Plasma-Wall Interactions

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25 September 2014

| with material supplied by:

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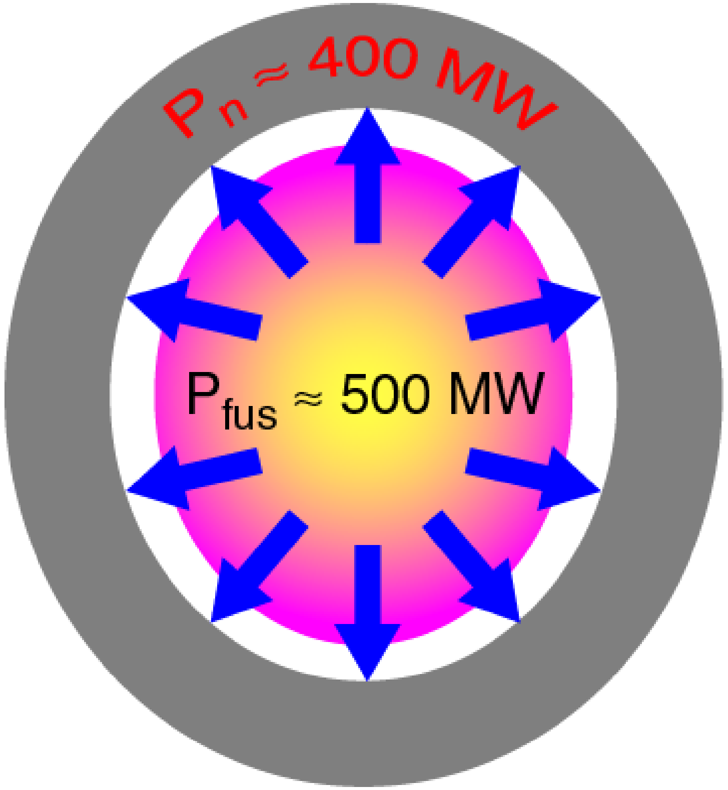
Outline

- Why do we need a wall?
- What are power and particle fluxes to the wall?
- Which are the fundamental processes during PWI?
- What are ITER-specific PWI issues?
- Summary

Why do we need a wall?

The role of material walls

Example ITER



$P_\alpha \approx 100$ MW

$P_{aux} \approx 40$ MW

1. VACUUM CONDITIONS

   Unlike the sun, a fusion plasma can only be maintained under ultra high vacuum conditions -

   base pressure ≈ O(10^{-8} mbar)

2. EXTRACTION OF POWER

   The α-particle power and auxiliary injected power used to heat the plasma must be finally extracted through the plasma facing wall

   Power carried by neutrons is converted to heat in blanket wall

   neutrons also breed tritium in blanket

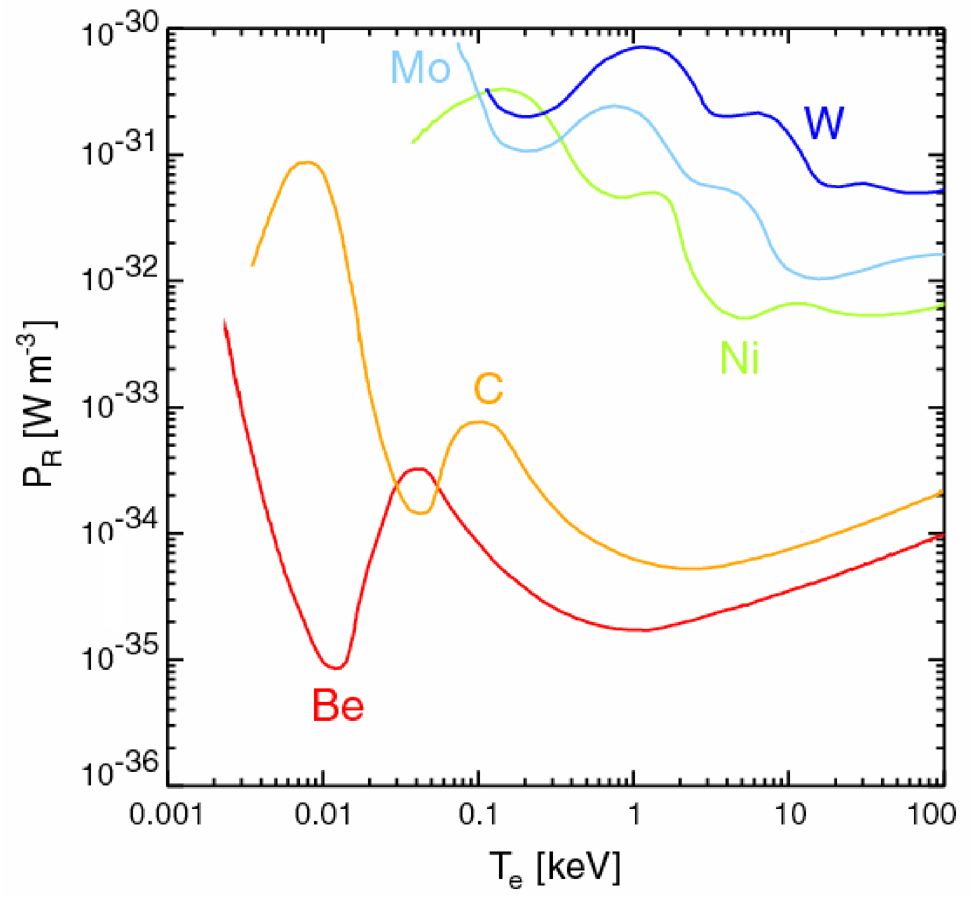
3. HELIUM REMOVAL

   The removal of the helium ash requires thermalisation and neutralisation of plasma ions

“Clean” D+T plasma: limited impurities

Impurities are not all fully ionized

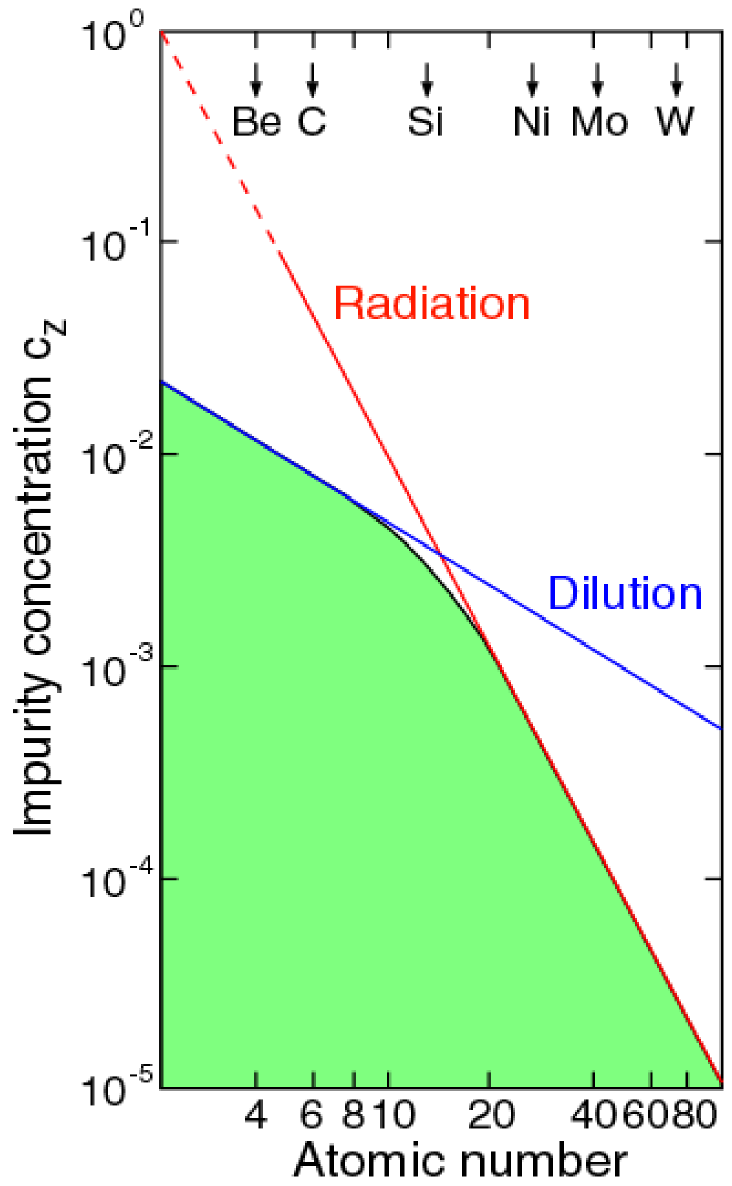
- Electronic transitions possible
- Power loss by radiation



"Clean" D+T plasma: limited impurities

Plasma is quasi-neutral

- Impurities dilute the plasma
- Each impurity of charge Z "displaces" Z-fuel ions



Power exhaust and limitation of the plasma

Heating power leaves the plasma in form of:

- radiation
- kinetic energy of escaping particles.

⇩

Direct contact of the plasma with the vessel walls must be avoided.

Imperfections in the magnetic configuration or displacement of the plasma might lead to concentrated heat deposition on areas that are difficult to control and cool.

⇩

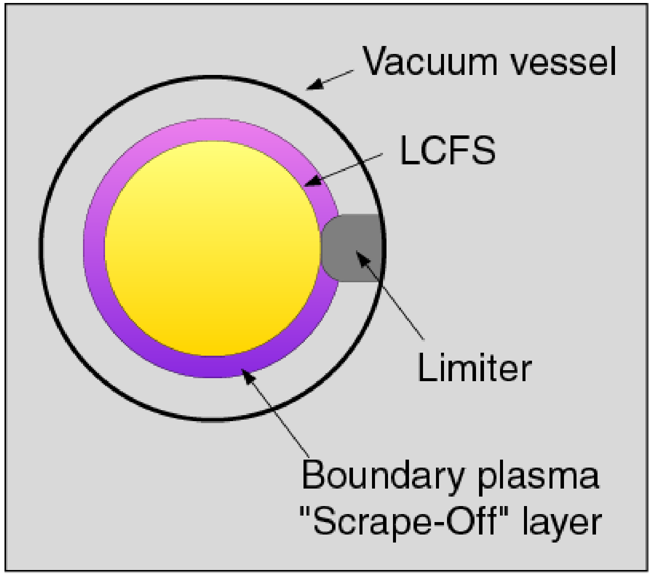
The plasma edge must be controlled (limited).

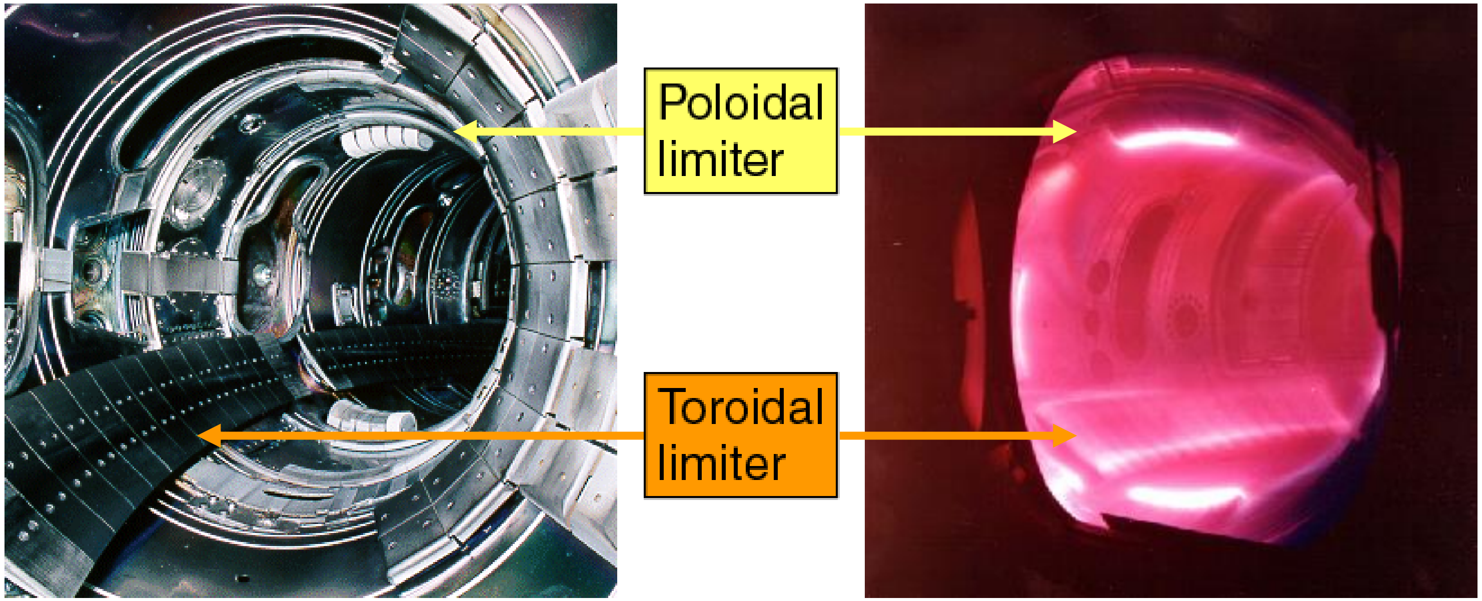
Plasma limiters

Limiter:
A material structure protruding from the main wall used to intercept particles at the plasma edge.

Last Closed Flux Surface (LCFS):
The magnetic surface that touches the innermost part of the limiter.

Scrape-off Layer (SOL):
The plasma region located in the limiter shadow i.e. between the LCFS and the vessel wall.

