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Development of models for plasma interactions with Be on the basis of dedicated experiments

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Outline

ERO simulations:

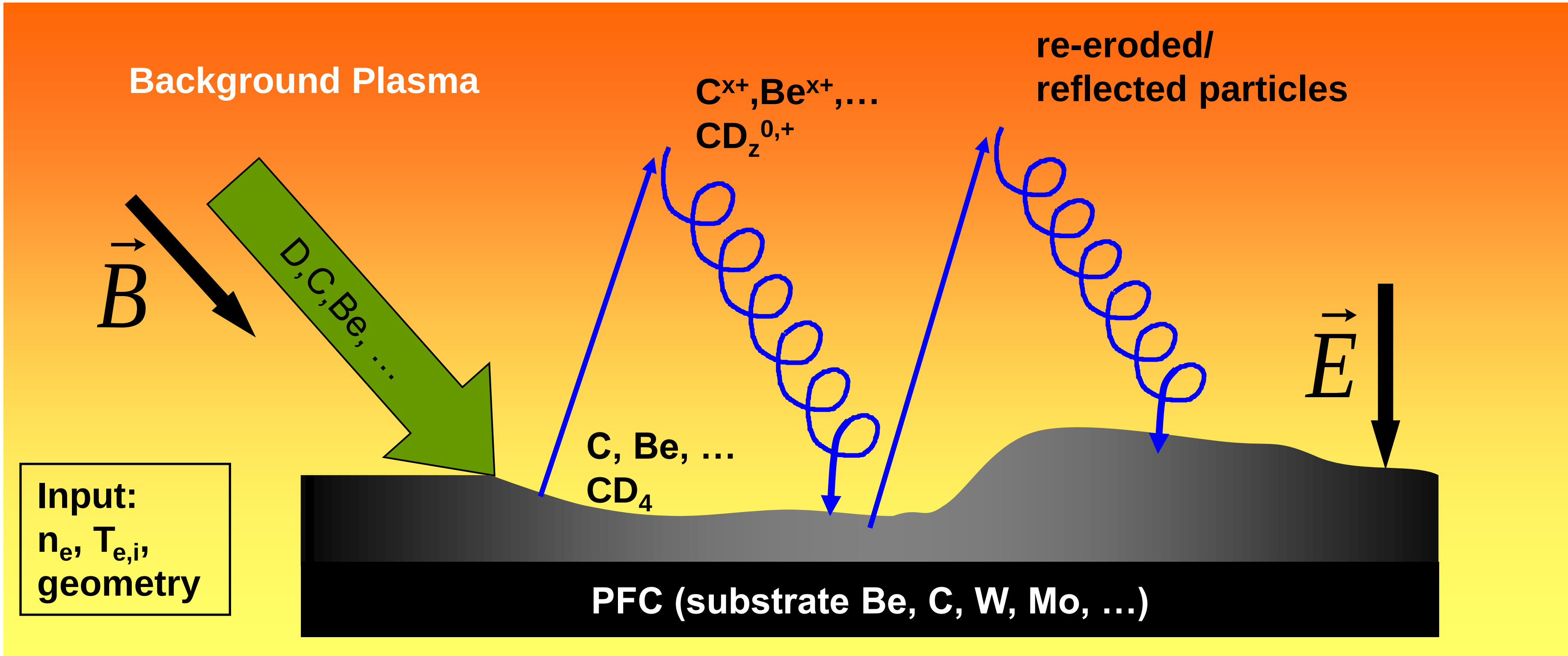
- Motivation: ITER FW erosion (sensitivity to erosion data)
  - *LIM/ERO code-code benchmark*
- PISCES-B (Be target erosion)
  - *Tracking of MS population*
  - *Be-D molecules*
- JET ITER-like wall (ILW solid Be limiter erosion)
- Other JET experiments (^{10}Be, divertor, QMB)

Further relevant experiments in FZJ:

- Laser techniques
- New linear devices
- Be proxy

ERO introduction

3D MC impurity transport code ERO



Local transport:

- ionisation, dissociation
- friction (Fokker-Planck), thermal force
- Lorenz force (including ExB component)
- cross-field diffusion

