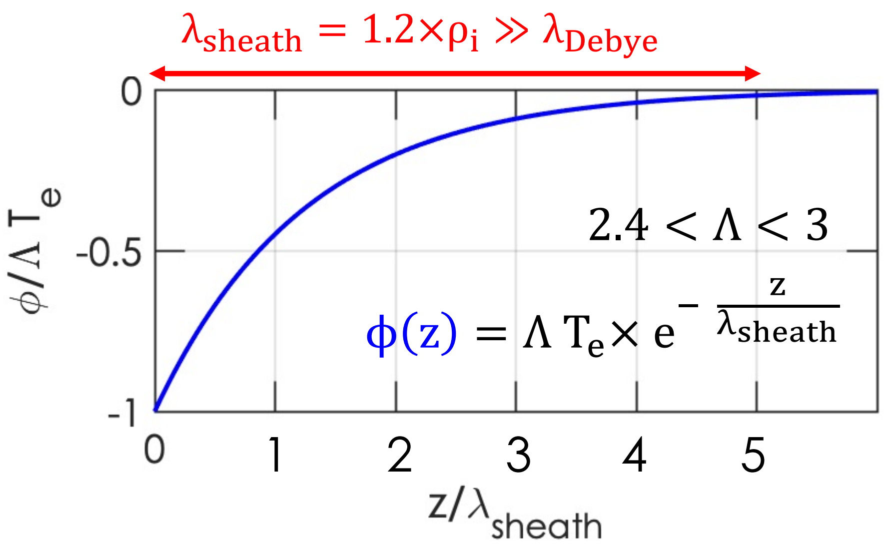

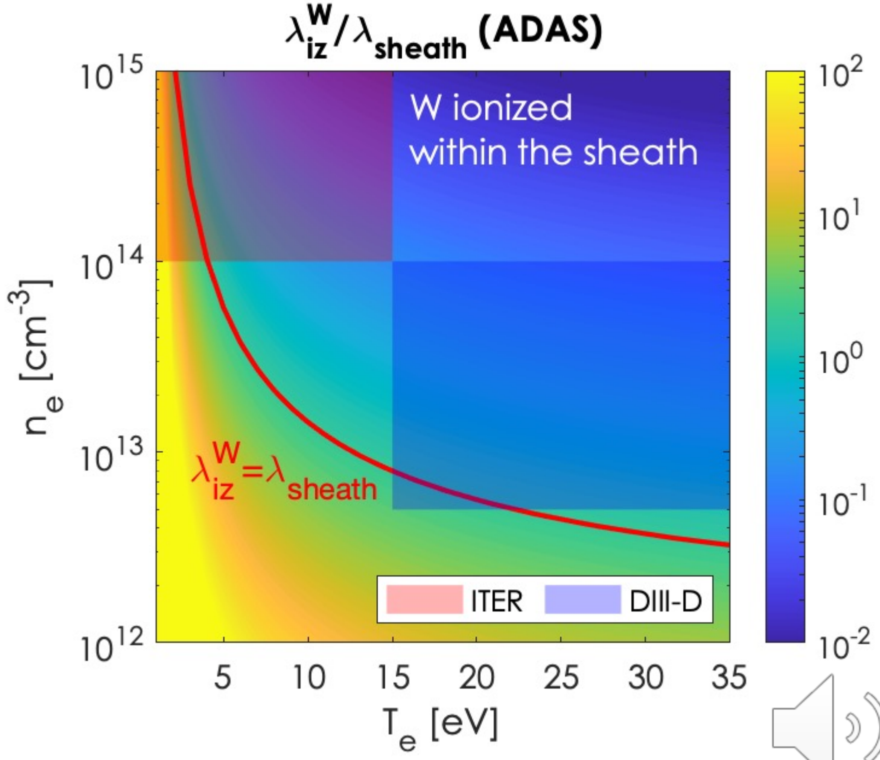

- **In ITER and DIII-D:**

  → **Sputtered neutral W ionized within the sheath :**

$$\lambda_{iz} \lesssim \lambda_{sheath} \lesssim \rho_W$$

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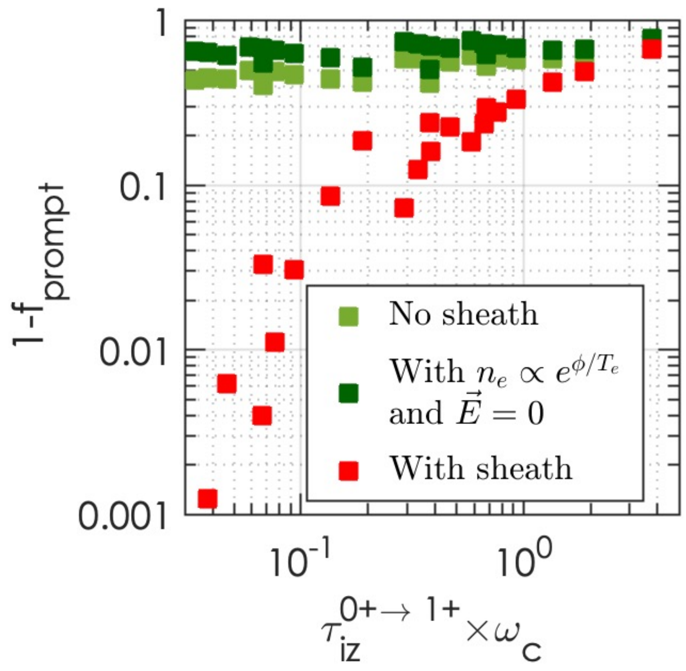
W prompt redeposition strongly enhanced by the sheath electric field because of the large inertia of W impurity

- **When W ionized within the sheath ($\lambda_{iz} \lesssim \lambda_{sheath}$), W prompt redeposition affected by Chodura sheath due to:**
  - increase of λ_{iz} due to the decay of n_e in the sheath

$$n_e(z) = n_{e,0} e^{\phi(z)/T_e}$$

  - acceleration of impurity toward material surface by the sheath electric field

- **Sheath electric field strongly enhances W prompt redeposition and has stronger effects than multiple W ionizations and decay of n_e in the sheath**



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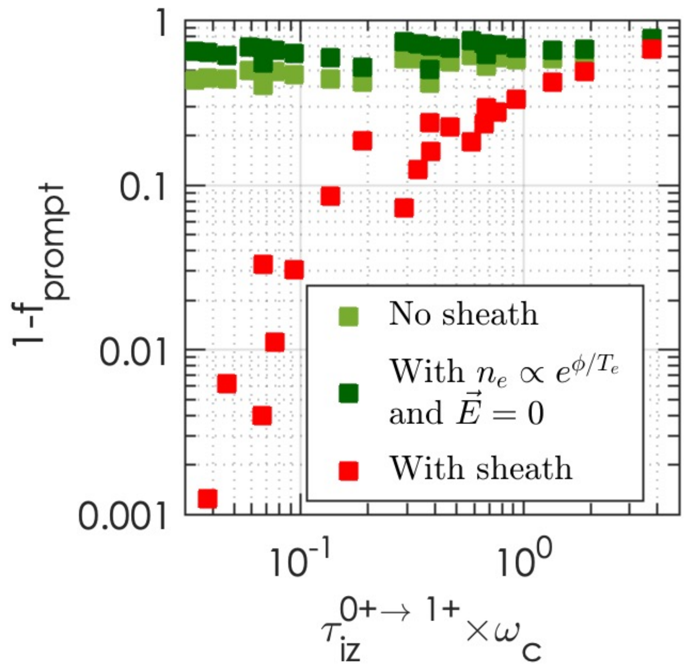
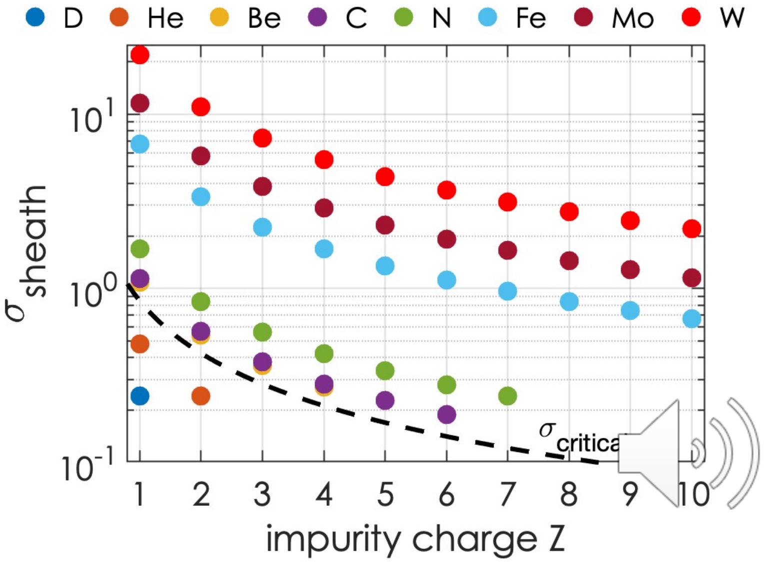
- **Electric field remains much stronger than Lorentz force despite high W charge state due to large W mass**