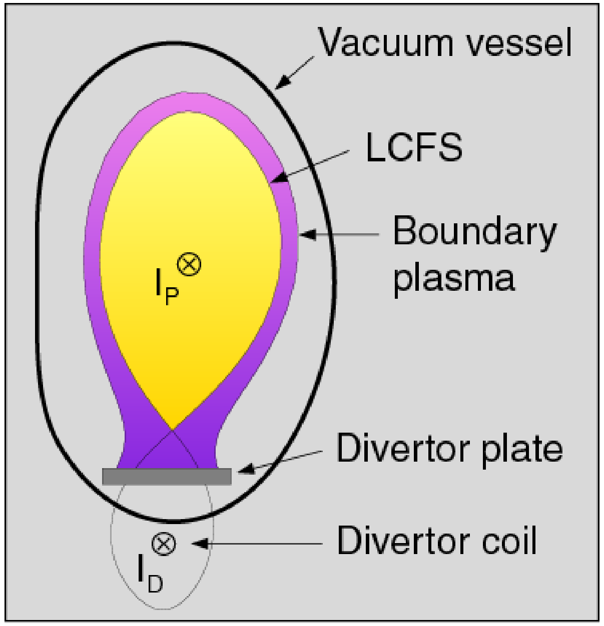


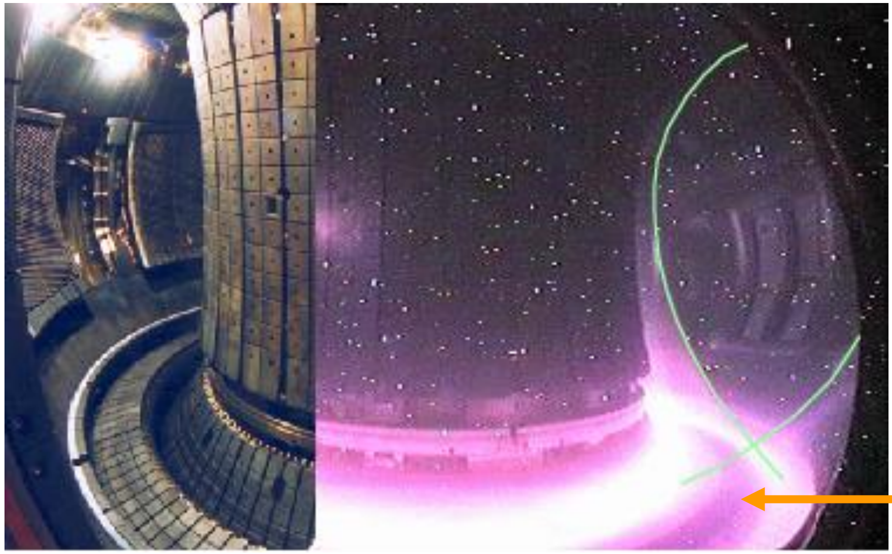


Plasma divertors

Divertor:
A separate region in the vacuum vessel to which escaping ions are exhausted || B by means of auxiliary magnetic coils.

The magnetic boundary between confined plasma and edge/divertor plasma is called **separatrix** ≡ LCFS





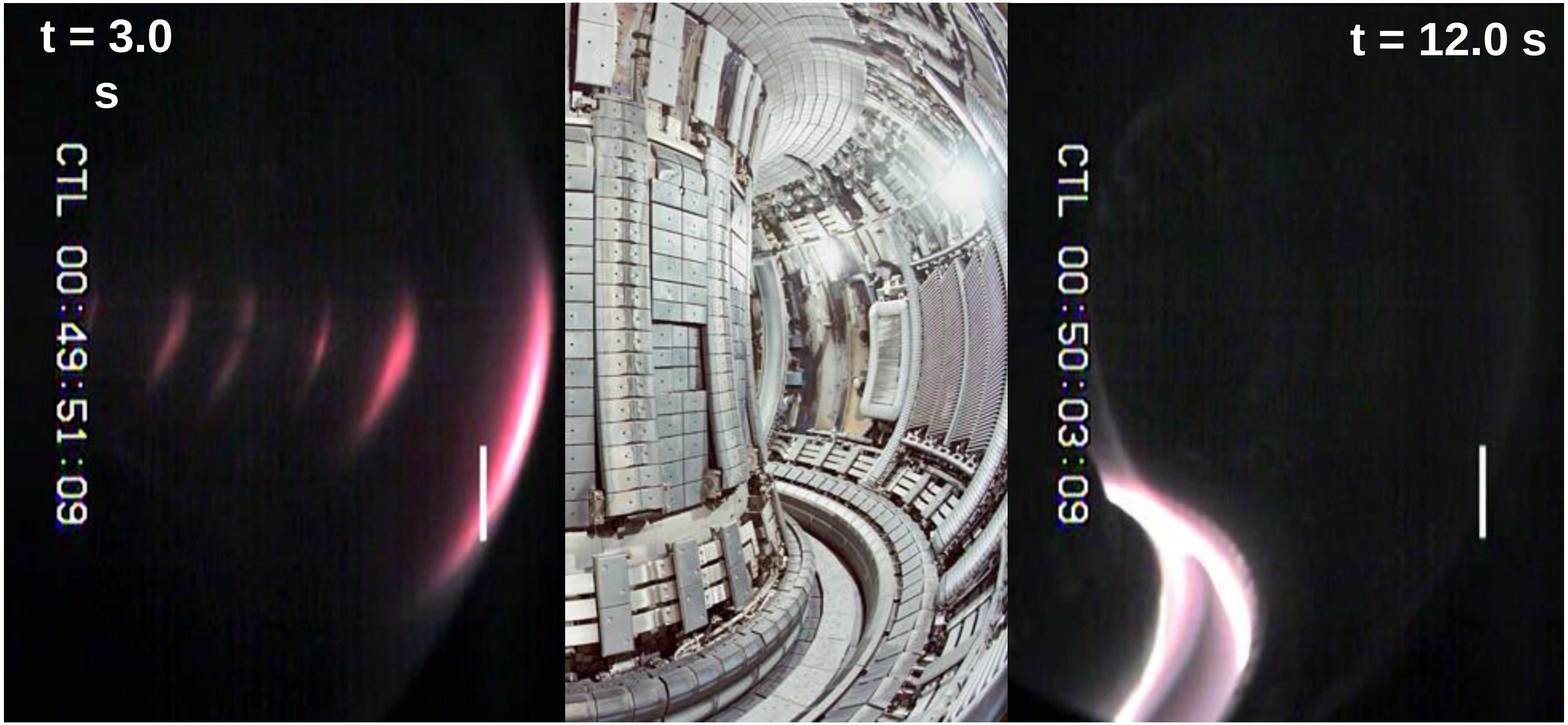
The divertor in ASDEX Upgrade

Limiter vs. divertor operation

Divertor tokamaks need limiters for discharge ramp-up and shutdown

Example: JET

#62218: plasma visible light emission

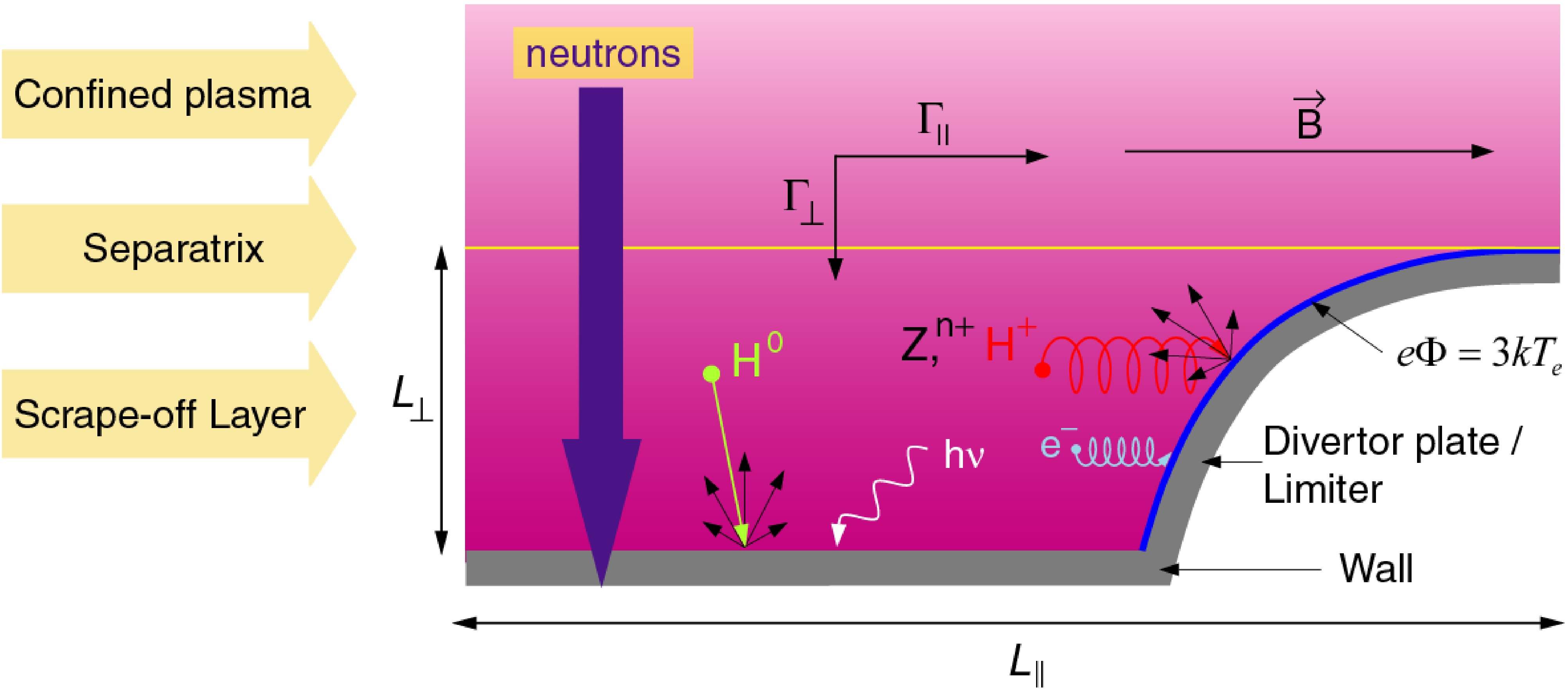


Limited **Diverted**

R.A. Pitts, EPS 2005

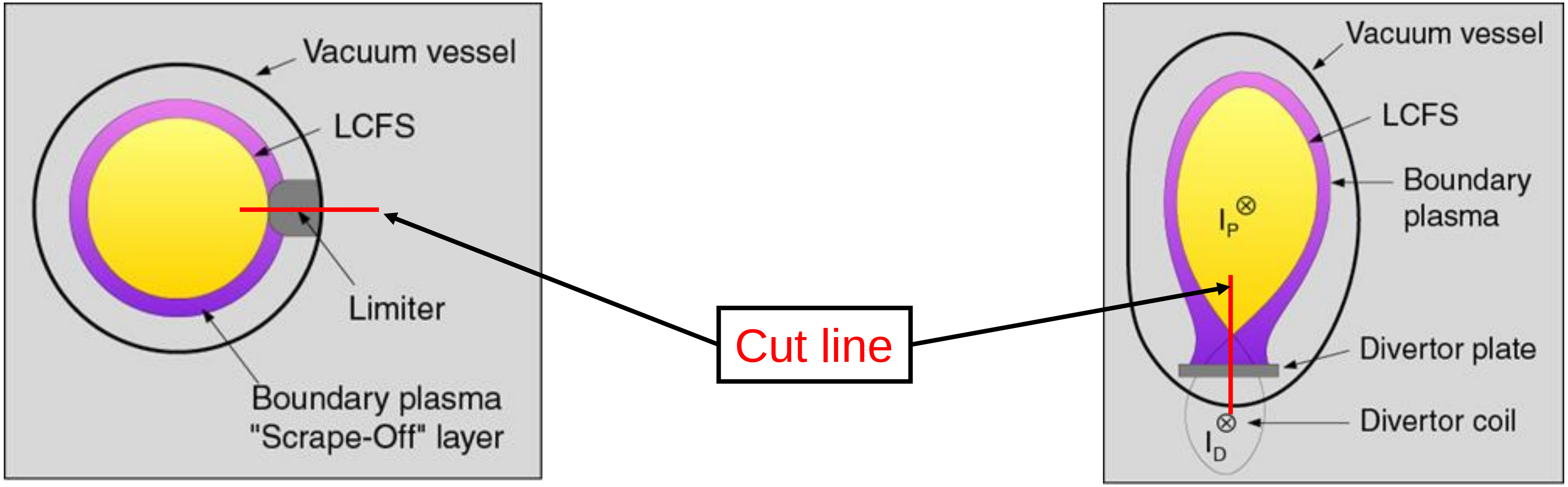
What are power and particle fluxes to the wall?

Plasma-material interactions

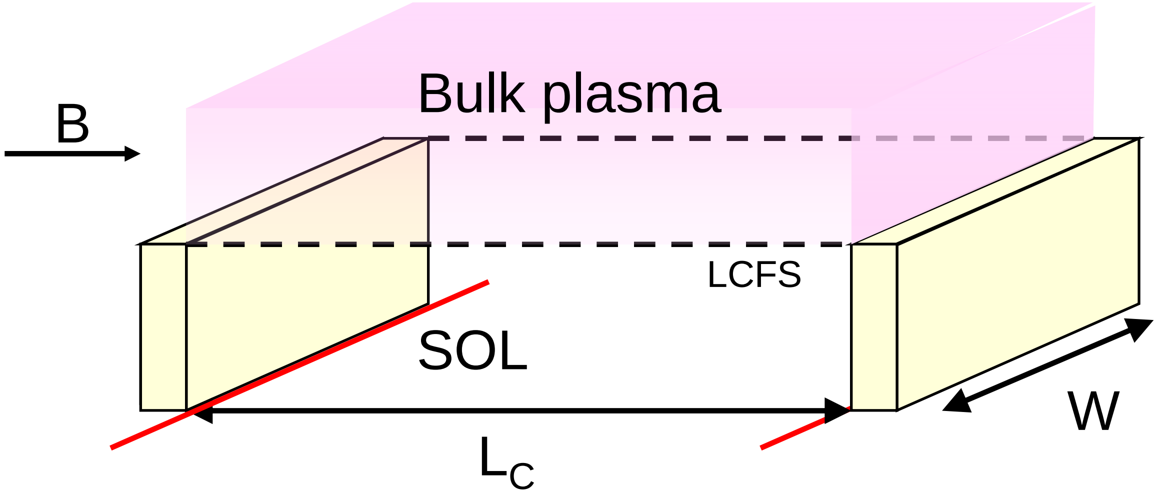


Edge plasma: particle flux to the wall

In both limiter and divertor plasmas wall elements are connected by field lines



In "field aligned" coordinates this can be drawn as a 2.5 dimensional problem

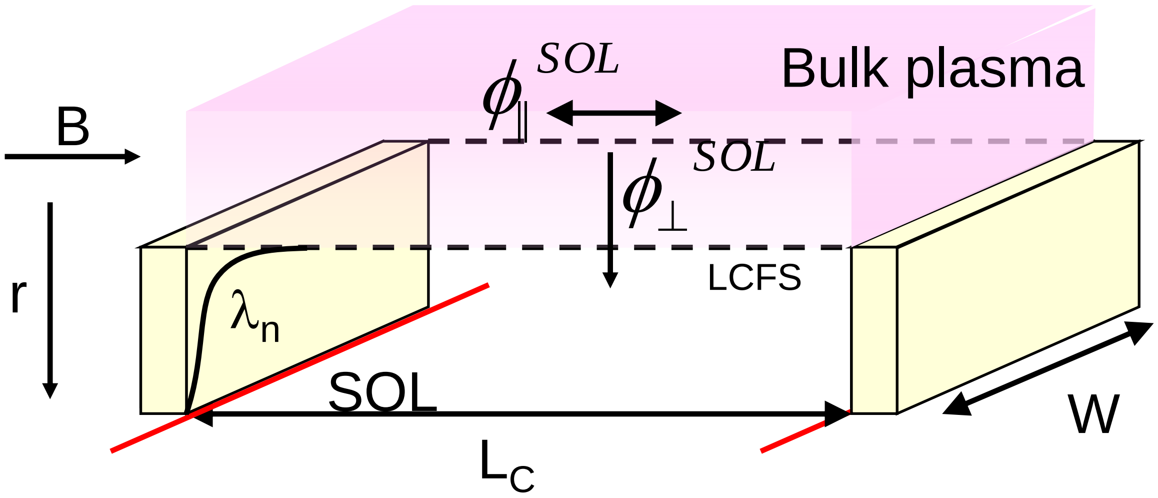


(Simplified) estimate of ion particle flux

$$\Phi_{\parallel}^{SOL} = 2W \int_{r_{LCFS}}^{\infty} n(r) c_s dr \quad \left(s^{-1}\right)$$

$$= 2W \int_{r_{LCFS}}^{\infty} n\left(r_{LCFS}\right) e^{-r/\lambda_n} c_s dr$$

$$\Phi_{\perp}^{SOL} = -D_{\perp}^{SOL} \left.\partial n / \partial r\right|_{LCFS} L_C W \quad \left(s^{-1}\right)$$