Plasma-surface interaction:

- physical sputtering/reflection
- chemical erosion (CD_4)
- (re-)erosion and (re-)deposition
- HMM and SDTrimSP surface models

ERO modelling strategy

Code development:

- *PSI & transport*
- *material mixing*
- *castellated surfaces*
- *atomic data, ADAS*

Benchmarking:

- ***PISCES-B (with beryllium)***
- ***JET ILW***
- *Pilot-PSI,* ***PSI-2, JULE-PSI***
- *TEXTOR, AUG,*
- *…*

Estimations for ITER:

- *tritium retention*
- *target & limiter lifetime*
- *impurities into plasma*

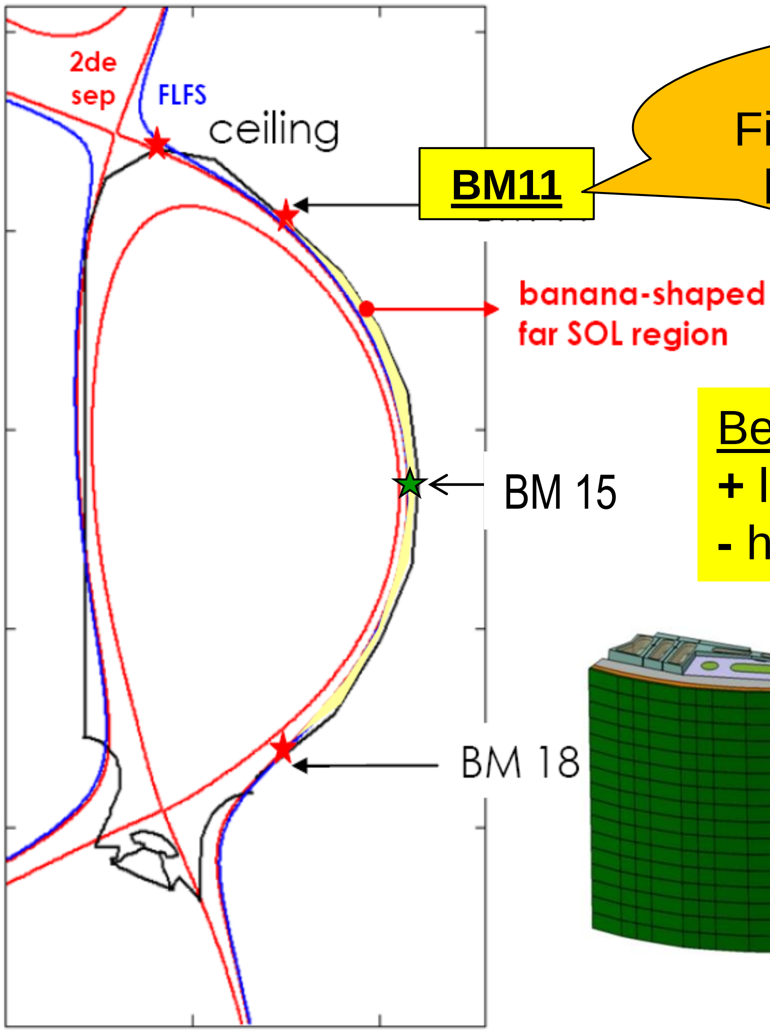
Coupling with other codes:

- *plasma parameters from: e.g. B2-Eirene, Edge-2D*
- *surface mixing: TriDyn, MolDyn*