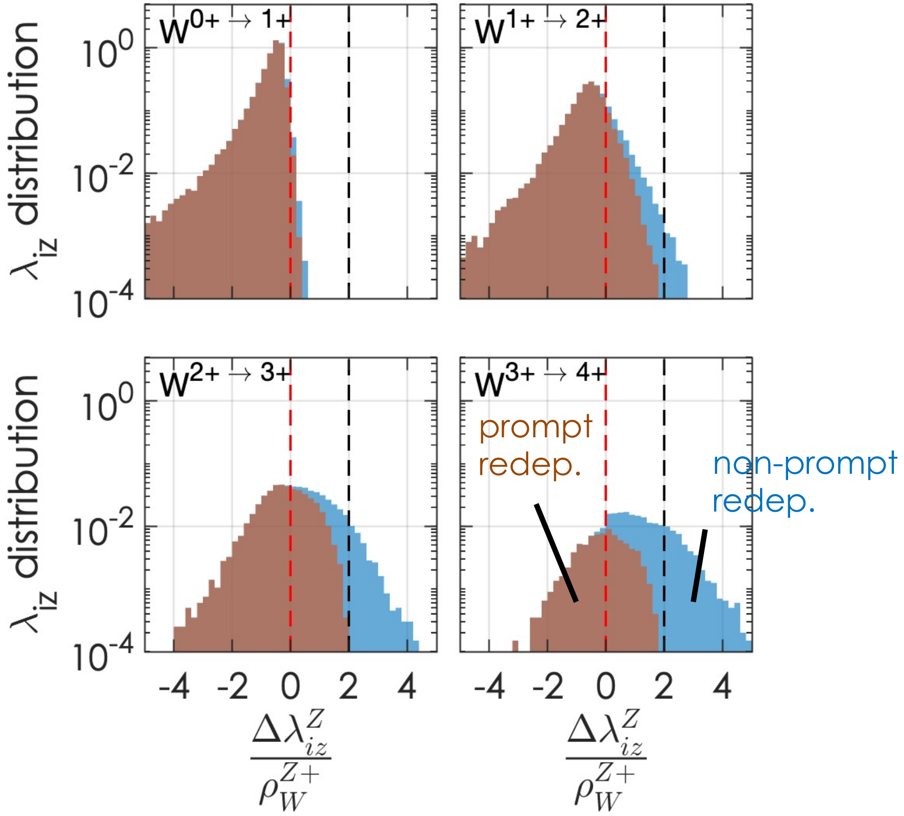
$$\sigma_{sheath}^{W} = \frac{Z\Lambda Te}{\frac{1}{2} m_W \omega_c^2 \lambda_{sheath}^2} > \sigma_{critical} = \left(\frac{E_{cutoff}}{E_{binding}}\right) / \Lambda Z$$

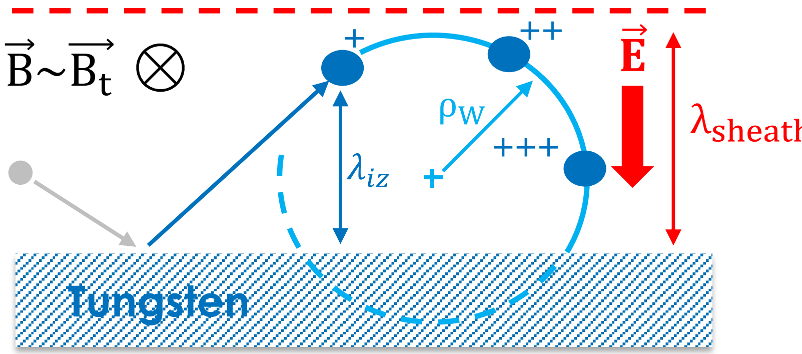




W prompt redeposition scales with the ratio of the neutral W ionization mean-free path over the sheath width

- **Only W impurity ionizing out of the sheath do not promptly redeposit because of the strong sheath electric field**





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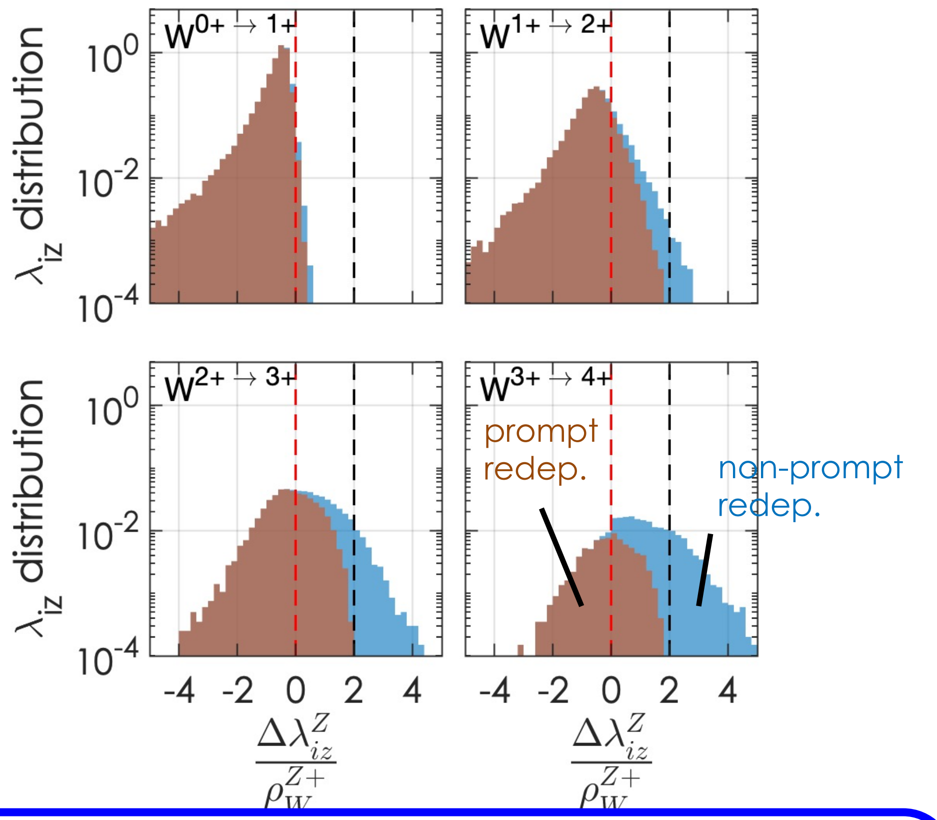

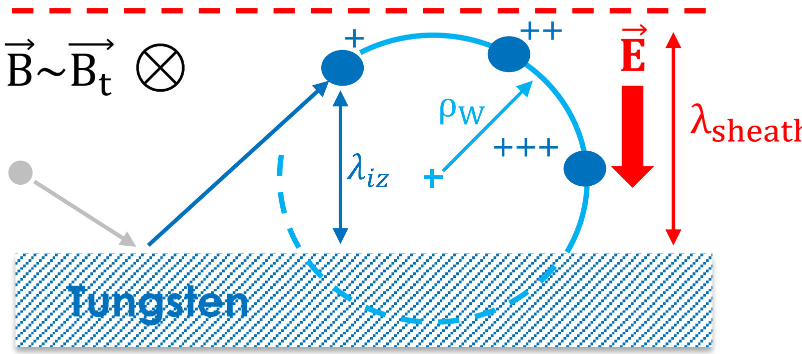

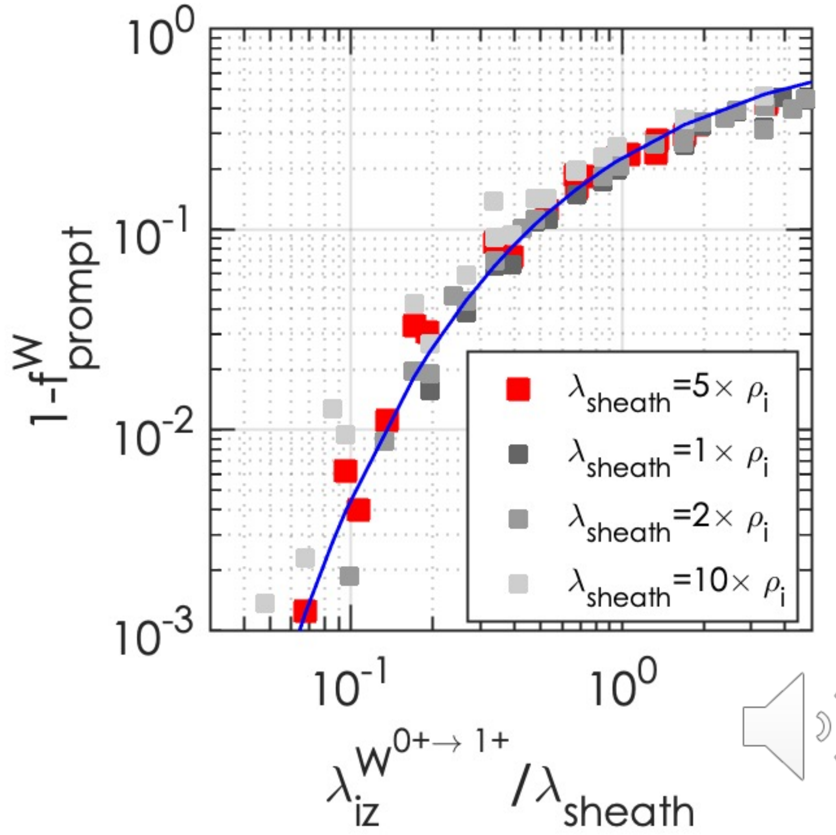

- **W prompt redeposition scales as the W neutral ionization mean-free path over the sheath width:**

$$\frac{\lambda_{iz}^{0+\to1+}}{\lambda_{sheath}} = \frac{<v_W>\tau_{iz}^{0+\to1+}}{\lambda_{sheath}}$$

New scaling law for W prompt redeposition with analytical formulation

- **Consequently, the fraction $1\text{-}f^{W}_{prompt}$ of W impurities non-promptly redeposited is correlated to the fraction f^{W}_{sheath} of W impurities ionized within the sheath:**

$$\mathbf{1 - f^{W}_{prompt} \approx \frac{1}{2}\sqrt{1 - f^{W}_{sheath}}}$$

- **f^{W}_{sheath} can be analytically expressed[1]:**

$$f^{W}_{sheath} = \int_0^{\left(\frac{\lambda_{iz}^{W^{0+\to 1+}}}{\lambda_{sheath}}\right)^{-1}} \Upsilon_{\xi_c}(\eta_b)d\eta_b \text{ where } \xi_c = \frac{E_c}{E_b}$$