Flux balance

$$\Phi_{\perp}^{SOL} = \varphi_{\parallel}^{SOL} \Rightarrow \lambda_n = \sqrt{2D_{\perp}^{SOL} L_C / c_S} \approx \mathrm{O}(0.01)\,\mathrm{m}$$

$$\Phi_{\parallel}^{SOL} = 2Wn\left(r_{LCFS}\right) c_s \lambda_n \approx \mathrm{O}\left(10^{21} - 10^{23}\right) \mathrm{s}^{-1}$$

Total flux entering the SOL from the bulk plasma is concentrated radially on length λ_n and toroidally on length W ~ 2πR

→ Flux amplification (~ x100!)
→ Very high power densities (~10 MW/m²)

<u>For comparison:</u>

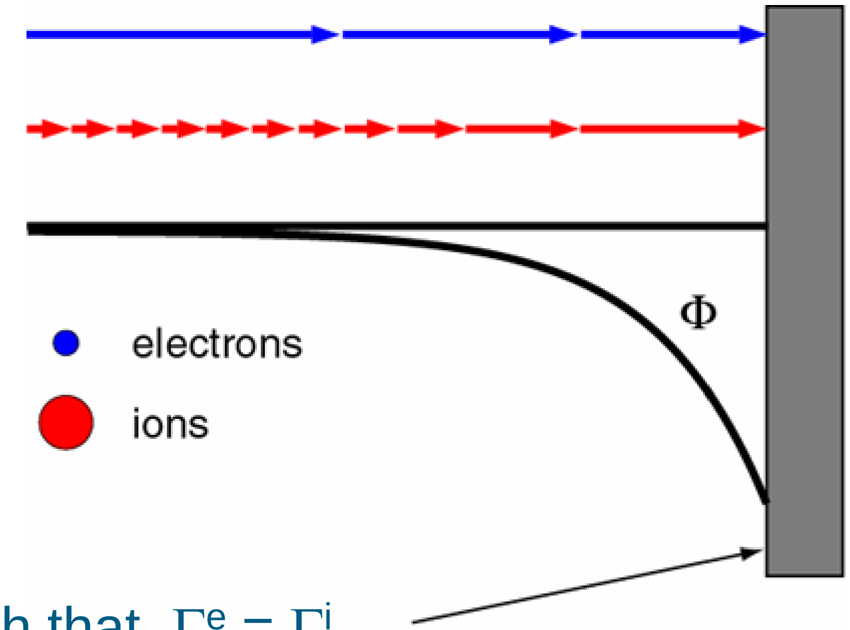
Hot plate	0.05-0.1 MW/m²
Oxy-acetylene torch	100 MW/m²

Particle energies: sheath acceleration

Energies of ions hitting the wall

Electrons much faster than ions
Flux Γ = density x velocity

→ More electrons hit the wall than ions
→ Wall charges up, repelling electrons



In equilibrium: electrostatic potential Φ such that $\Gamma^e = \Gamma^i$

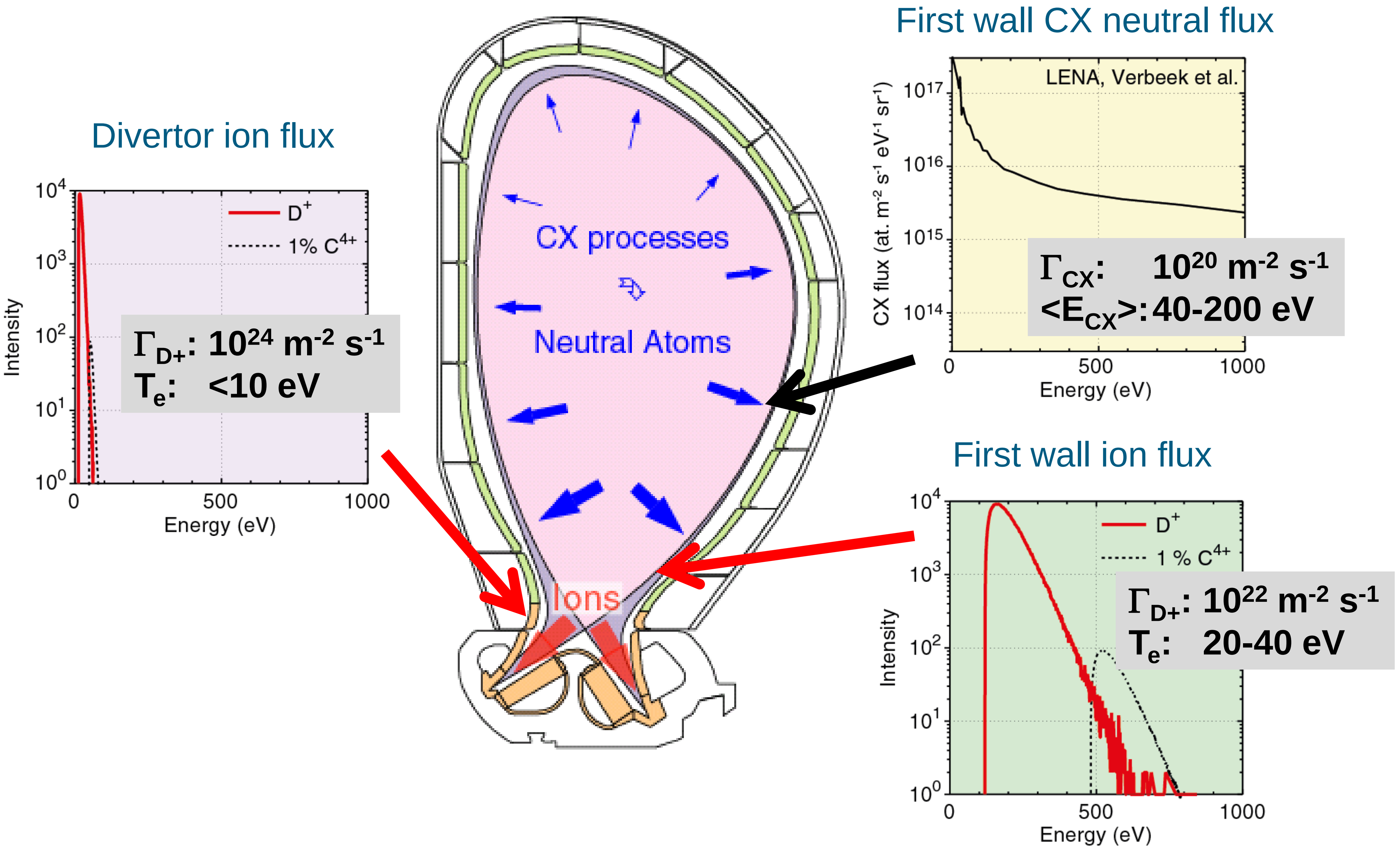
- For hydrogen plasmas $\Phi \sim 3T_e$
- Positive ions of charge q gain 3 q T_e while traversing the sheath

e.g. $T_e = 20\,eV$

$D^+ \rightarrow 60\,eV$

$C^{+4} \rightarrow 240\,eV$

First wall: Particle fluxes and energies

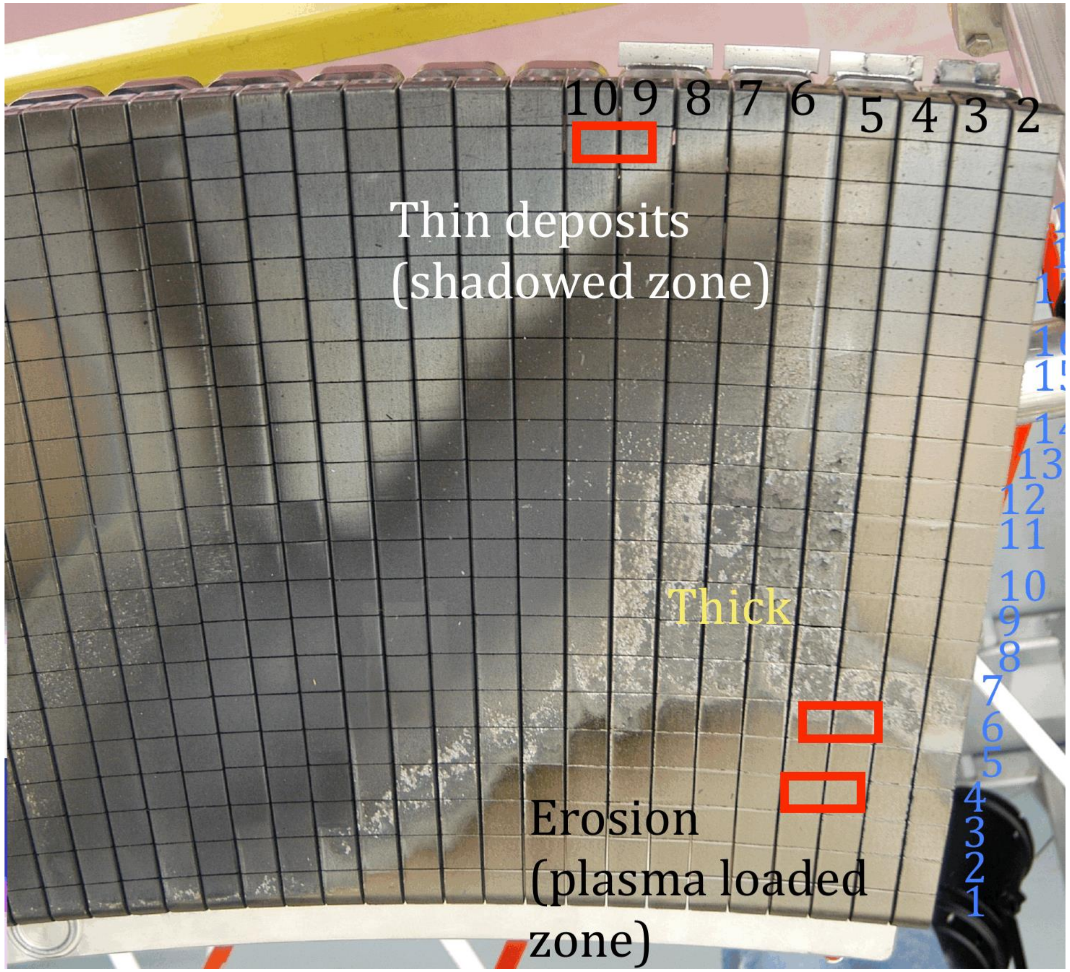


Stationary particle fluxes

Spatially very inhomogeneous

⮱

3-D modelling is necessary **also** in tokamaks



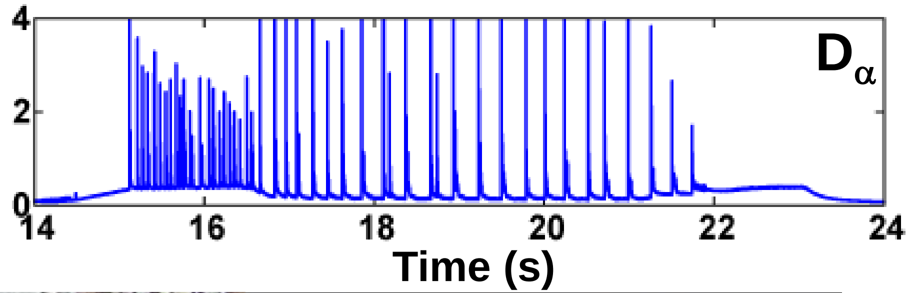
Particles escaping from the confined plasma cover vast range of flux and energy