D Borodin et al, Phys. Scr. **T145** (2011) 014008

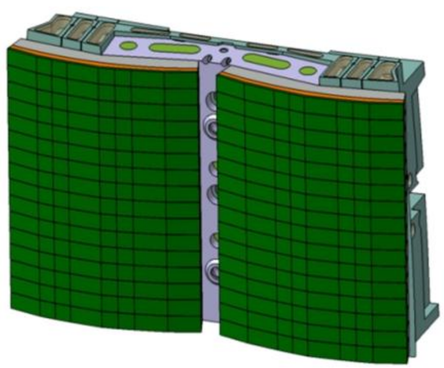
ERO ITER FW life time predictions

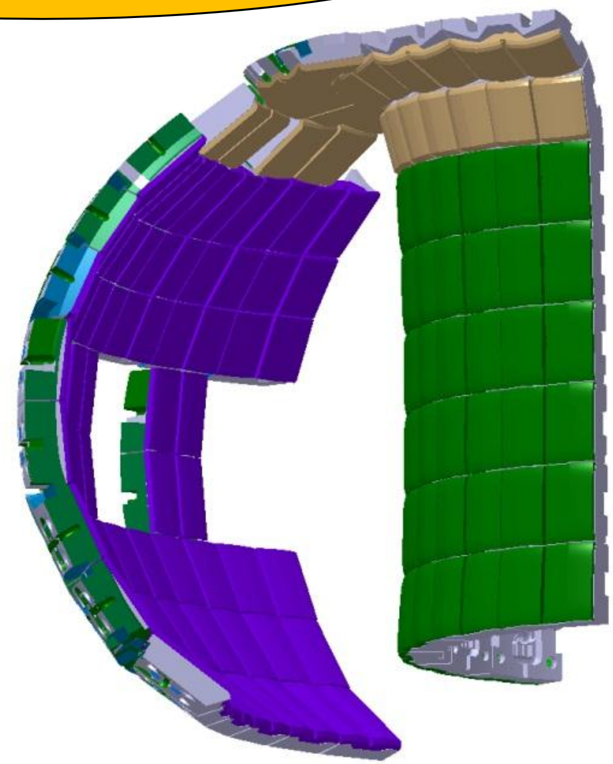
ITER Be wall – BM erosion



FLFS close to 2nd separatrix =>
First PFC ***life time*** estimates assuming
limiter-like contact on outboard BM11

Be
+ low Z
- high erosion





- *Blanket module (BM) shapes optimized for heat loads (P.C.Stangeby)*

Aim – predictive modelling of ITER, including first wall life time

LIM code results

[S.Carpentier et.al, PSI-19, J.Nucl.Mater. (2010)]

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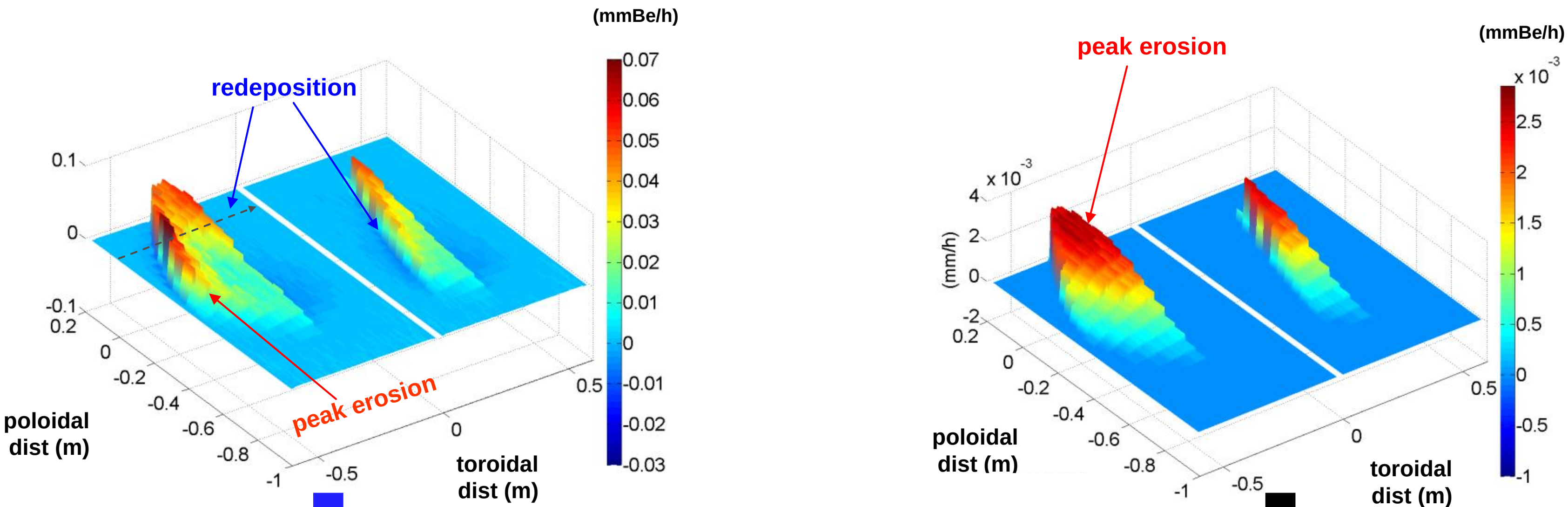
2D Net erosion-redeposition patterns on BM11