[1] J. Guterl CPP 2020 [2] J. Guterl NME 2021

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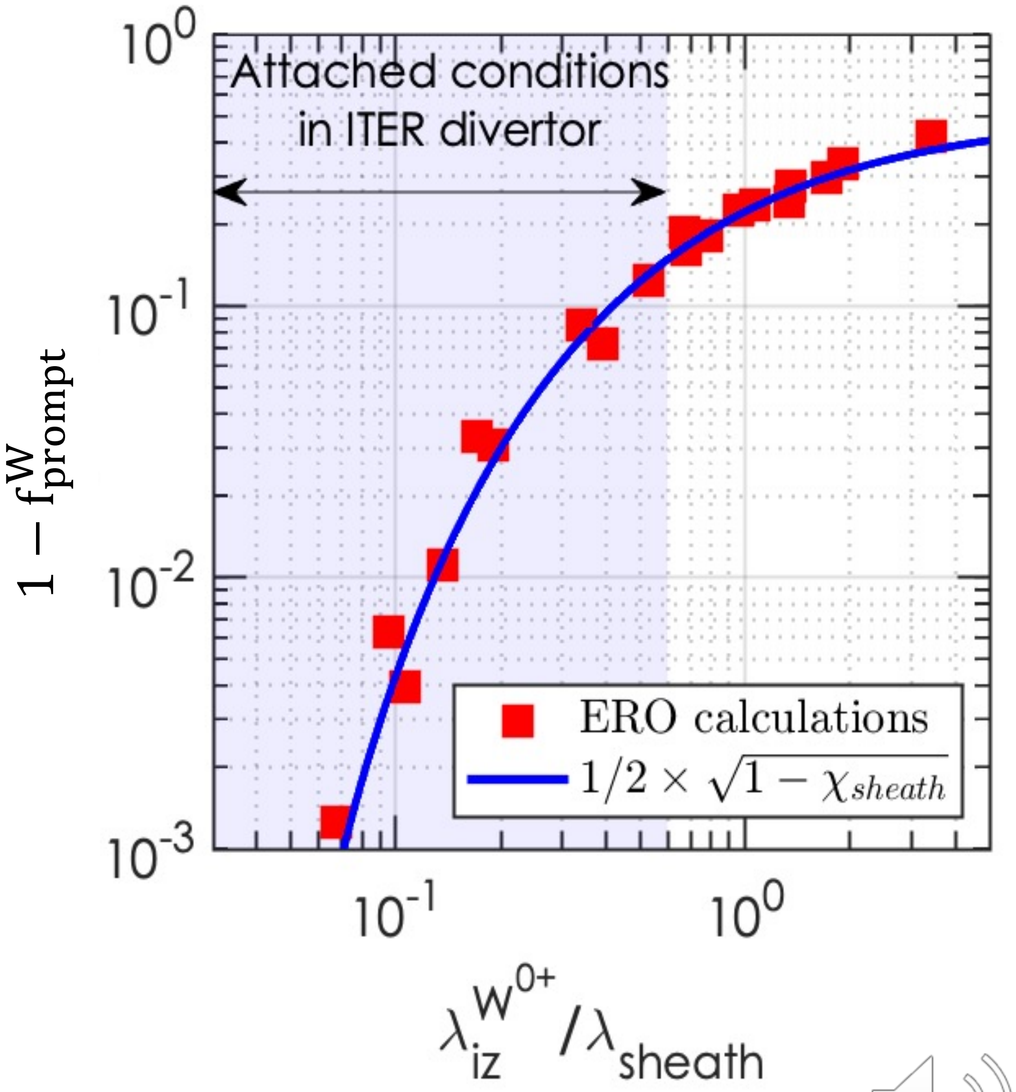

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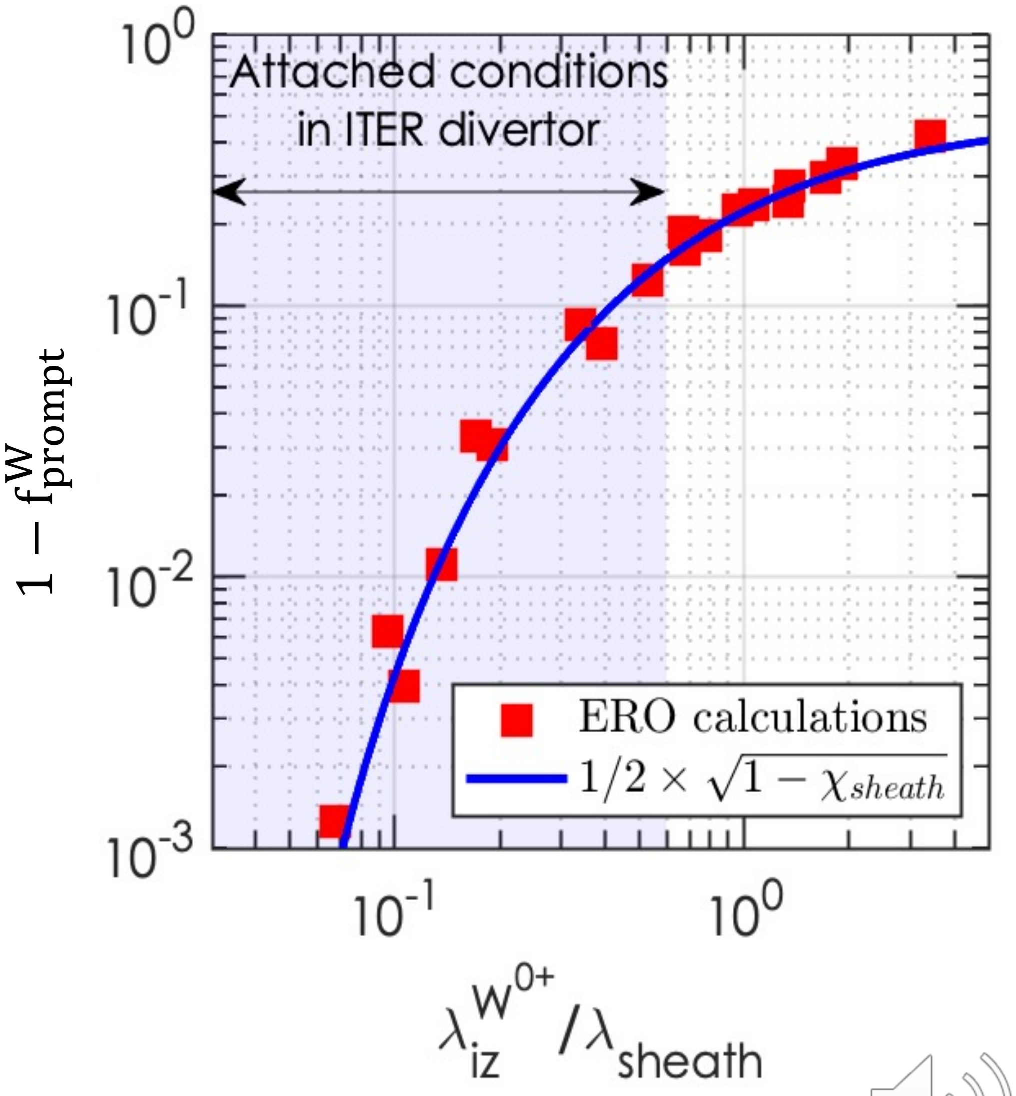
- **New robust analytical scaling law for W prompt redeposition[2]**
- **Tungsten prompt redeposition governed by:**
  - $\lambda_{iz}^{W^{0+\rightarrow 1+}}$: tungsten ionization rates
  - λ_{sheath}: width of the sheath
  - E_c: tail of the energy distribution of sputtered W particles, determined by energy of particles impinging on W PFCs



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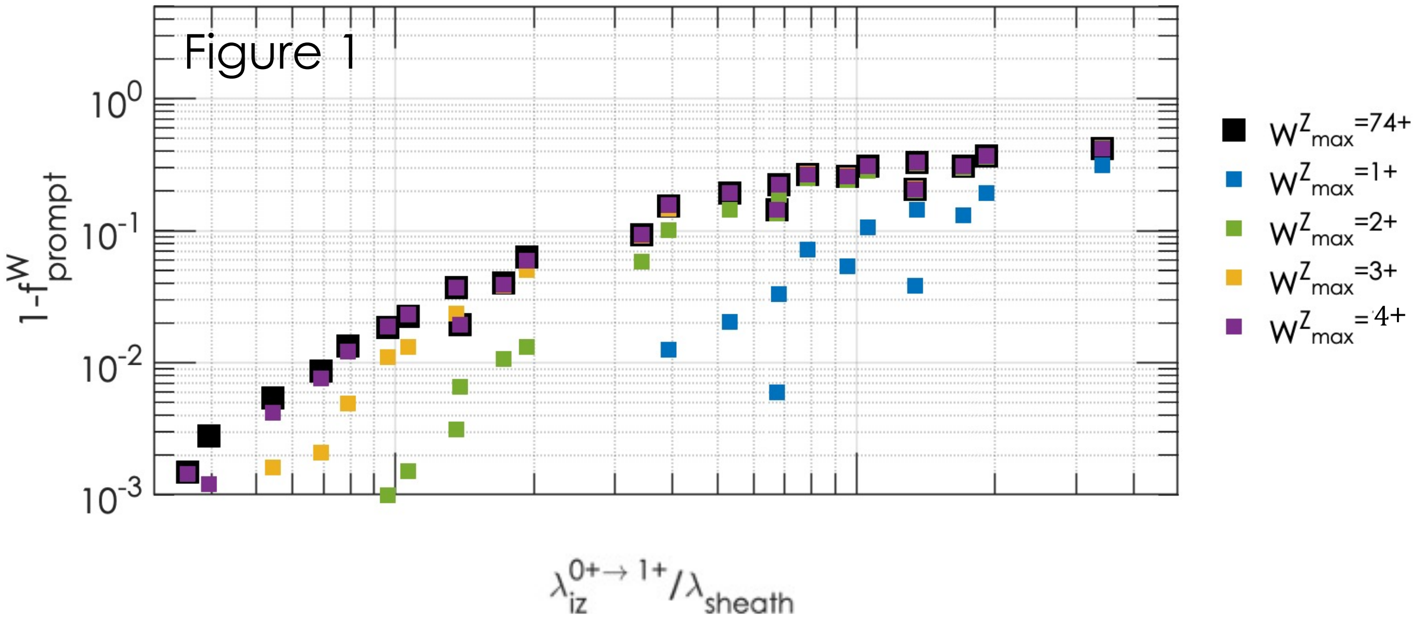
W prompt redeposition not directly correlated to the multiple ionizations of W impurities during their first gyro-orbit