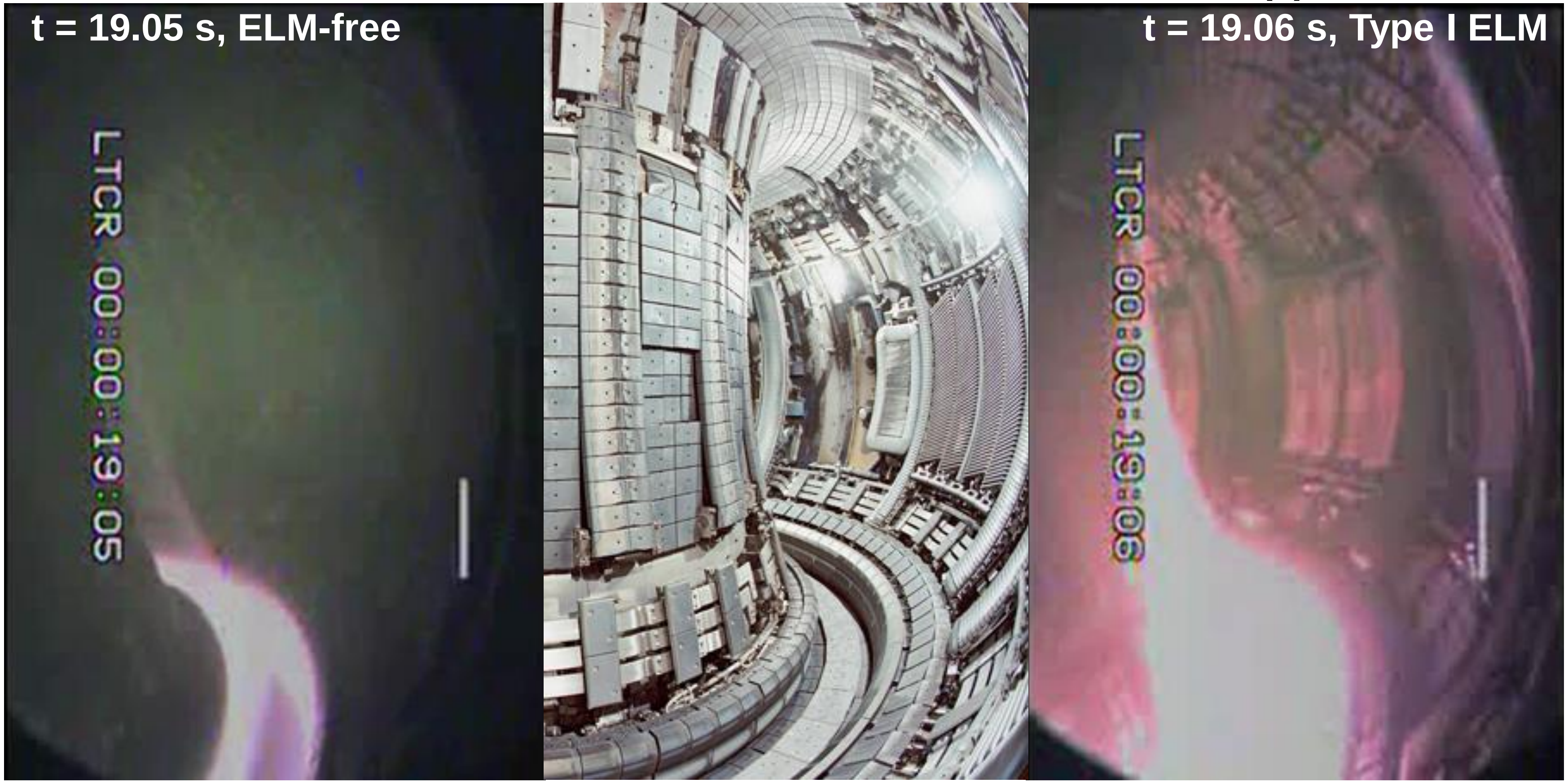
⮱

No uniform engineering and plasma physics boundary conditions

Transient flux excursions

Plasma instabilities can lead to transient heat load excursions

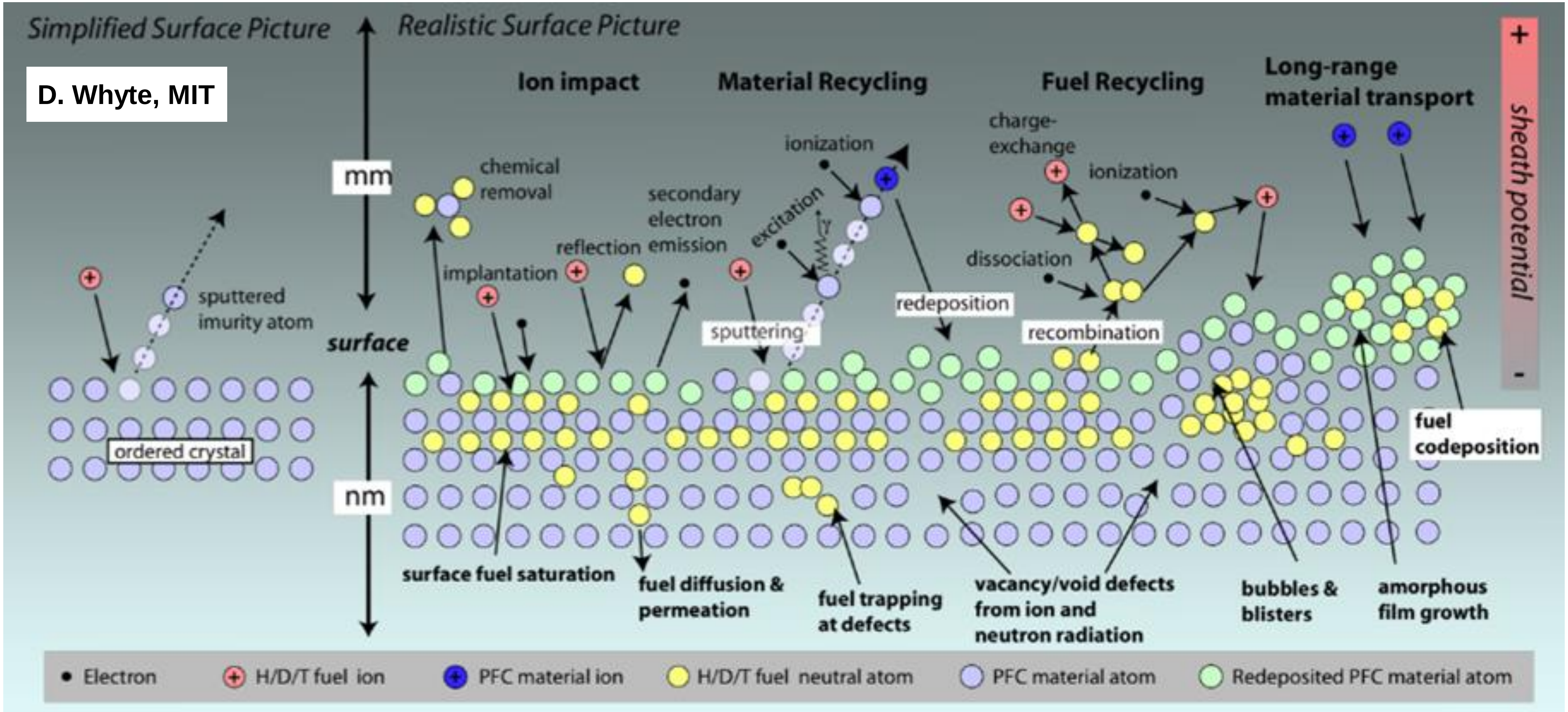




JET #62218

Which are the fundamental processes during PWI?

Fundamental PWI processes



- Rates for individual processes change as surface evolves (towards equilibrium?)
- Surface compounds ("mixed materials") formed with different properties compared to pure elements
- Surface processes and plasma properties are interlinked: impurity fluxes, transport, temperatures, compositions, hydrogen isotope retention …

Fundamental PWI processes

Plasma-wall interactions comprise coupled processes spanning orders of magnitude in time and length scales

- Physical sputtering and implantation
- Chemical sputtering and reactions
- Radiation enhanced sublimation
- Photon induced desorption
- Evaporation and sublimation
- Altered thermomechanics
- Melting and splashing
- Arcing
- Neutron induced damage and transmutations
- Material mixing and migration
- Hydrogen isotope retention and release
- Heating and cooling, transport

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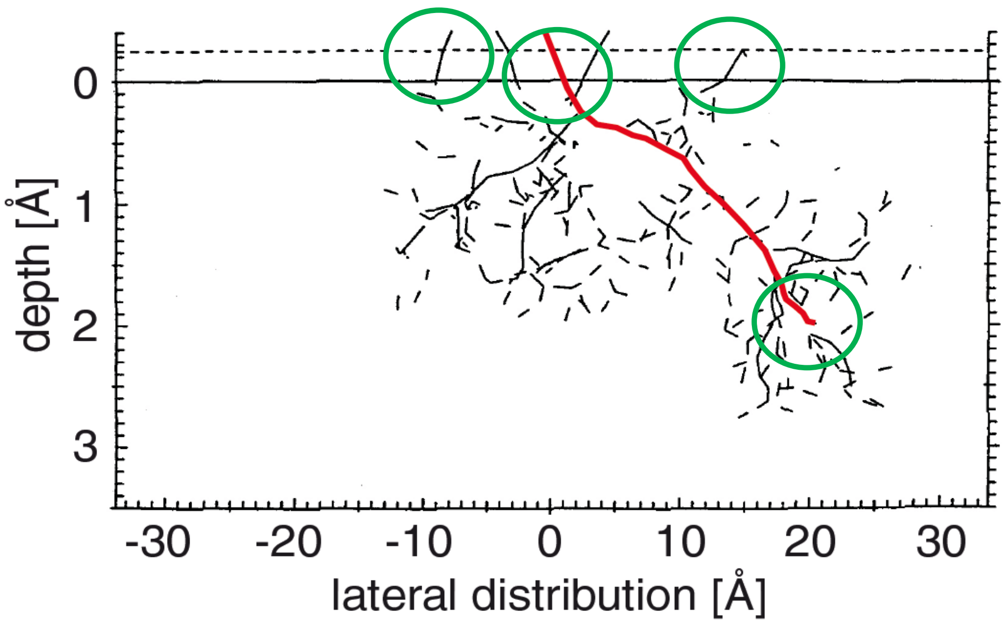
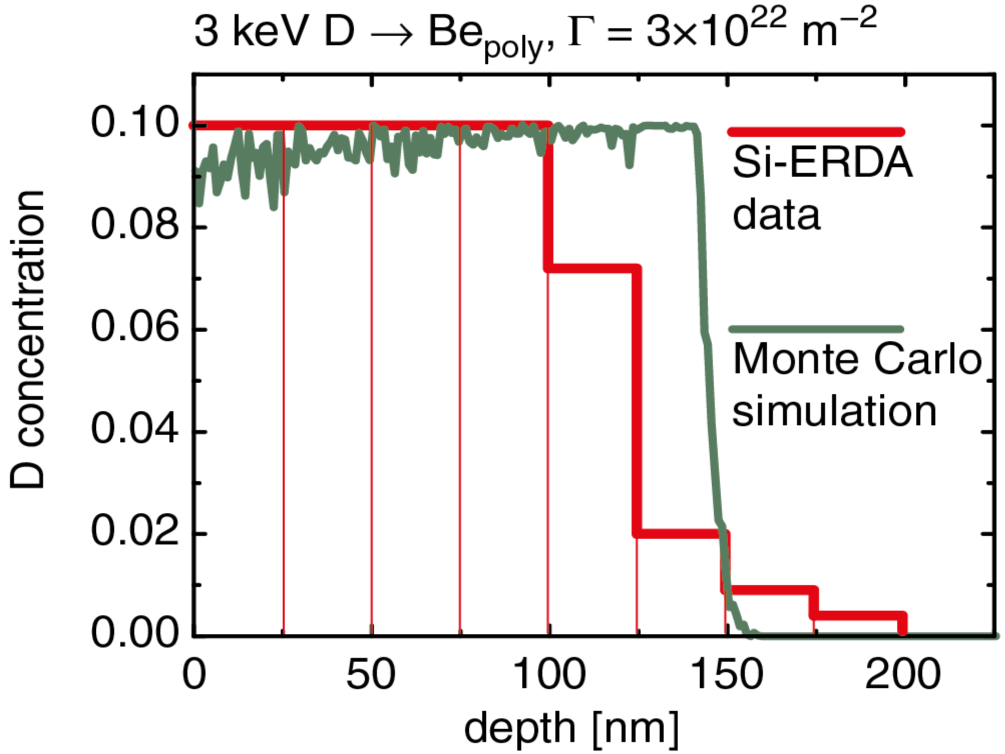
Physical sputtering and implantation

Collision cascade





- Primary and secondary knock-on atoms
- Sputtering
- Energy loss: stopping
- Defects: point defects, vacancies, dislocations

  dpa: displacements per atom
- Projectile trapping

- Simulation: binary collision approximation
- Implantation profile reproduced

Limit (→ Molecular Dynamics simulations)

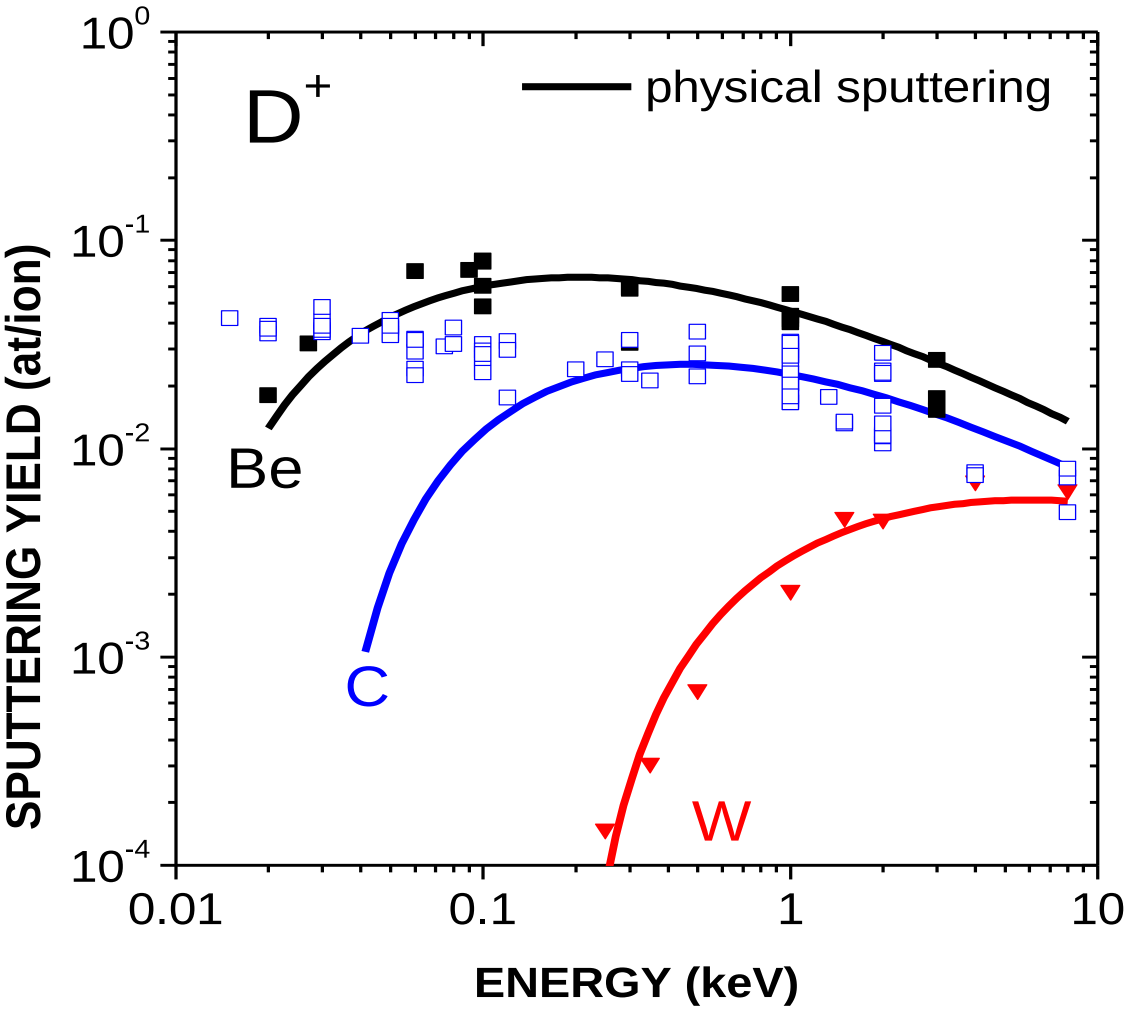
- Low kinetic energies (< 20 eV)
- Molecules