High density case

Low density case

- ✓ $\langle Y_{eff} \rangle$ ~ 7%, ~50% particles locally redeposited
- ✓ Net peak erosion ~ 0.06 mm/h
  - ➔ PFC lifetime ~ 1500 shots
- ✓ T-retention* ~ 0.083 gT/h for one module
  - ~ 3 gT/h for 36 BM11-18
  - ➔ Limit ~ 1920 shots

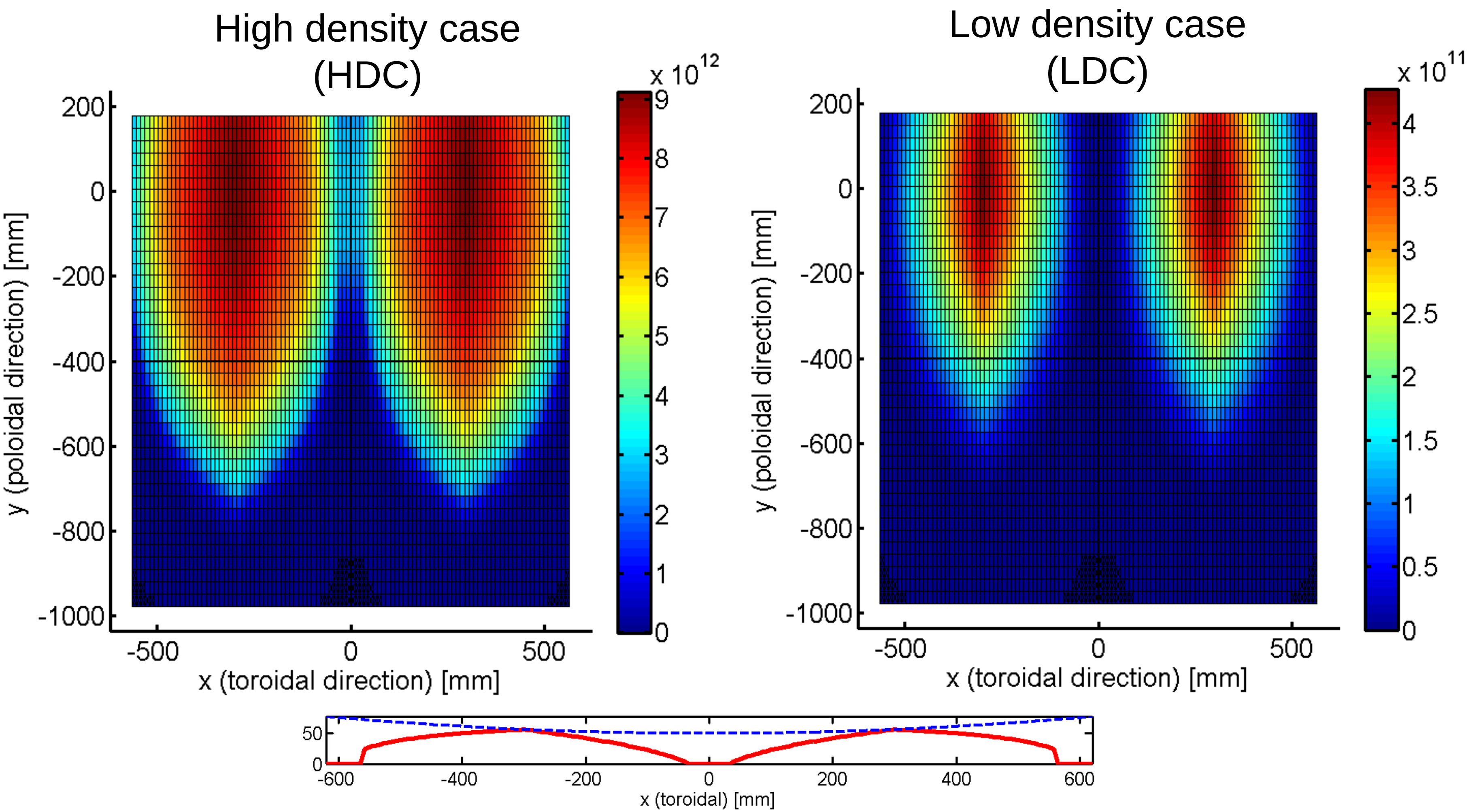
(assuming: 50:50 D:T plasma, maximum safety limit ~640g)