- **<u>How to monitor tungsten prompt redeposition and net erosion in tokamak divertors?</u>**

- **Multiple ionizations of W impurities during their first gyro-orbit still critical to allow W impurities to prevent re-entering in the sheath region and avoid prompt redeposition (fig. 1) …**



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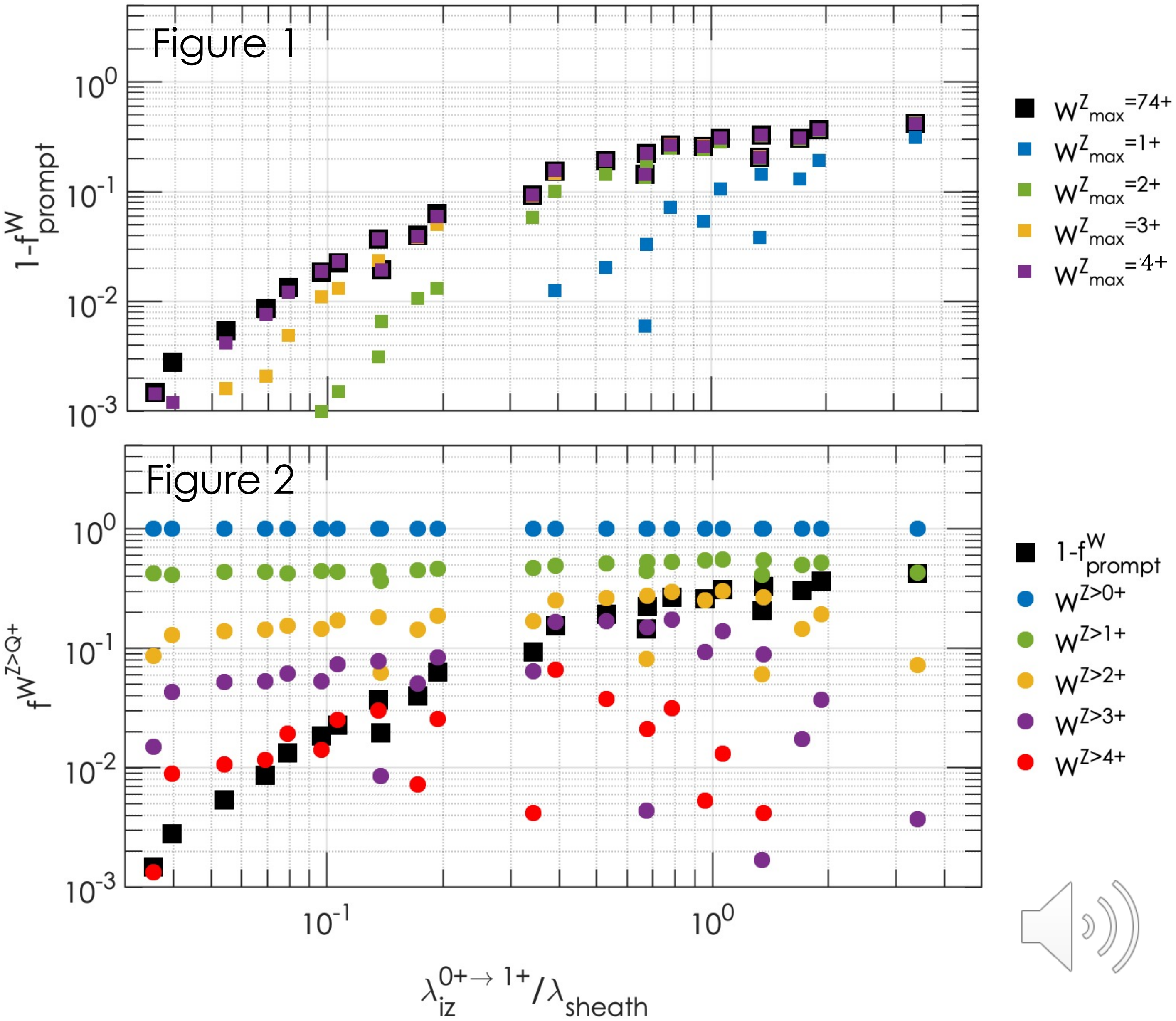
- **… but no global correlation between tungsten prompt redeposition and W ionization events across divertor conditions (fig. 2) !**

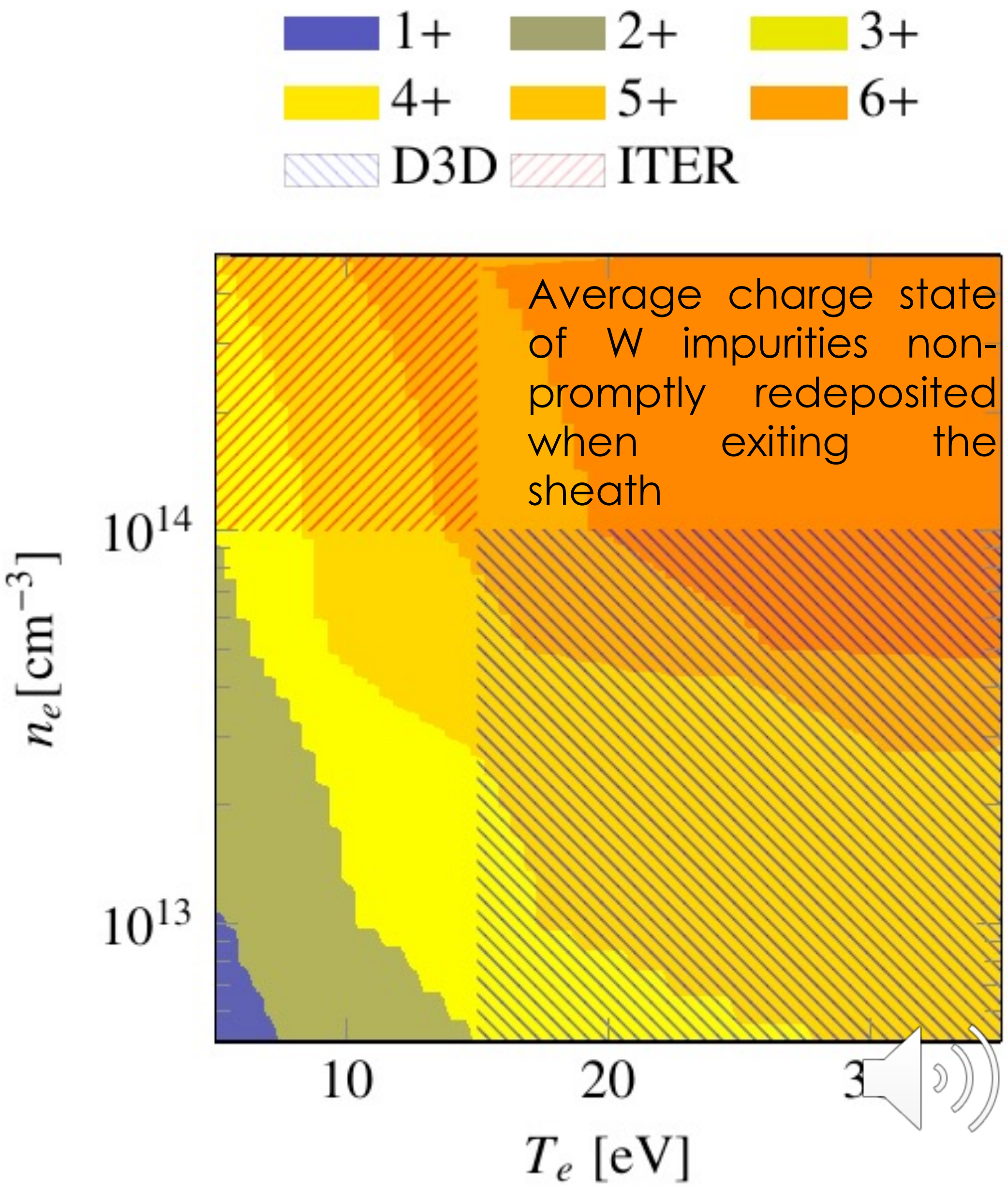


In-situ monitoring of W net erosion in ITER divertor requires spectroscopic measurements of emissions from W-III, W-IV and W-V lines

- In absence of global correlation between ionizations and prompt redeposition of W impurities, spectroscopic measurement of multiple emission lines required to monitor W net erosion

- In-situ monitoring of W net erosion only possible through spectroscopic measurements of W-III, W-IV and W-V emission lines

- Dominant charge-states for non-promptly redeposited W impurities expected to be similar in current tokamaks, e.g. DIII-D, and in future fusion devices (ITER) operating at higher divertor plasma density



In-situ monitoring of W erosion through S/XB coefficients strongly affected by the ionization and emission of sputtered W impurities within the sheath region

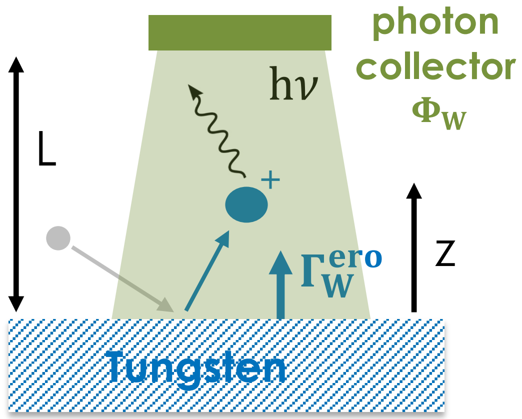
- **W gross erosion flux given by** $\Gamma_W^{ero} = \int_0^L S_{iz}^{W^{0+}\rightarrow W^{1+}}(T_e, n_e)\, n_{W^{0+}}\ n_e\, dz$