Sputtering yield

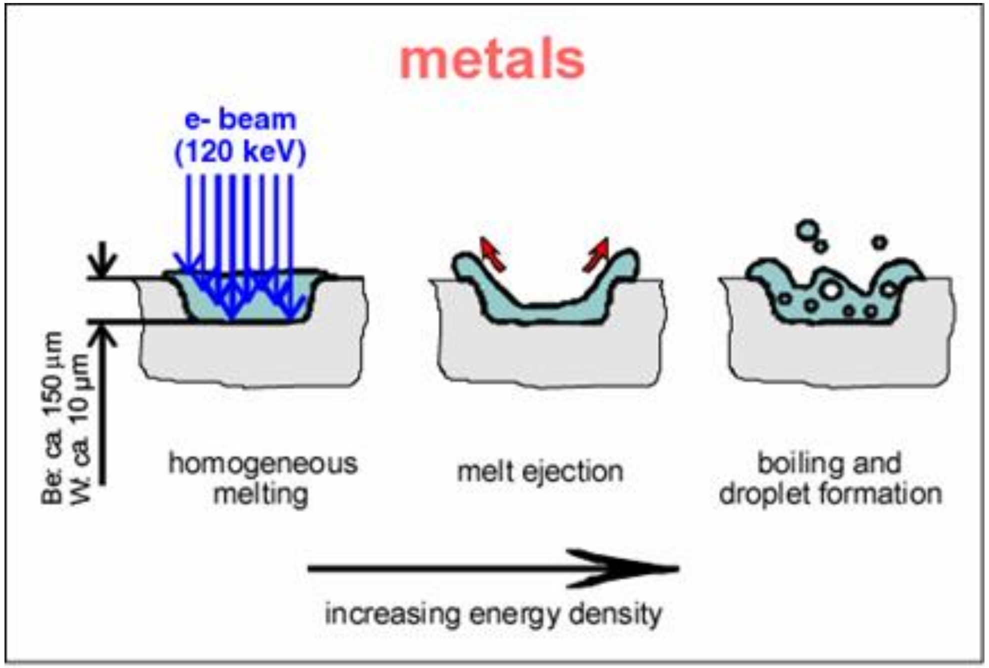
$$Y = \frac{\text{\# eroded atoms}}{\text{\# of projectiles}}$$

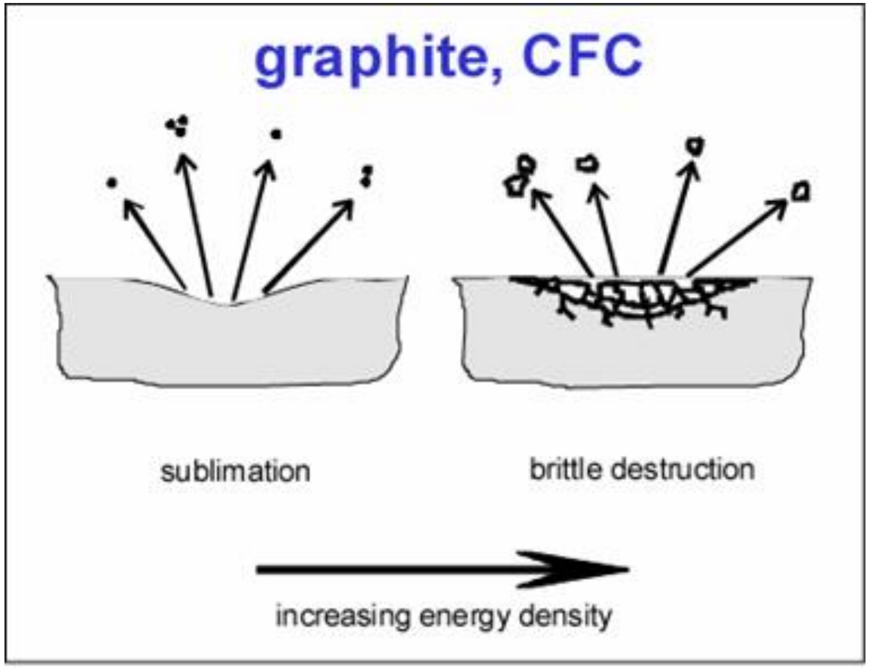
- Physical sputtering: threshold energy
- Maximum yield

- Carbon: chemical erosion: NO threshold hydrocarbon chemistry



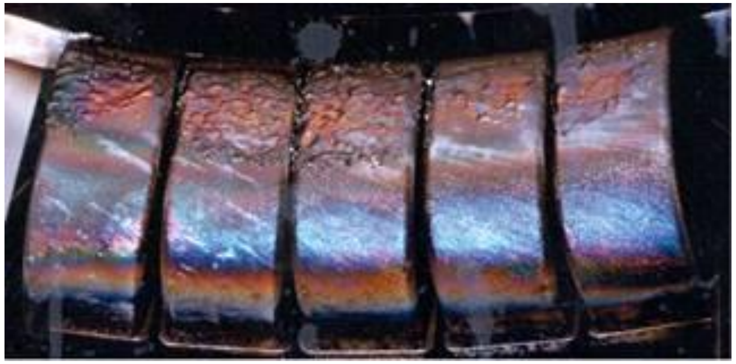
Extreme power loads: Melting and splashing





FOR METALS:
Splashing
Formation of droplets
Formation of dust

FOR CARBON:
Above a certain power load (threshold) emission of debris
➩ *BRITTLE DESTRUCTION*

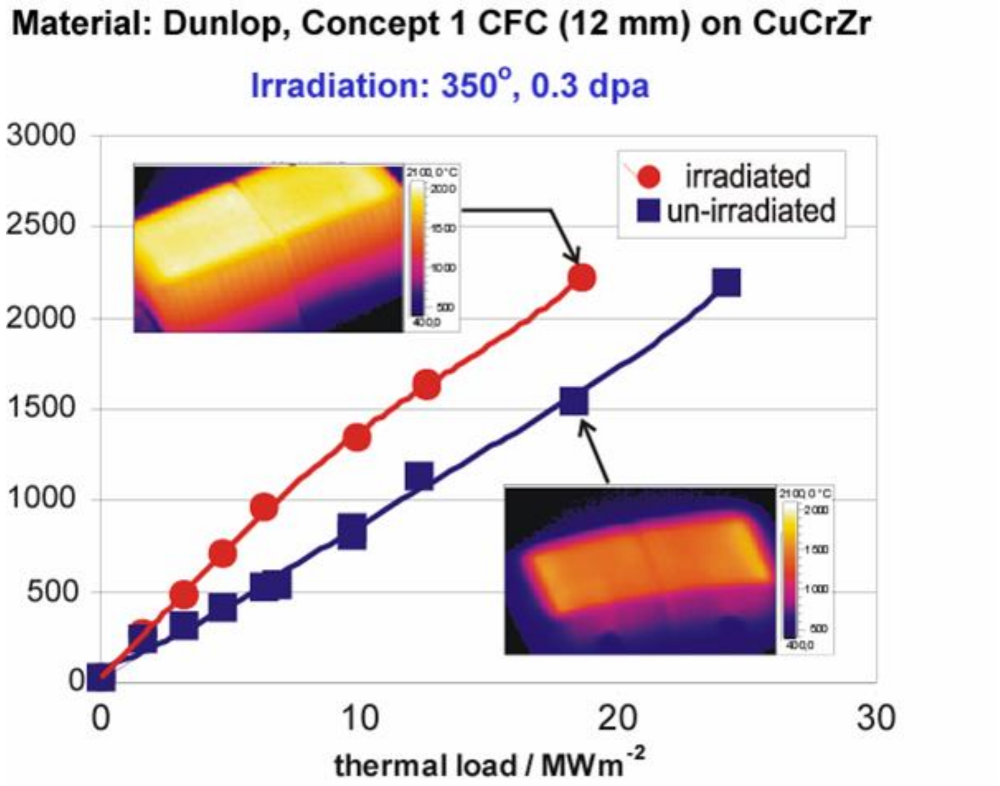


What are ITER-specific PWI issues?

Neutron induced damage, transmutations

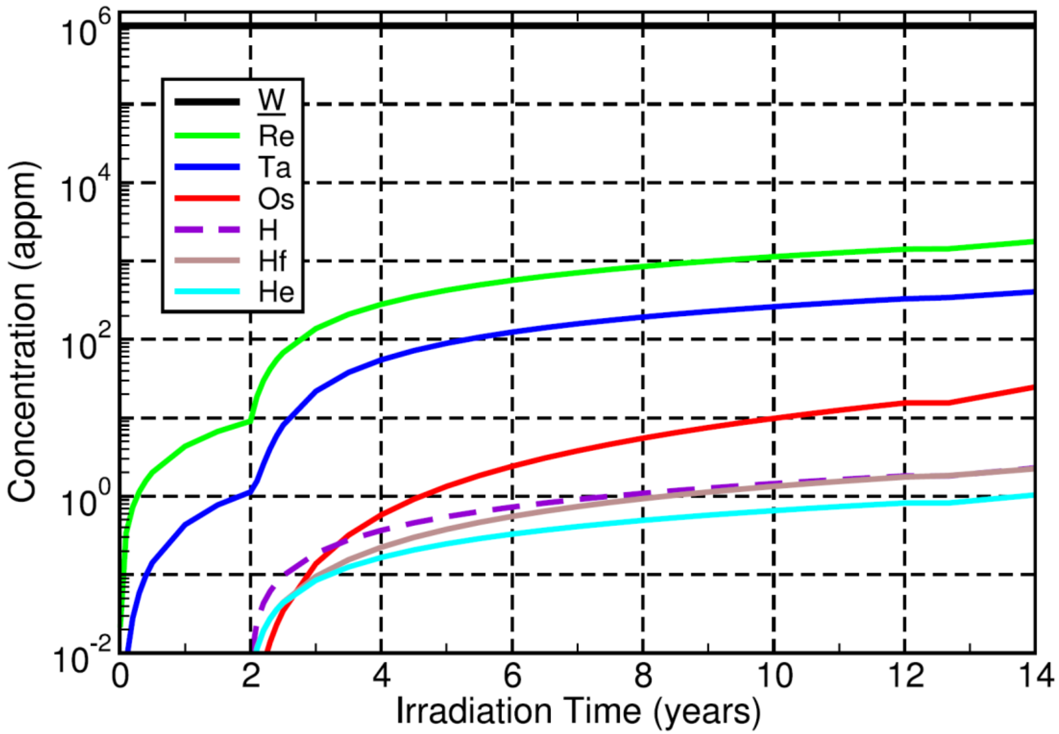
Production of lattice defects

- Reduced thermal conductivity



Transmutations

- Formation of new elements (alloys)



ITER: PWI with multi-element walls

Multi-element first wall:

ITER: Be – W
JET: ITER-like First Wall
W7-X: C – steel
DEMO: W-based alloys

Dynamic evolution of surface composition

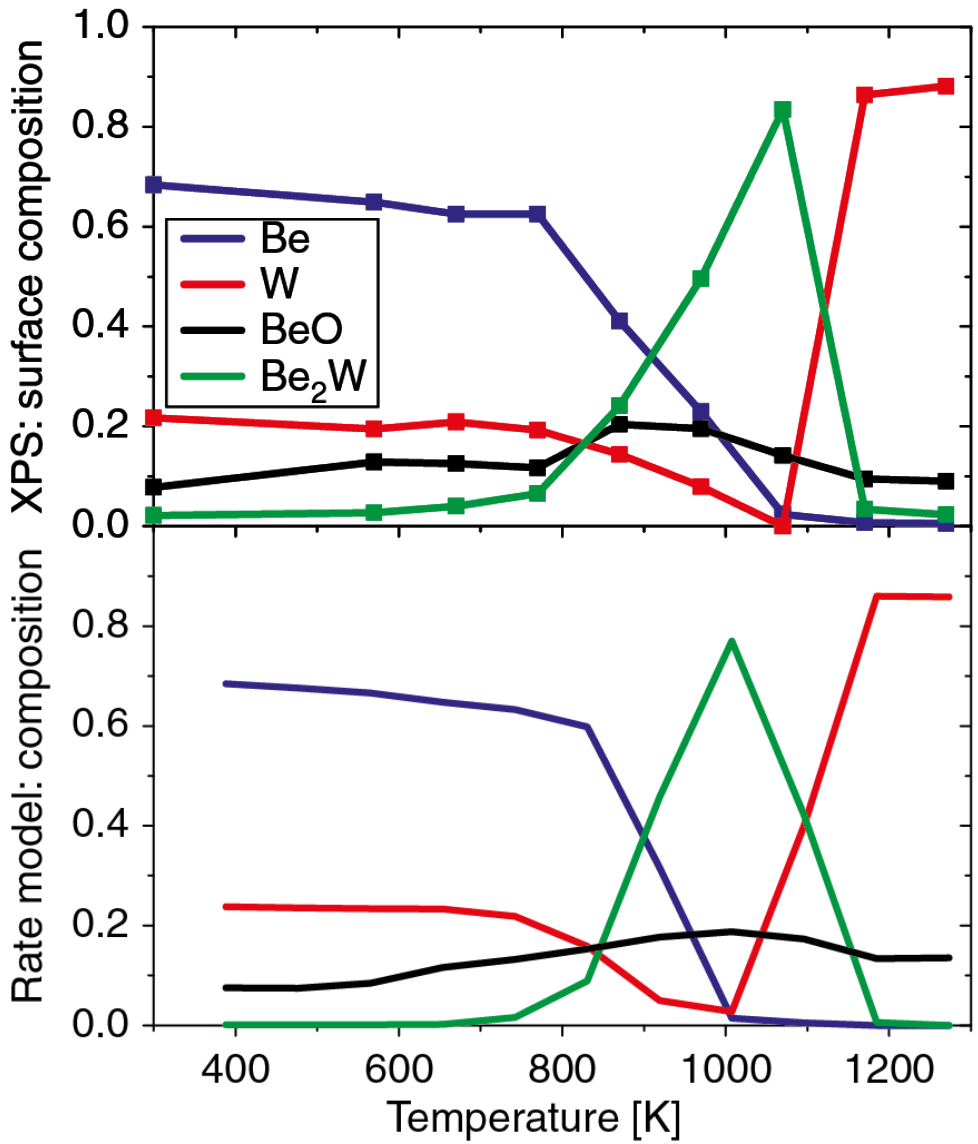
- strongly alters physical and chemical first wall properties (erosion, melting, hydrogen inventory, …)
- influences plasma performance by impurity concentration and transport

→ Integrated modeling of plasma scenarios including dynamic wall evolution

Two ingredients required:

- Model of background plasma, providing particle and energy fluxes to/from the wall (fusion device!)
- Model of physical and chemical surface processes (laboratory!)