- ✓ $\langle Y_{eff} \rangle$ ~ 6%, ~10% particles locally redeposited
- ✓ Net peak erosion ~0.0025 mm/h
  - ➔ PFC lifetime ~ 36 000 shots
- ✓ T-retention* < 1.3 mgT/h for 36 BM11-18

* 2D estimation of (D+T)/Be = f(T_{surf}, E_{imp}, Γ_D/Γ_{Be})
[PICSES-B scaling law, G. De Temmerman, R. Doerner]

Important issue for ITER: benchmark with ERO focusing on life time

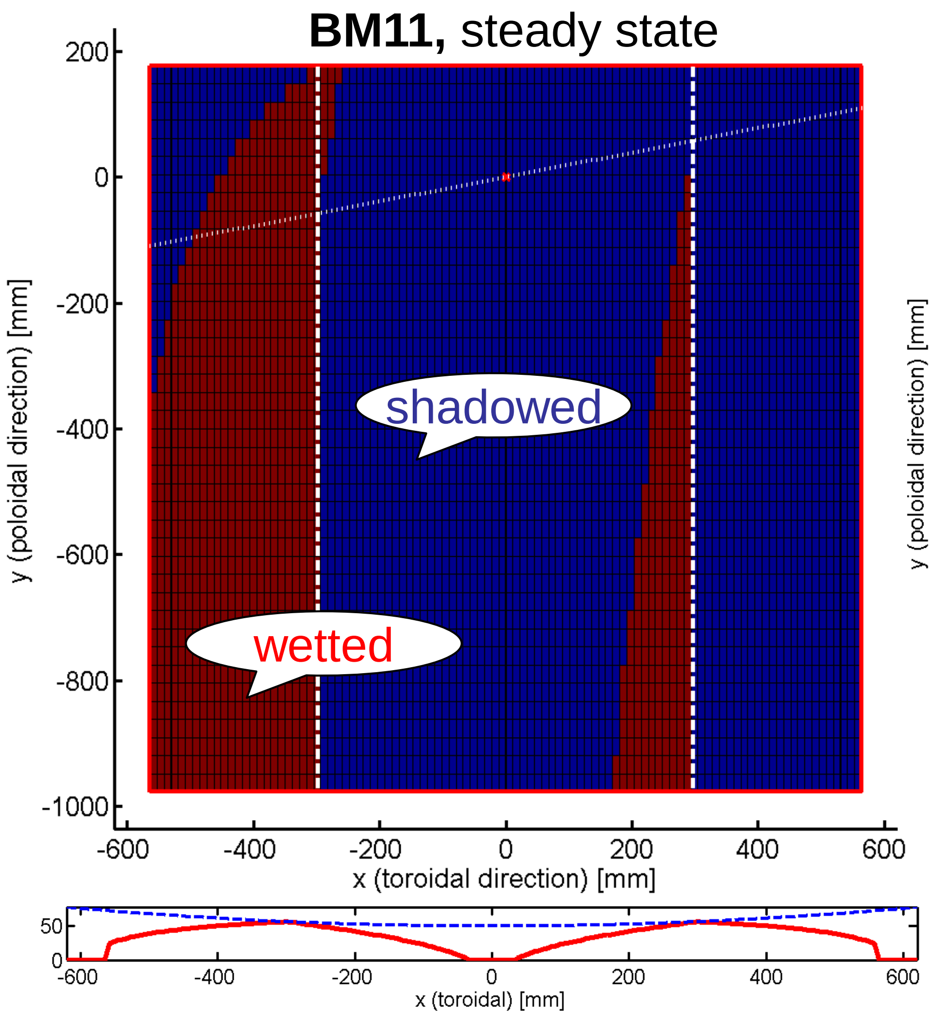
Plasma parameters at limiter surface

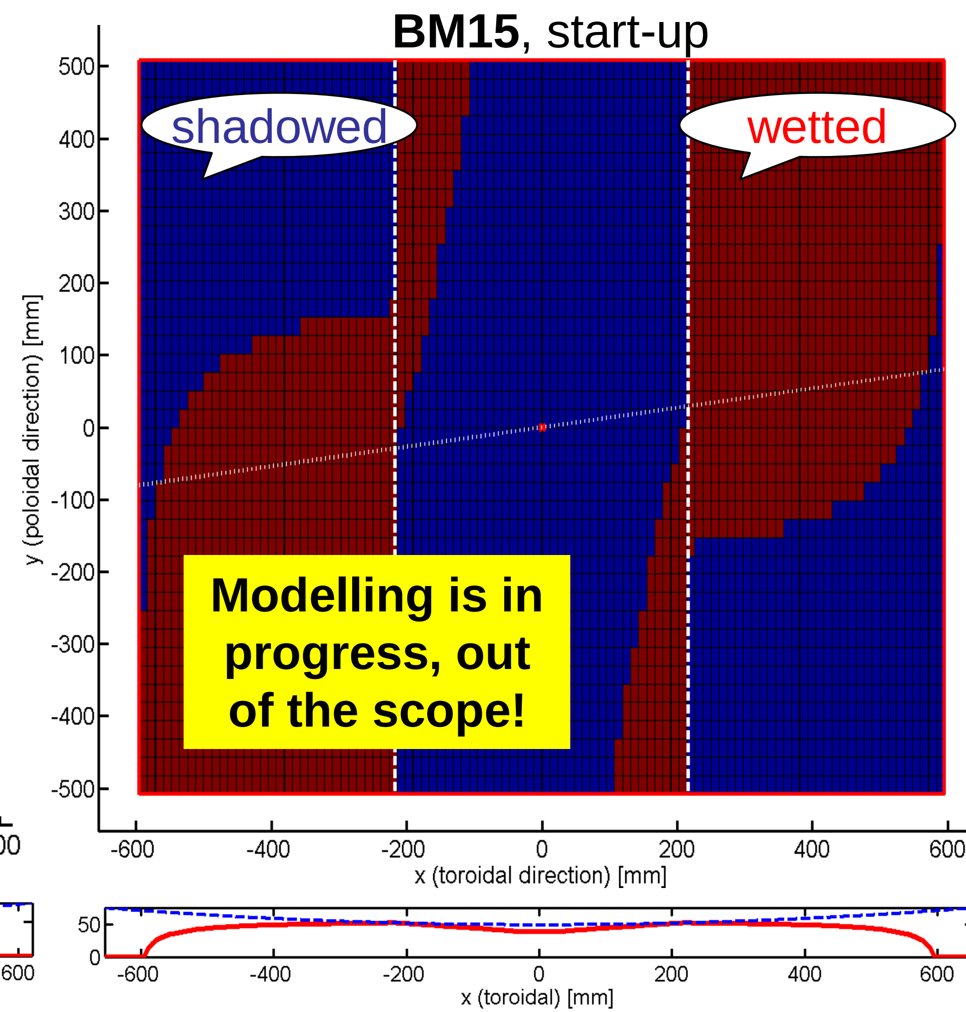


$T_e = 10eV = const$
$T_i = 20eV = const$

$T_e = 7.1eV = const$
$T_i = 18.6eV = const$

Shadowing patterns (LIM and ERO)