- Introducing the photon emissivity coefficient $\sigma_{photon}^{W^{0+\rightarrow 1+}}$, W gross erosion flux can be inferred using the S/XB coefficient[1]

$$\Gamma_W^{ero} = \int_0^L \underbrace{\frac{S_{iz}^{W^{0+\rightarrow 1+}}(T_e,n_e)}{\sigma_{photon}^{W^{0+\rightarrow 1+}}(T_e,n_e)}}_{S/XB^{W^{0+\rightarrow 1+}}} \times \underbrace{\sigma_{photon}^{W^{0+\rightarrow 1+}}(T_e, n_e)\, n_{W^{0+}} n_e dz}_{\Phi_W}$$

- It is usually assumed $\lambda_{sheath} < \lambda_{iz}^{W^{0+\rightarrow 1+}}$, such that $\Gamma_W^{ero} = S/XB^{W^{0+\rightarrow 1+}} \times \Phi_W$

- **But when** $\lambda_{iz}^{W^{0+\rightarrow 1+}} < \lambda_{sheath}$, $\Gamma_W^{ero} = \underbrace{\frac{\int_0^L S_{iz}^{W^{0+\rightarrow 1+}}(T_e,n_e(z))\, n_{W^{0+}}(z) n_e(z)\, dz}{\int_0^L \sigma_{photon}^{W^{0+\rightarrow 1+}}(T_e,n_e(z))\, n_{W^{0+}}(z) n_e(z) dz}}_{< S/XB^{W^{0+\rightarrow 1+}} >_{eff}} \times \Phi_W$



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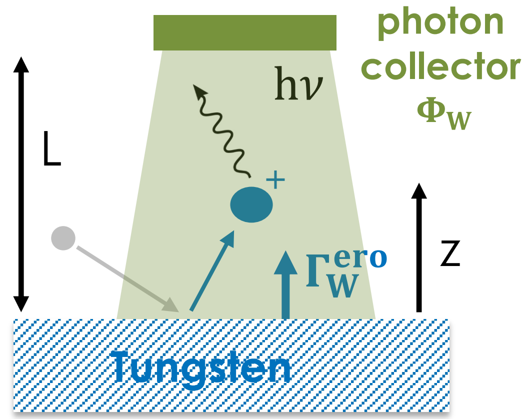
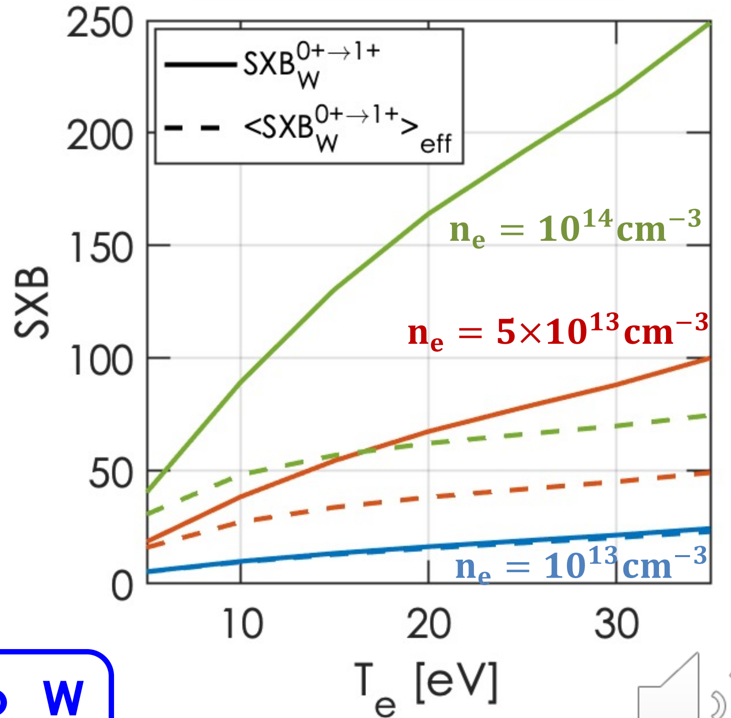


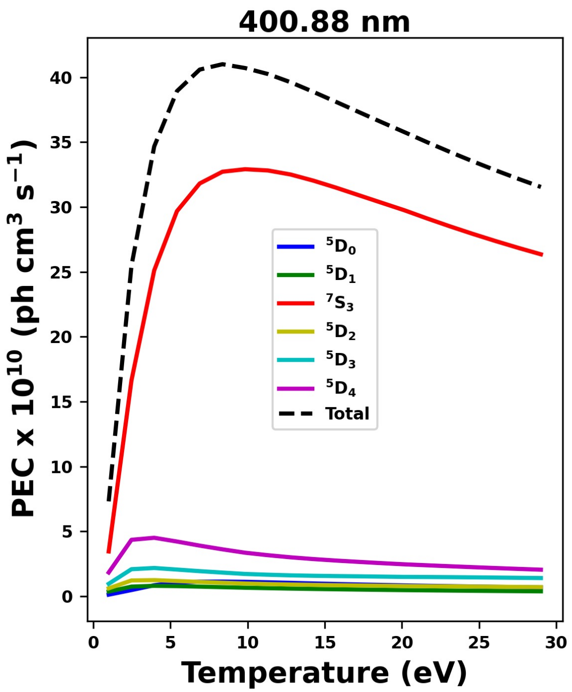


Reduction of the effective SXB coefficients at high n_e due to W ionization and emission within the electric sheath[2]

[1] K. Behringer PPCF 1989
[2] J. Guterl CPP 2020

Transient W metastable states also shown to impact S/XB coefficients

- Using excitation rates from a new non-perturbative Dirac R-matrix electron-impact calculation for WI[1] , it can be shown[3]:
  - **W I PECs for intense spectra lines are dominated by a single metastable level*,****
  - **Total value of the ionization coefficient for neutral tungsten is relativel insensitive to changes in the metastable fraction**



[1] Smyth *et al.* Phys. Rev. A 2018 [2]Johnson *et al. PPCF* 2020 [3] C. Johnson *et al. NME* 20..

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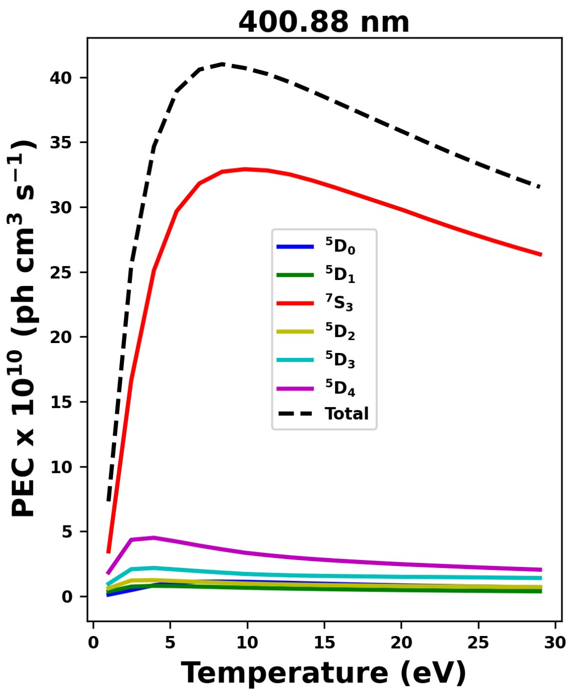
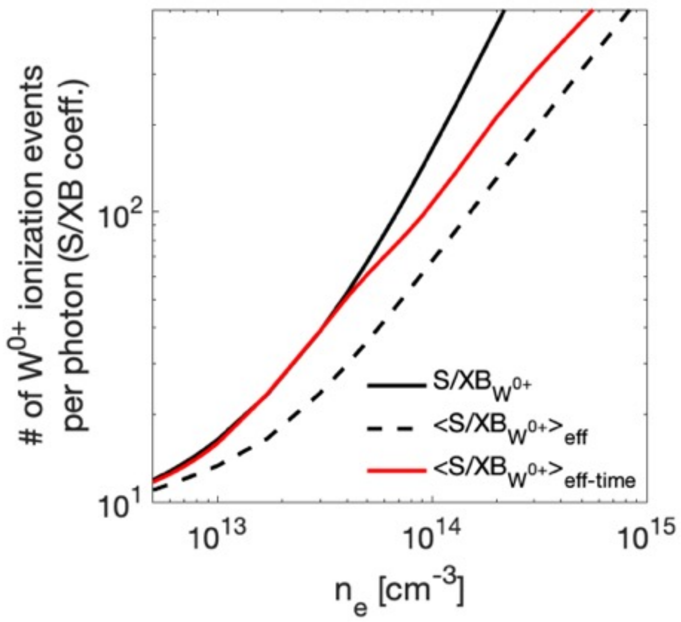