Atomistic reaction data: System Be – W



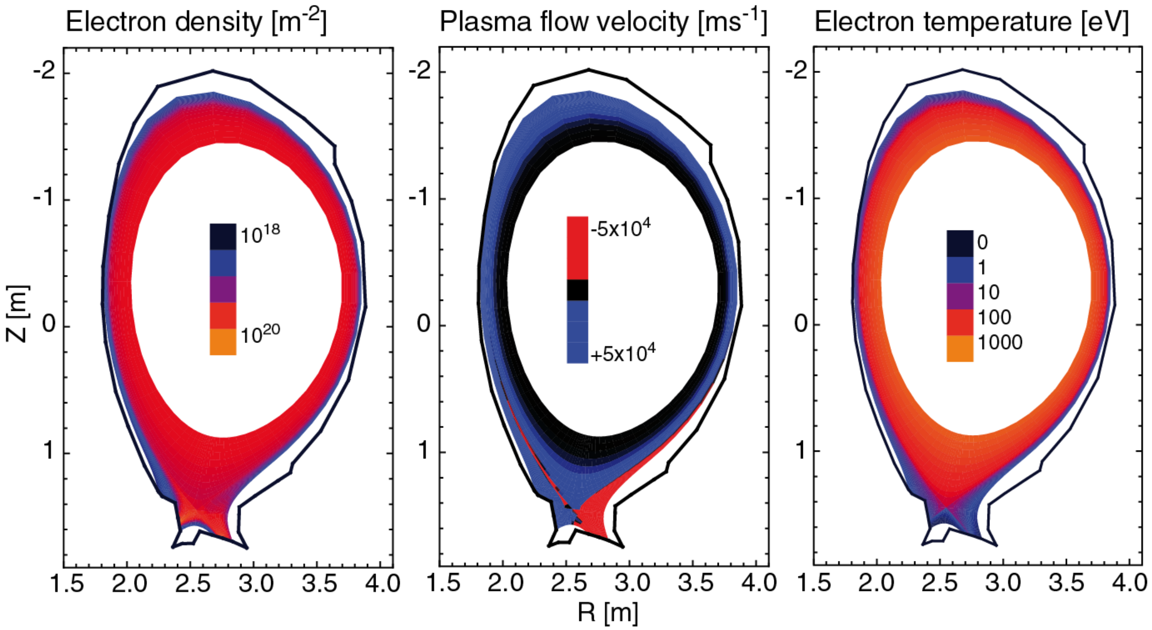
Lab experiment (UHV):
2.5 nm Be on W_{poly}

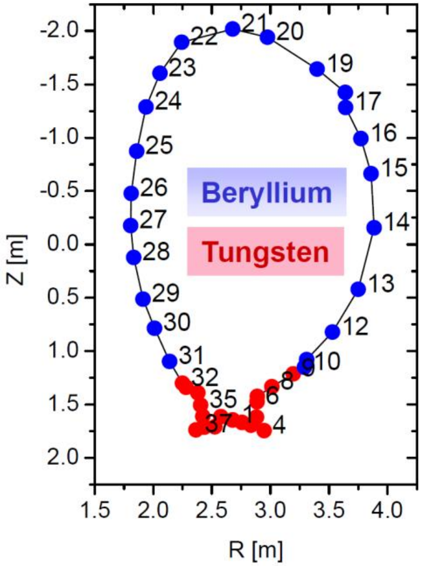
- Alloy formation and decomposition
- Quantitative XPS measurements

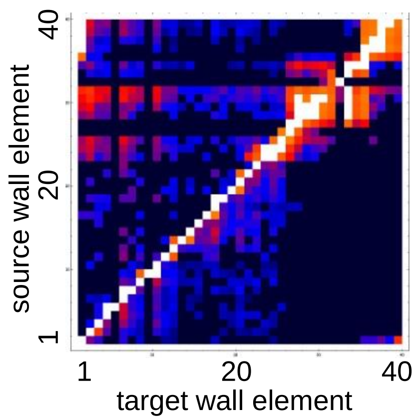
Forward calculation: reaction front model

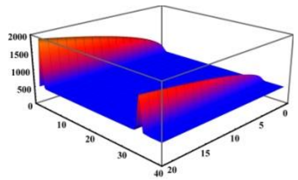
- Be diffusion in Be_2W
- $Be_2W \rightarrow 2\ Be + W$
- $Be + O \rightarrow BeO$
- etc.
- $[C]^z = [A]^x\ [B]^y\ k\ \exp\left(\frac{-E_a}{k_B\ T}\right)$gen:

Background plasma and impurity transport









JET #78647 EDGE2D/EIRENE

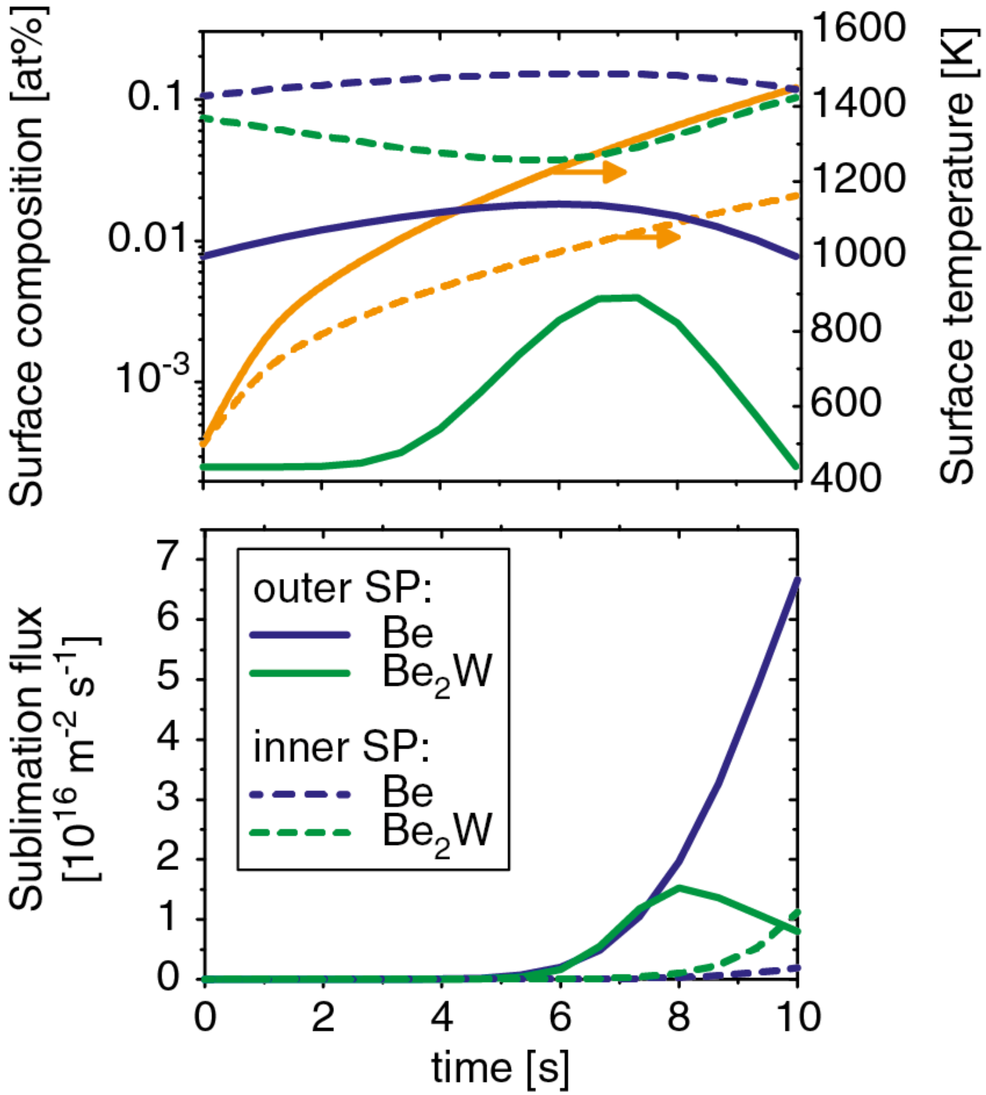
- L-mode
- Standard calculation grid
- Verified by experiment

Wall elements and transport

- Materials: Be und W
- DIVIMP redistribution matrix
- Dynamic surface temperature

➔ Solve rate equation system for each wall element

Surface composition at strike point during discharge



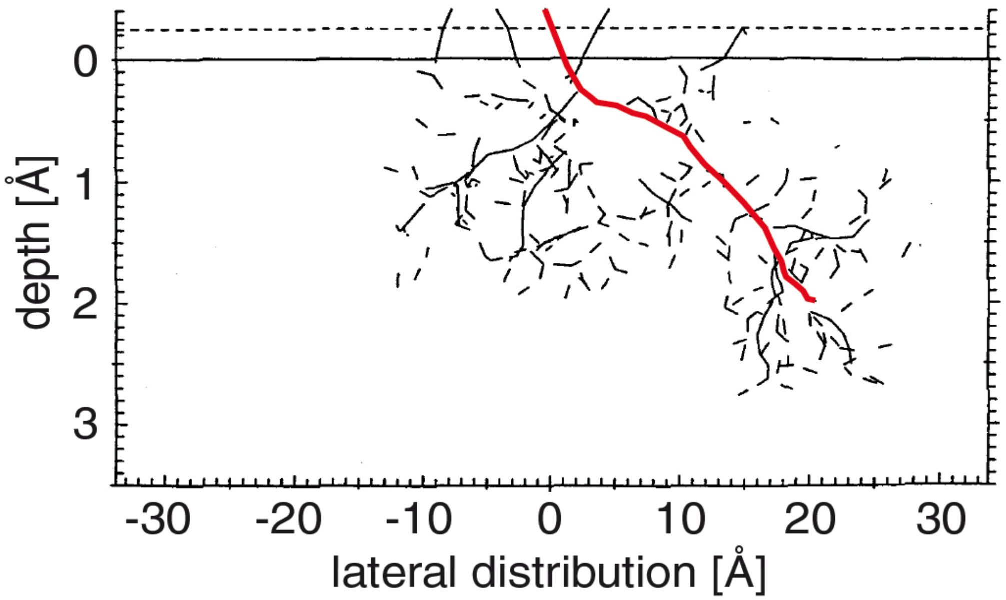
Composition at divertor strike point and sublimation flux

- Periodic: Deposition and erosion at inner strike point
- Be flux into plasma from outer strike point

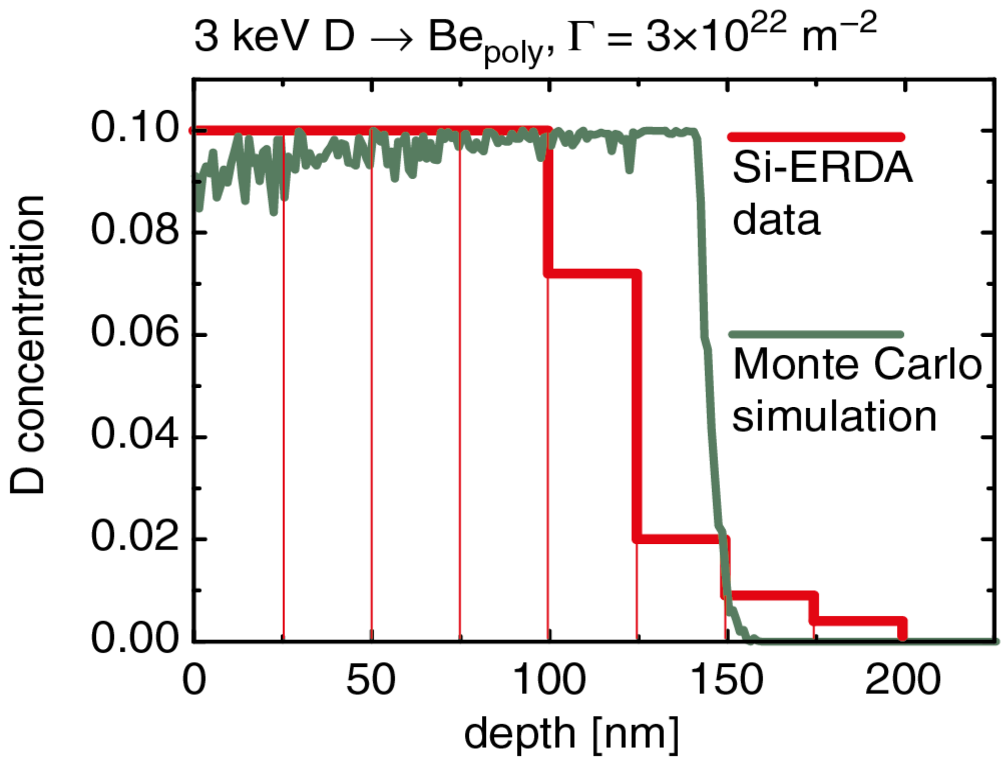
➔Dynamic composition based on a static plasma scenario!