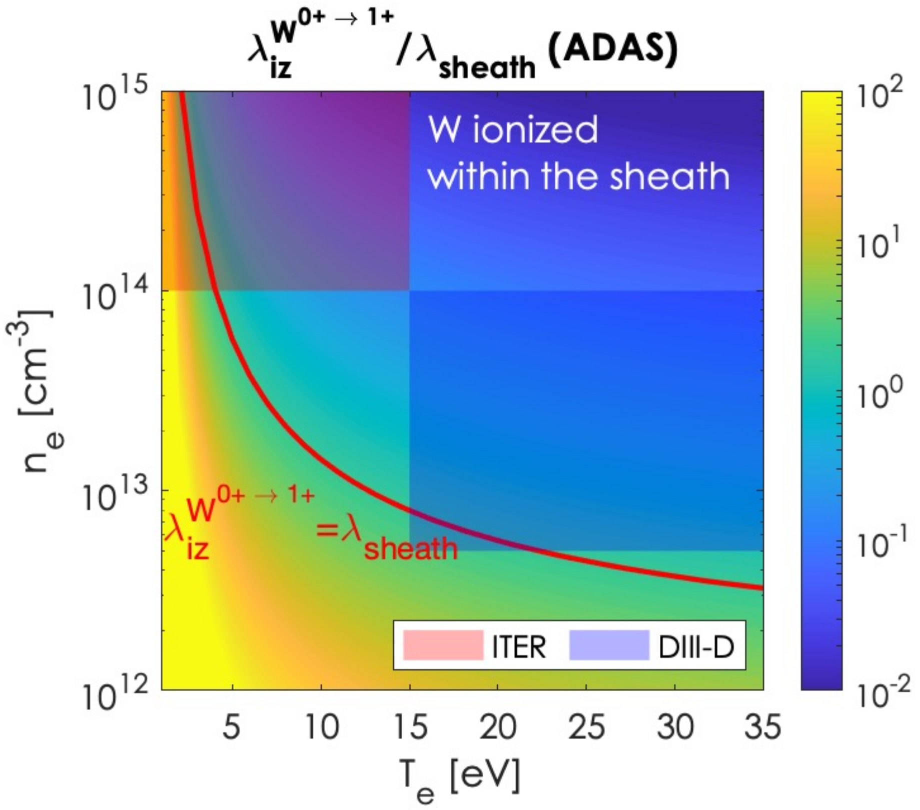


- Using the new collision-radiative solver ColRadpy[3] :
  - **Time dependent effective S/XBs can deviate significantly from steady-state due to non-equilibrium population of metastable state**

[1] Smyth *et al.* Phys. Rev. A 2018 [2]Johnson *et al. PPCF* 2020 [3] C. Johnson *et al. NME* 20…

Predictive modeling for W net erosion in divertors can be validated with innovative experiments in DIII-D

- W prompt redeposition governed by the ratio of W neutral ionization mean-free path over the sheath width: $\lambda_{iz}^{W^{0+\to 1+}} / \lambda_{sheath}$
- **Divertor plasma conditions in DIII-D significantly different than in ITER but values of $\lambda_{iz}^{W^{0+\to 1+}} / \lambda_{sheath}$ are similar**
  - **Regime of W prompt redeposition similar for DIII-D and ITER divertor conditions**



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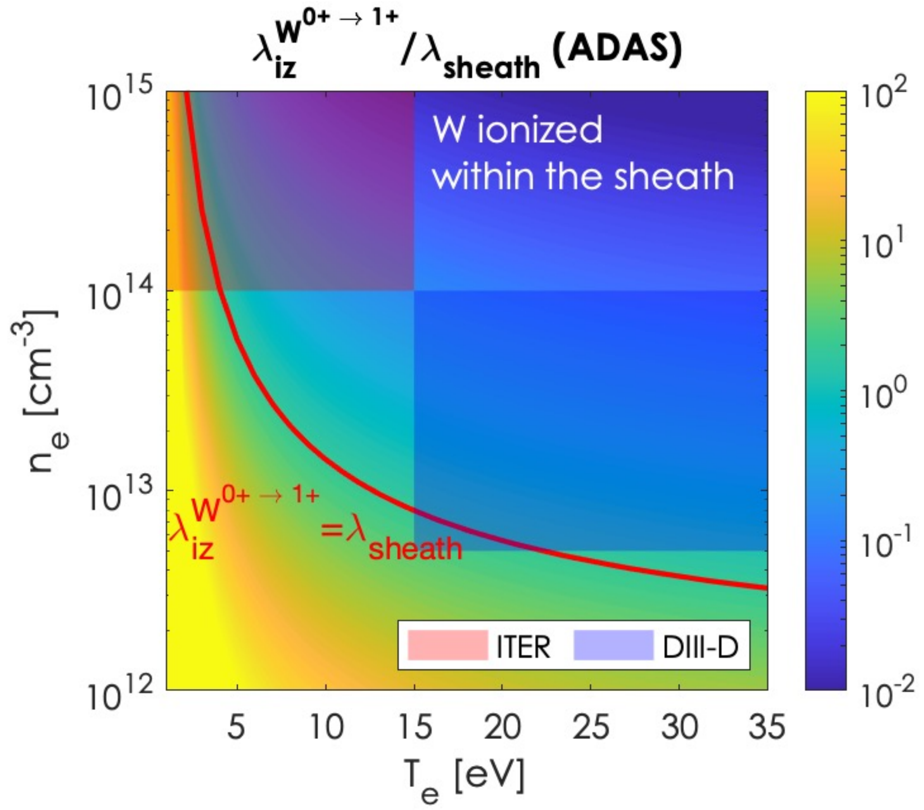
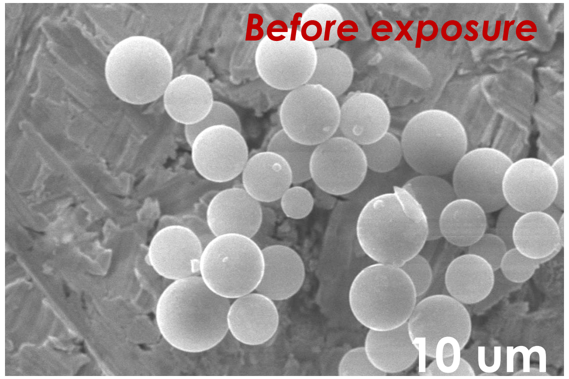
Experiments conducted at DIII-D to validate predictive modeling of W net erosion and assess physics parameters governing W net erosion:

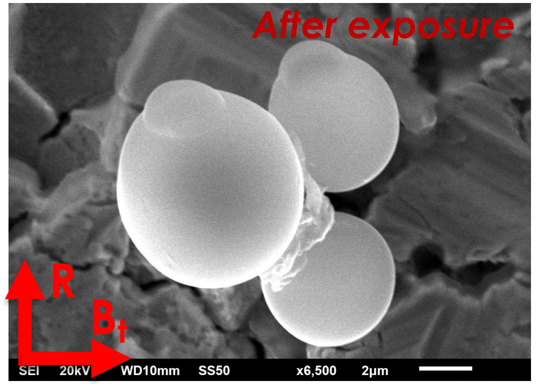
- Experimental estimations of the sheath width
- Direct measurement of W net erosion



Experimental estimation of the sheath width in the DIII-D divertor from the erosion of carbon micro-spheres

- Sheath width λ_{sheath} at divertor targets numerically estimated with PIC and kinetic simulations[1]: $\boldsymbol{\lambda_{sheath} = 1.2 \times \rho_i}$
- **Innovative experiments conducted in DIII-D to assess the sheath width :**
  - Angles of incidence of C impurities on divertor target inferred from small C deposition caps observed on C micro-spheres after exposure
  - ERO simulations show that angle of incidence of carbon impurities mainly determined by sheath width





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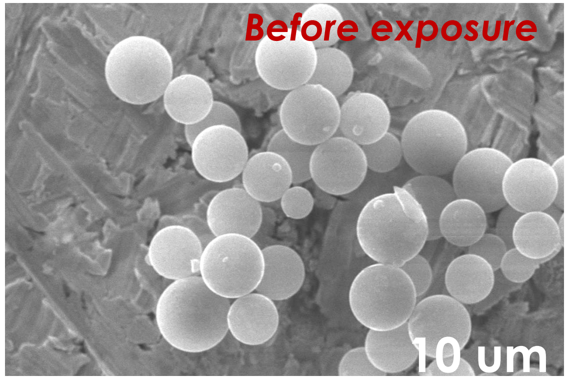
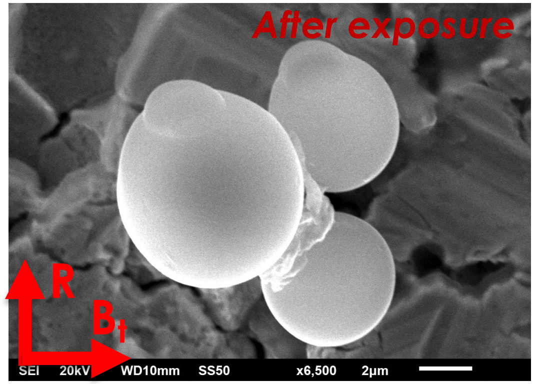
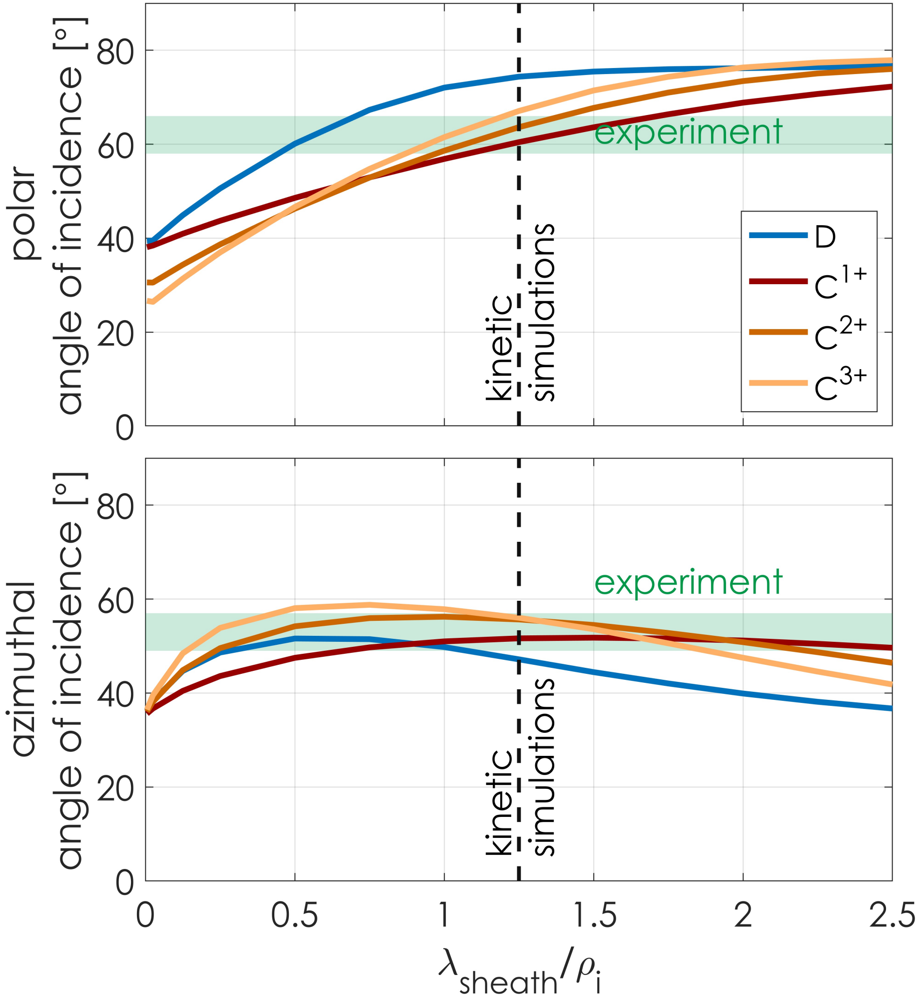