Hydrogen isotope retention and release

Simulation of collision cascade with Monte Carlo codes (TRIM)



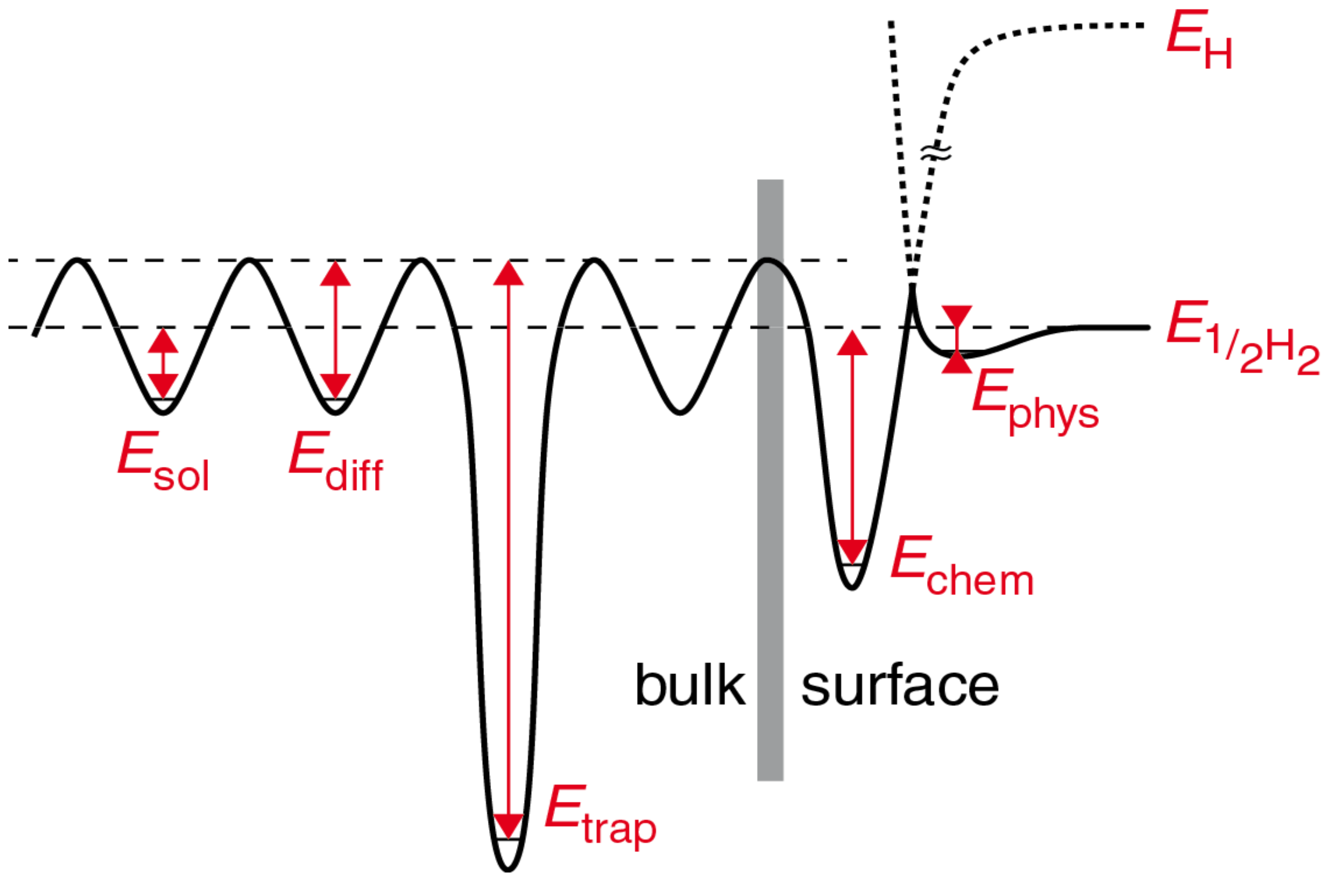
Result: Depth profile



Thermal release

Elementary steps

- diffusion of H in the solid
- trapping and release of H from binding sites (defects)
- recombination and desorption of H_2 from the surface



Thermal release

Described by **Diffusion-Trapping Model**

Local elementary reactions (trapping / release of H)

- thermally activated processes

with:

n_i: number density of each species

k: reaction rate constant

E_a: activation energy

$$R = n_i\, k\, \exp\left(\frac{-E_a}{k_B\, T}\right)$$

Diffusion:

driven by concentration gradient

(1st Fick's law)

$$\mathbf{j_i} = -D_i \operatorname{grad} n_i$$

local concentration change:

Diffusion described by continuity equation

(2nd Fick's law)

$$\frac{\partial n_i}{\partial t} = -\operatorname{div} \mathbf{j_i}$$

Particle flux at desorption

Partial differential equation:

considers both diffusion and elementary reactions

$$\frac{\partial n_i}{\partial t} = -D_i \operatorname{div}(\operatorname{grad} n_i) + \sum R^{\text{source}} + \sum R^{\text{sink}}$$

Example:

n_i: concentration of mobile (dissolved) $\mathrm{H}^{\text{mobile}}$

R: rates for trapping and release at traps $\square^{\text{trap}}$

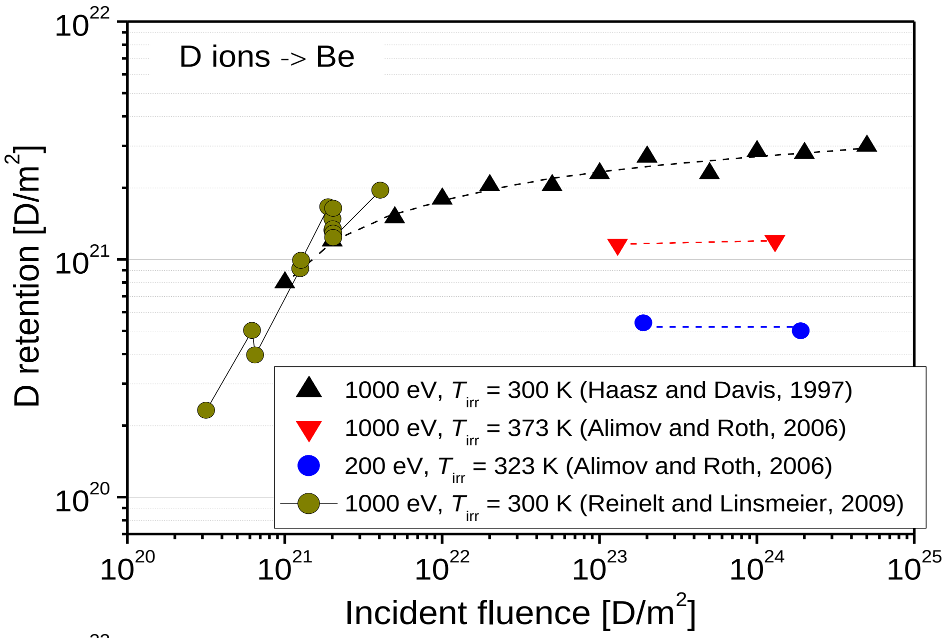
PDE describes H diffusion and the reaction: $\mathrm{H}^{\text{trap}} \rightleftharpoons \mathrm{H}^{\text{mobile}} + \square^{\text{trap}}$

$\Rightarrow$ Consider arbitrary elementary reactions

Description of the thermal release by a system of coupled differential equations

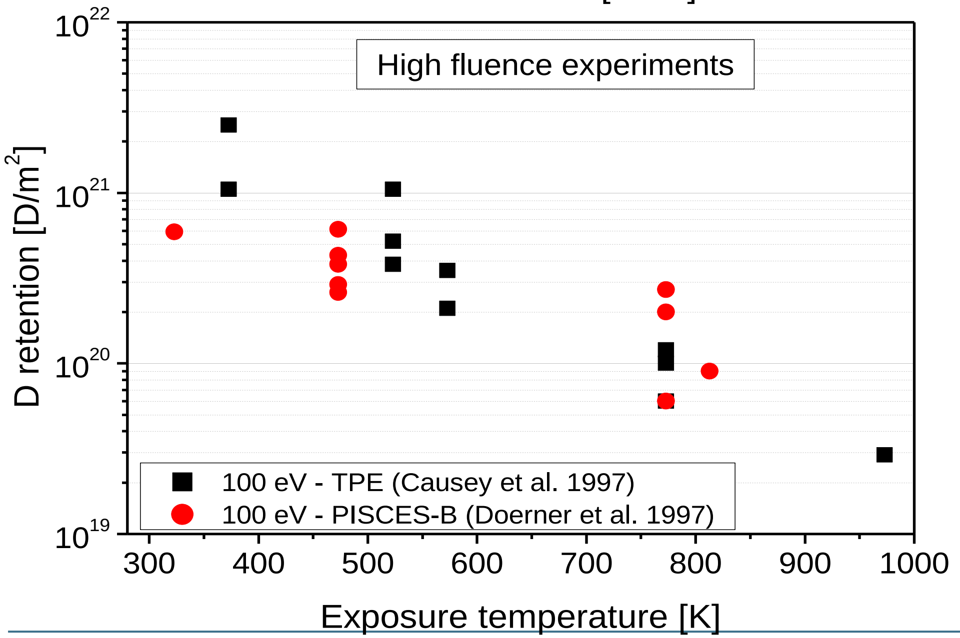
Tritium inventory in Be

Tritium in Be: saturation



D retention demonstrates saturation.
For 1 keV D ion irradiation, the saturation is observed at a fluence of 10^{22} D/m^2.

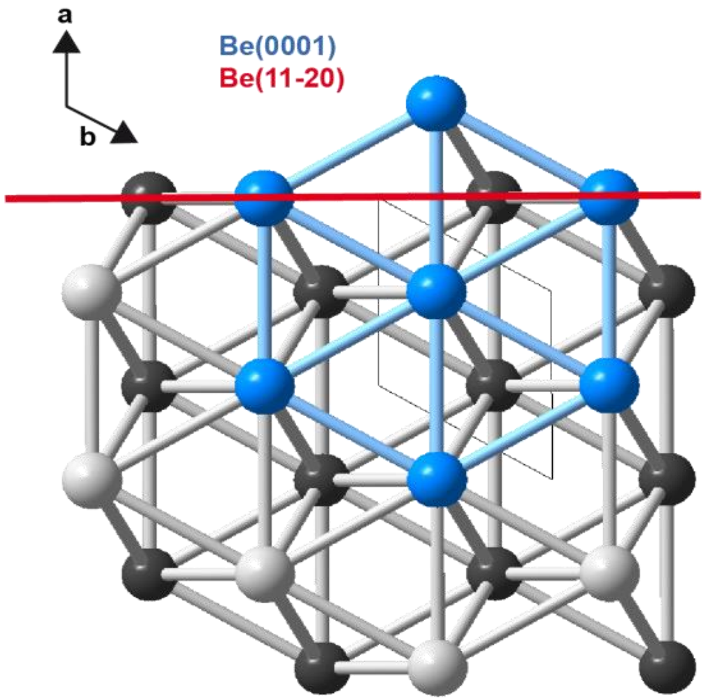
For D is trapped in the implantation zone with negligible diffusion into the bulk.



When the irradiation temperature increases, the D retention decreases.

From review of R. Anderl et al., J. Nucl. Mater. 273 (1999) 1

D diffusion in beryllium



Be crystal lattice

Be(0001) plane ll to surface

Be(11-20) plane ⊥ to surface

- Beryllium has **not an “ideal” hcp** structure. Be-Be distances are closer in <0001> than perpendicular to it (e.g. <11-20>)
- DFT (Density Functional Theory) calculations show anisotropy in transport processes with respect to Be basal planes

Modeling: 2D coupled rate equations

Strategy

- Solve a coupled reaction diffusion system (CRDS) consisting of an arbitrary number of diffusing species *i=A,B,C…* in 1, 2 or 3 dimensions
- Solve system of partial differential equations for the time dependent 2D depth profile $\rho(x,z,t)$ [m^{-3}]

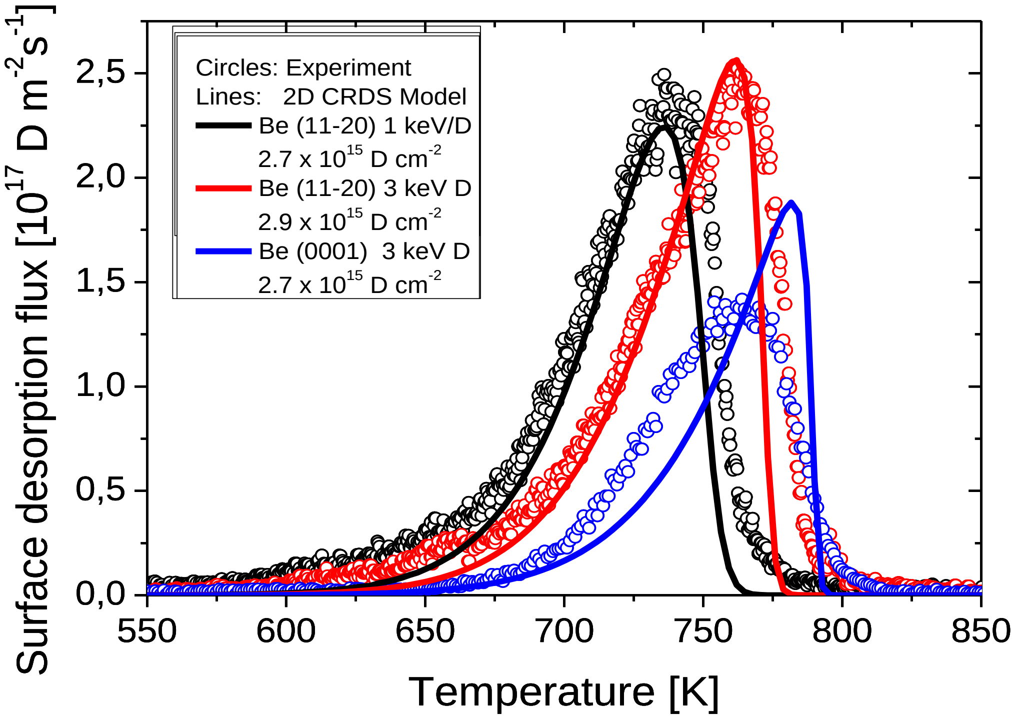
$$\frac{\partial \rho_A(x,z,t)}{\partial t} = \frac{\partial}{\partial x}\left(D_x(T(t))\frac{\partial \rho_A(x,z,t)}{\partial x}\right) + \frac{\partial}{\partial z}\left(D_z(T(t))\frac{\partial \rho_A(x,z,t)}{\partial z}\right) +$$

$$+\sum \Gamma_i^{Form}(\rho_{A,B,C\dots}) - \sum \Gamma_i^{Annihilation}(\rho_{A,B,C\dots}) + \Gamma_i^{Source}(x,z,t)$$

$$A + B \rightarrow C \qquad\qquad C \rightarrow A + B$$

$$\Gamma_1(\rho_A,\rho_B,t) = k_1\rho_A\rho_B \exp\left(-\frac{\Delta E_1}{k_B T(t)}\right) \qquad \Gamma_2(\rho_C,t) = k_2\rho_C \exp\left(-\frac{\Delta E_2}{k_B T(t)}\right)$$

TPD of D implanted in Be single crystals



TPD spectra and 2D-CRDS simulations after implantation of D at 1 keV/D and 3 keV/D in Be(0001) and Be(11-20)

Only one type of trap!

R. Piechoczek et al., J. Nucl. Mater. 438 (2013) S1072

1. Desorption temperature shift for different implantation energies
2. Desorption temperature shift for Be(0001) and Be(11-20)
3. Less D retention in Be(0001) than in Be(11-20)

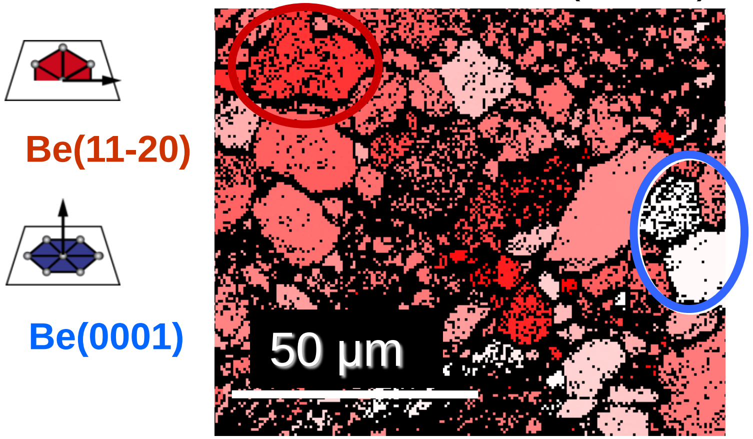
→

1. Deeper implantation → longer diffusion path to the surface → higher TPD peak temperature
2. Anisotropy of Be lattice → 2D anisotropic modelling required to implement results from DFT calculations
3. Dynamics during D implantation (MV+SI annihilation and trapping in MV) determines retention

TPD from Be polycrystal

Identical parameters also applied for polycrystalline Be

SEM (EBSD)



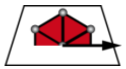
- Shift for Be_{poly} reproduced with no retrapping: fast grain boundary diffusion

R. Piechoczek et al., J. Nucl. Mater. 438 (2013) S1072

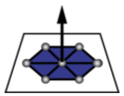
TPD from Be polycrystal

Identical parameters also applied for polycrystalline Be

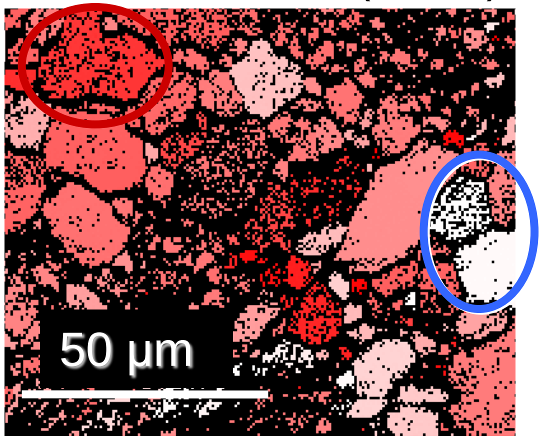
SEM (EBSD)



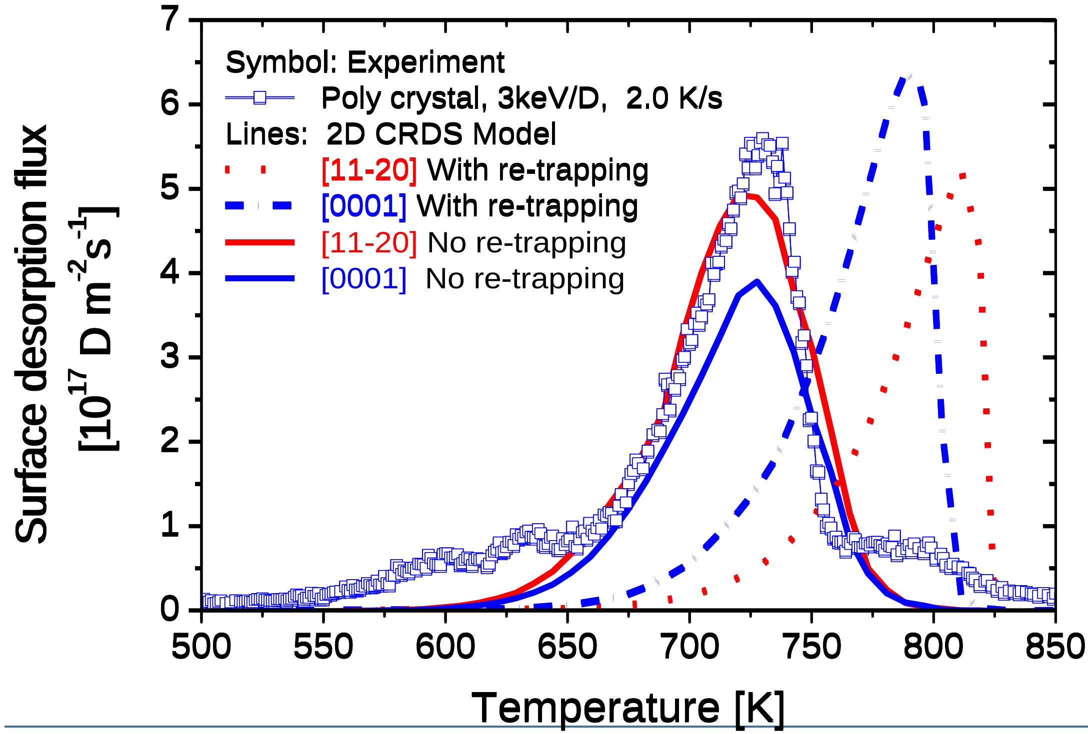
Be(11-20)

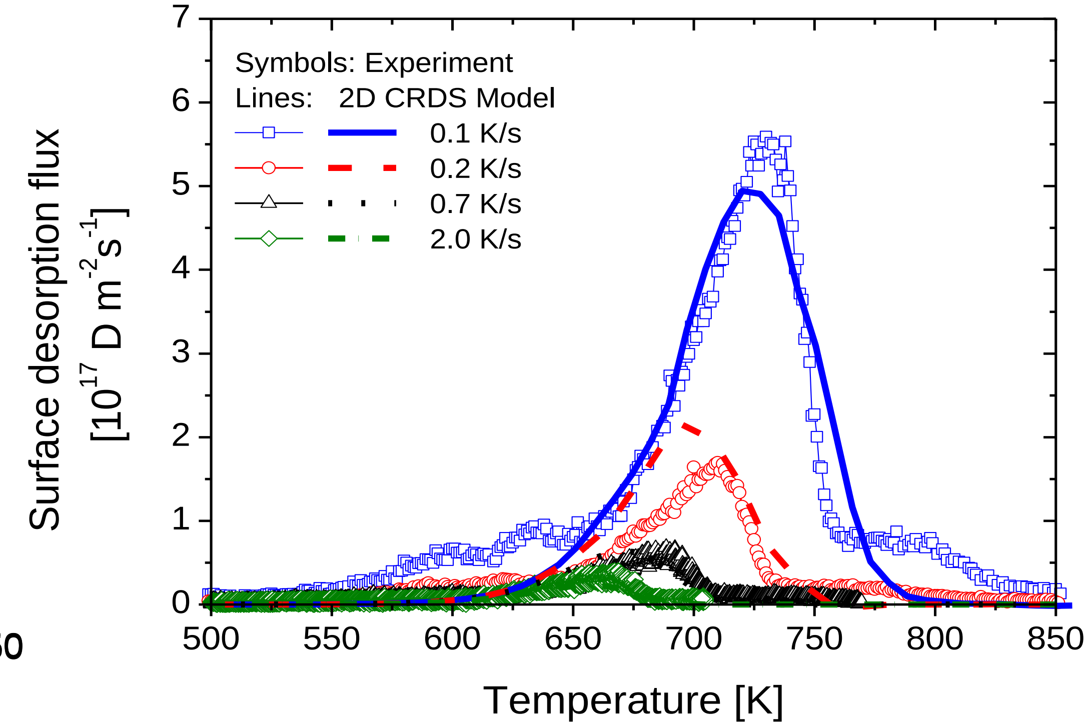


Be(0001)



- Shift for Be_{poly} reproduced with no retrapping: fast grain boundary diffusion
- heating ramp variation reproduced: no (self)trapping during heating





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Parameters for D release and diffusion

Experimentally and DFT determined parameters for full description

		ν	ΔE_{act} [eV]	ΔE_{act} [eV]
		CRDS	CRDS	DFT [Allouche]
Diffusivity ∥ Basal Plane	*Mobile Hydrogen* H_{mob}	**3.11E-06**	**<0.4***	**0.2**
	Mono vacancy MV	**3.11E-06**	**0.7**	**0.7**
	Self interstitial SI	**3.11E-06**	**0.4**	**0.4**
	Trapped Hydrogen H_{trap}	**-**	**-**	
Diffusivity ⊥ Basal Plane	H_{mob}	**7.68E-06**	**<0.4***	**0.4**
	MV	**7.68E-06**	**0.7**	**0.7**
	SI	**7.68E-06**	**0.004**	**0.004**
	H_{trap}	**-**	**-**	
Trapping	$H_{mob} + MV \rightarrow H_{trap}$	**1.00E+13**	**0.4**	**0.4**
Detrapping	$H_{trap} \rightarrow H_{mob} + MV$	**1.00E+11***	**1.75**	**1.75**
Annihilation	$MV + SI \rightarrow$ -	**1.00E+13**	**0.004**	**0.004**
Self trapping	$H_{mob} + 1\ H_{trap} \rightarrow 2\ H_{trap} + SI$	**1.00E+13**	**0.4**	**0.4**

Anisotropy in diffusion of self-interstitials crucial for modeling!

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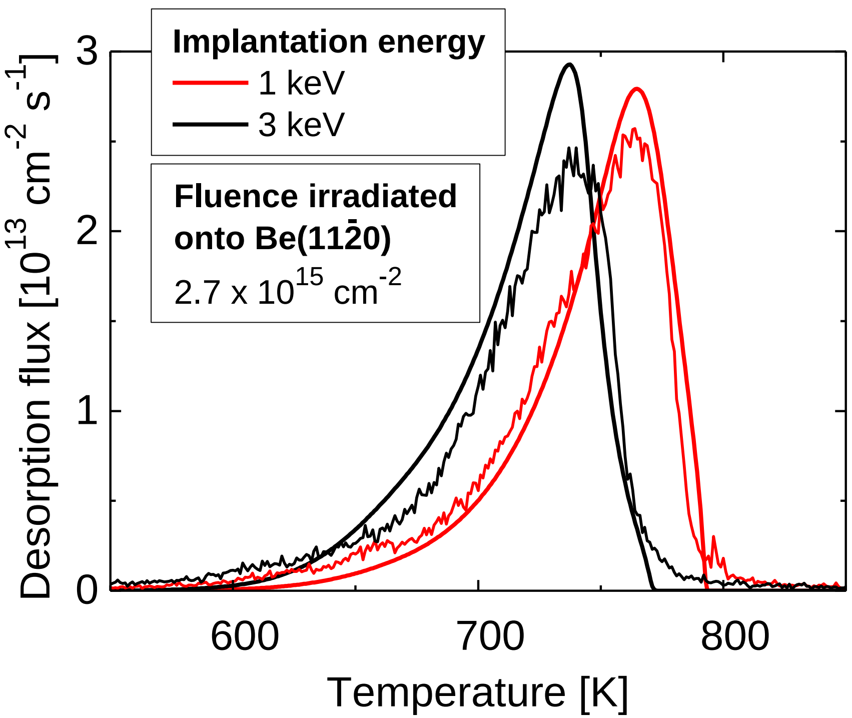
Experiment: Desorption von D_2 from Be

Determination of paramaters by forward calculation

- Different single processes
- Numerical solution of PQE with boundary conditions (implantation profile, desorption of D_2 molecules from surface)
- Comparison to experiment

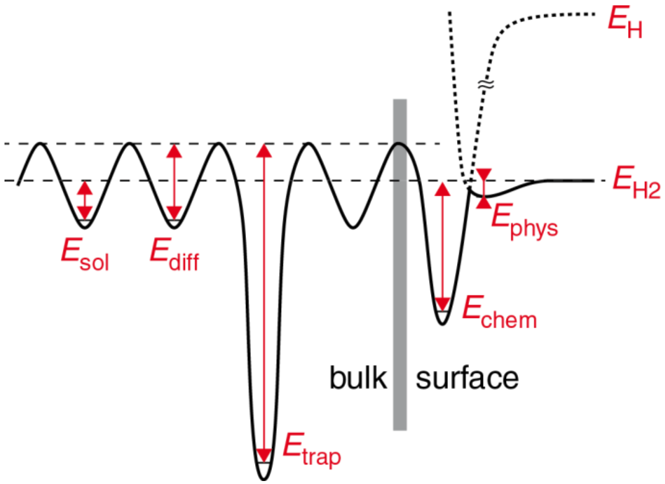


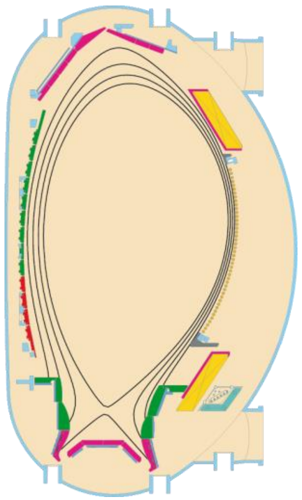
Single processes	E_a
Diffusion of D	0.3 eV
Diffusion of $\square^{trap}$	1.2 eV
Release $D^{trap} \rightarrow D^{mob} + \square^{trap}$	1.85 eV
Release $D^{mob} + \square^{trap} \rightarrow D^{trap}$	0.3 eV
Self release $D^{mob} + D^{trap} \rightarrow 2\,D^{trap}$	0.3 eV

Hydrogen isotope retention and release

Full and detailed detailed description of H isotope retention and release

- Investigation of single steps in the relevant
  - Fluence ranges
  - Temperature ranges
  - Particle energy ranges





Global modeling with respect to the various regions of a fusion device

Summary

The wall of a magnetic fusion device is essential to its operation

- Maintain clean vacuum
- Provide power and particle exhaust

The wall is exposed to high particle and power fluxes leading to large number of coupled processes that span many length and time scales

- Erosion, material migration, re-deposition
- Mixed material formation
- Hydrogen isotope retention and release

ITER will be first machine with extended D-T burning plasma

- Neutrons will lead to additional (deep) traps and transmutations

Plasma-wall interaction processes are a key challenge on the way to a fusion power plant