- **λ_{sheath} inferred from the measurement of the angle of incidence of C ions impinging on divertor target in excellent agreement with kinetic simulation[1] of the sheath on divertor targets!**
- **Similar experiments conducted with micro-trenches**

[1]D. Coulette *PPCF* 2016

Experimental validation of model for W prompt redeposition and net erosion in DIII-D divertor with DiMES

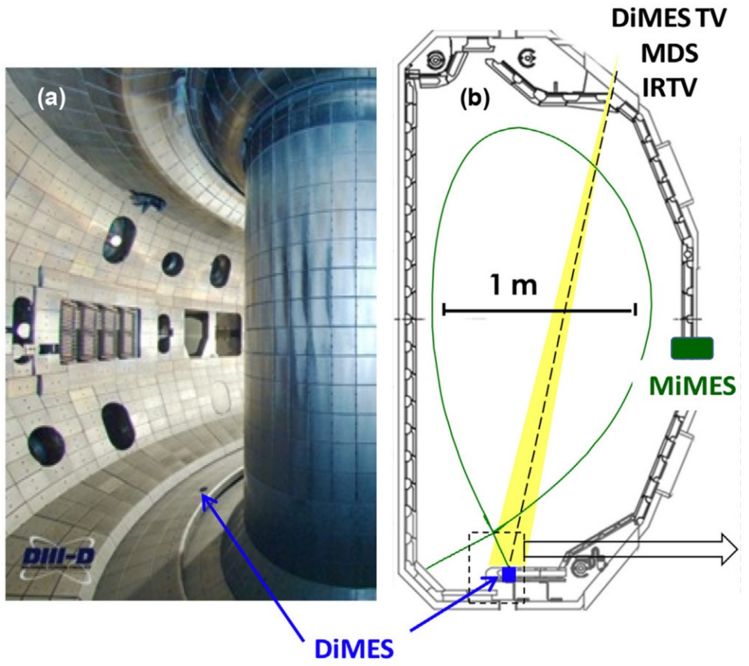
- The Divertor Material Evaluation System (DiMES) allows for exposure of material samples in the lower divertor of DIII-D under well-diagnosed plasma conditions

- Experimental estimations of W net erosion through small/large dots DiMES experiments in DIII-D[1,2]:

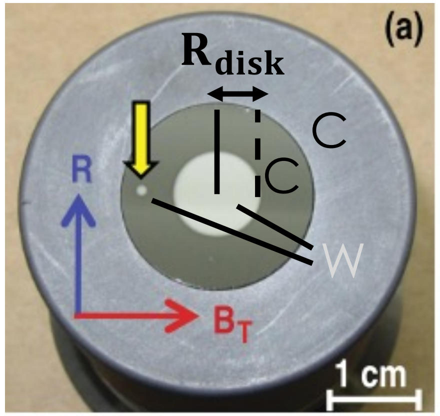
$$< \Gamma_W^{net} >_{R_{disk}} = \Gamma_W^{gross}\left(1 - \xi_{redep}(R_{disk})\right)$$

ξ_{redep}: Fraction of W redeposited on W sample

- Strong dependency of ξ_{redep} on R_{disk} when $R_{disk} \sim \lambda_{redep} \sim 1mm$



DiMES with small and large W dots[1]



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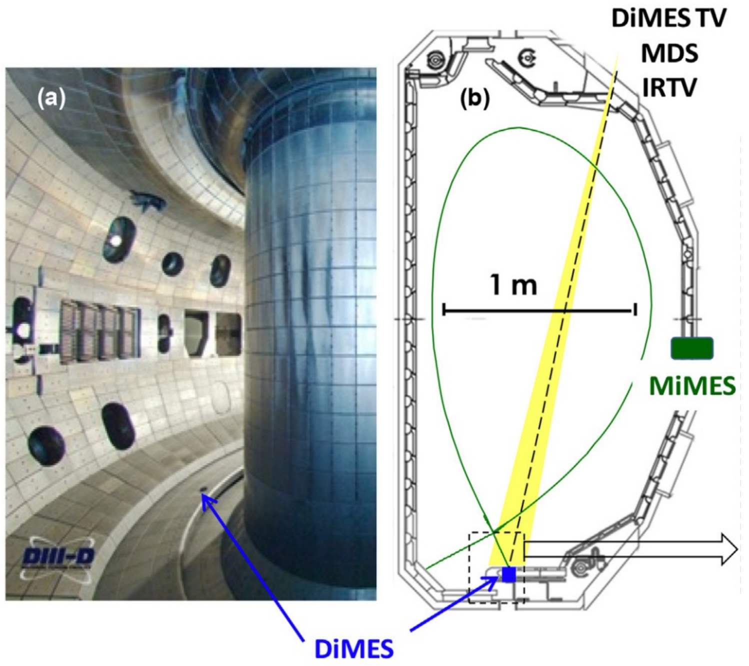
- **Experimental validation of model for W prompt redeposition and net erosion through comparison of net erosion from small and large W dots exposed in DIII-D divertor with DiMES**

$$\frac{< \Gamma_W^{net} >_{large\ disk}}{< \Gamma_W^{net} >_{small\ disk}} = \frac{\Gamma_W^{gross}\left(1 - \xi_{redep}(R_{large})\right)}{\Gamma_W^{gross}\left(1 - \xi_{redep}(R_{small})\right)}$$



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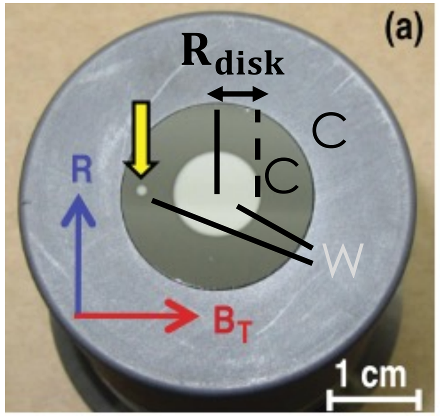

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Reduced model of W prompt redeposition and net erosion in agreement with experimental measurements of W net erosion in DIII-D

- **Reduced model with few characteristic parameters $(\beta_{redep}, \lambda_{redep})$ developed to analyze small/large dots DiMES experiments**

W ionization rates, energy distribution, n_e, T_e, sheath, B field

$\beta_{redep}, \lambda_{redep}$

$$\frac{< \Gamma_W^{net} >_{\text{large disk}}}{< \Gamma_W^{net} >_{\text{small disk}}} = \frac{1 - \xi_{redep}(R_{large})}{1 - \xi_{redep}(R_{small})}$$

[1] J .Guterl PPCF 2019

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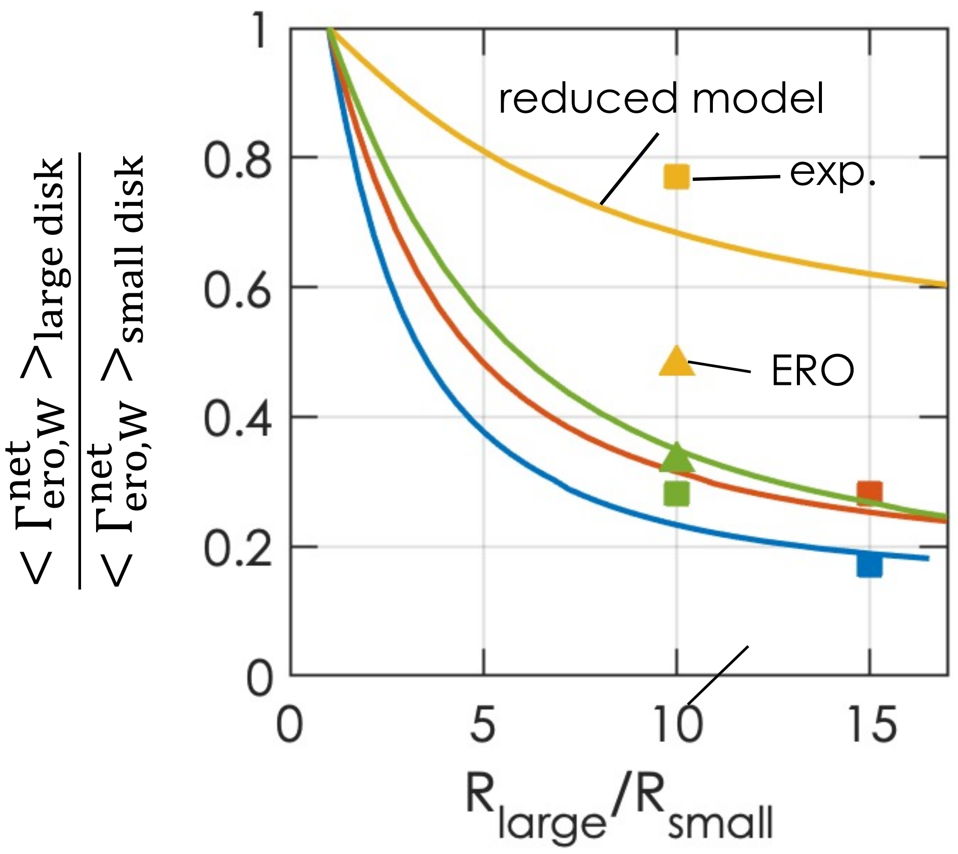

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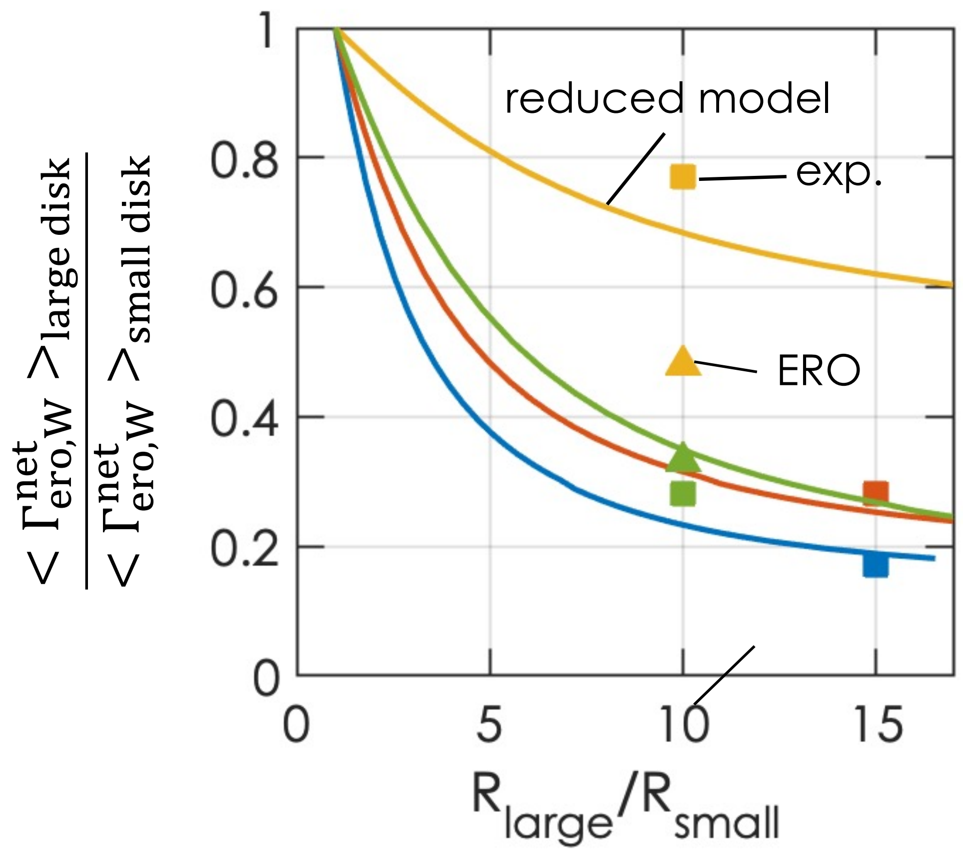
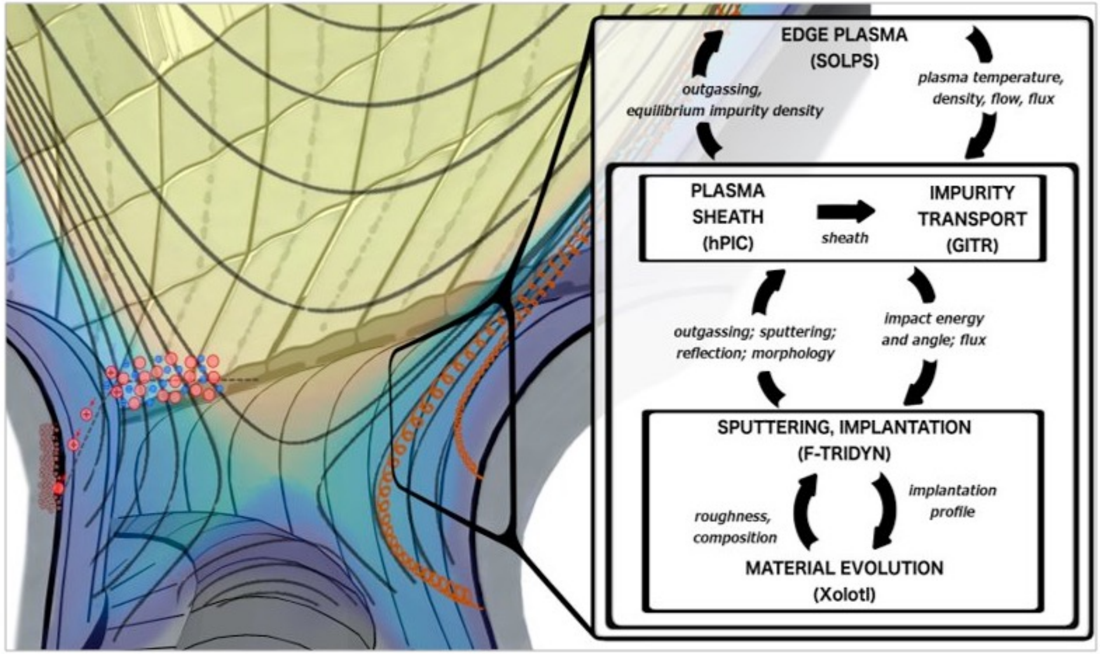


- **Reduced model in good agreement with experimental measurements in various plasma conditions and with comprehensive ERO model[1]**
- **Experimental framework available in DIII-D for quantitative assessment of critical parameters controlling W prompt redeposition and net erosion (W ionization rates, PEC)**

[1] J .Guterl PPCF 2019

PSI-SciDAC: development and integration of HPC simulation tools capable of predicting W PFCs lifetime and impact on plasma performance

- **Large US multi-institutions project led by B. Wirth to predict the performance and impact of dynamic W PFC material[1]**
  - Development and integration of suite of coupled plasma and materials modeling tools to predict **multi-scale PFC evolution and feedback to the boundary plasma**
  - Active framework to apply **uncertainties quantification to PMI codes and workflow[2]**
- Recent focus on modeling of **Be-W system**
- An example of workflow for W divertor PFCs[3,4]:
  - Boundary plasma: SOLPS
  - Plasma sheath: hPIC
  - 3D trace impurity transport: GITR
  - Erosion, surface morphology: F-TryDyn
  - Material evolution due to H, He implantation: Xolotl



[1] Psi-SciDAC [2] O. Cekmer Int. Journ. Uncertain. Quantif. 2018 [3] A. Lasa Physica Scripta 2020 [4] FY2018 report

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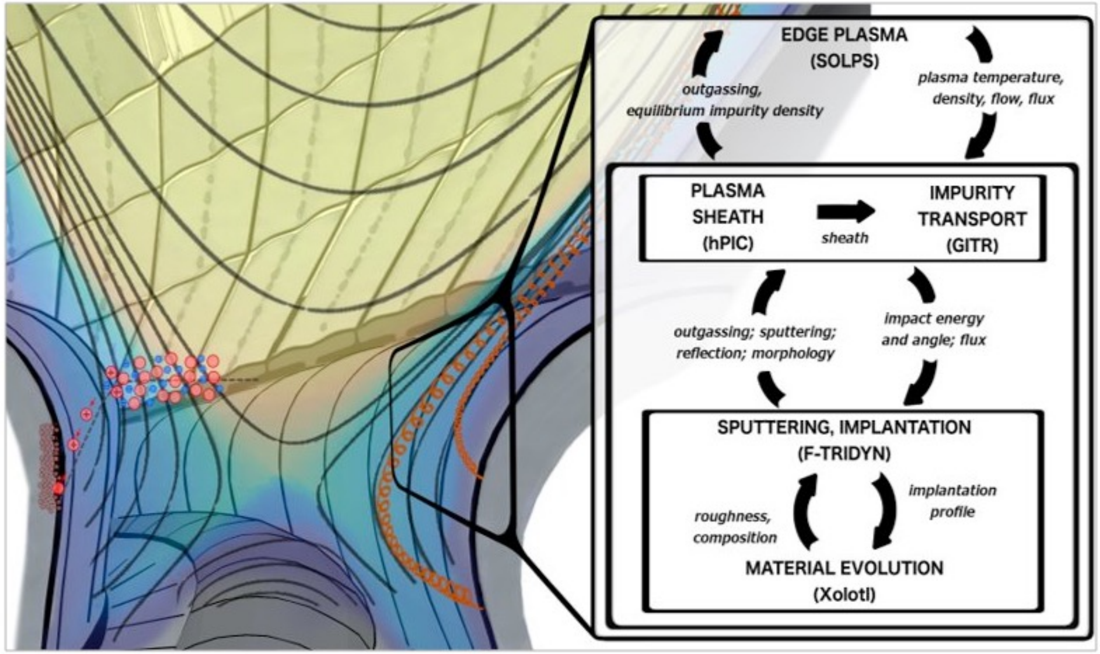

- **HPC simulations tools developed in the PSI-SciDAC project can support ITER goals for PMI modeling**
  - **Framework for collaboration?**

[1] Psi-SciDAC [2] O. Cekmer Int. Journ. Uncertain. Quantif. 2018 [3] A. Lasa Physica Scripta 2020 [4] FY2018 report

Summary

- **Tungsten(W) prompt redeposition in tokamak divertors is mainly governed by the ratio of the ionization mean-free path of sputtered neutral W particles over the sheath width:**
  - ***New scaling law for W prompt redeposition with analytical formulation***
- **In-situ monitoring of W net erosion in divertors requires *monitoring photon emissions associated with the ionization of W impurities in charge states Z > 2+, typically W-III, W-IV and W-V lines for ITER***
- **Parameter governing W prompt redeposition has similar values for divertor plasma conditions in DIII-D experiments and in ITER far-SOL:**
  - ***Experiments conducted at DIII-D to validate predictive modeling of W net erosion in ITER divertor and beyond***
    - **Measurement of sheath width from erosion of carbon micro-spheres**
    - **Measurement of W prompt redeposition through small/large dots experiments**
- **HPC simulation tools for W/Be PMI modeling W available through the PSI2-SciDAC project**