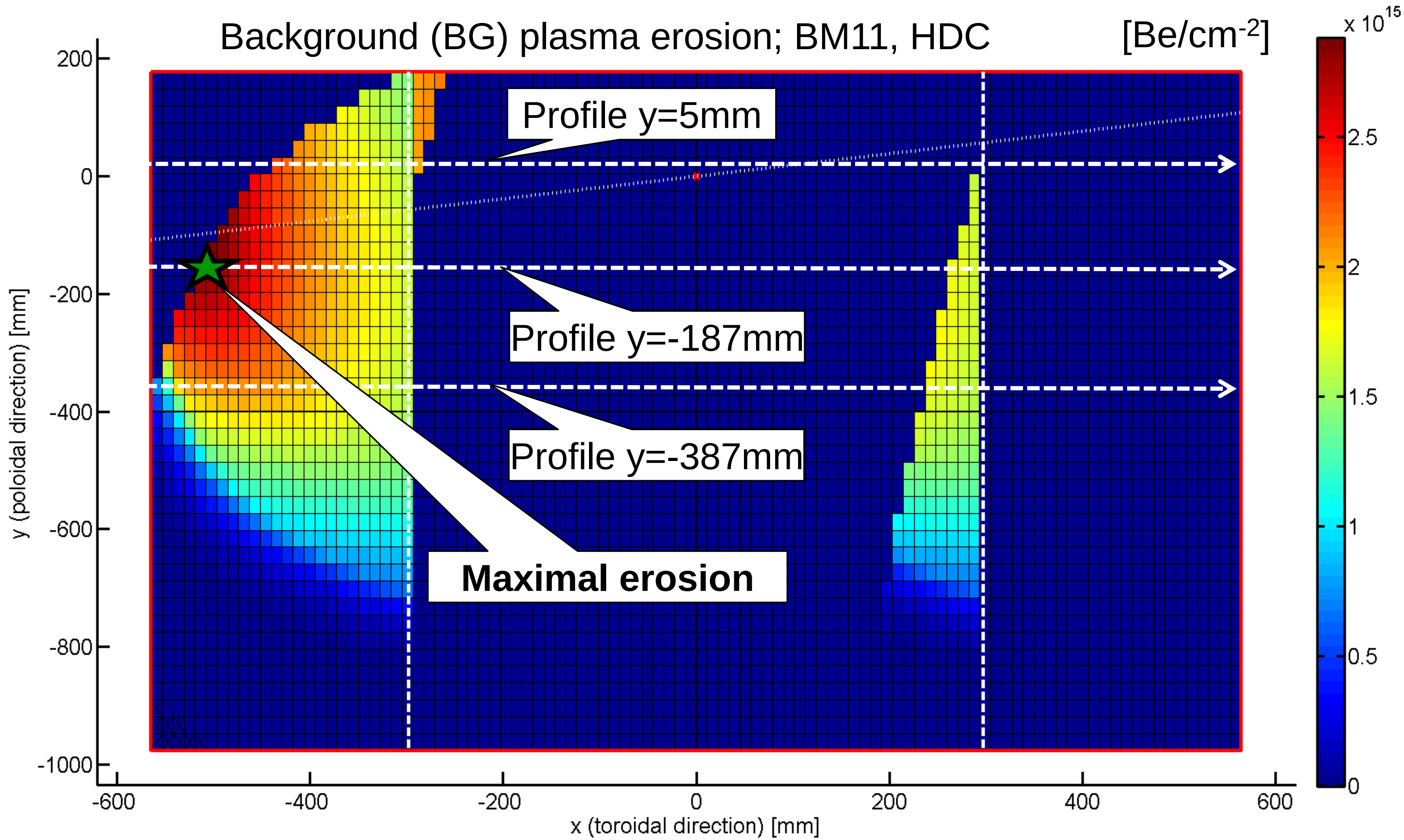




In shadowed areas we assume no BG erosion and re-deposition of intrinsic Be impurity

Shaping and shadowing implemented in the parametric form for any BM

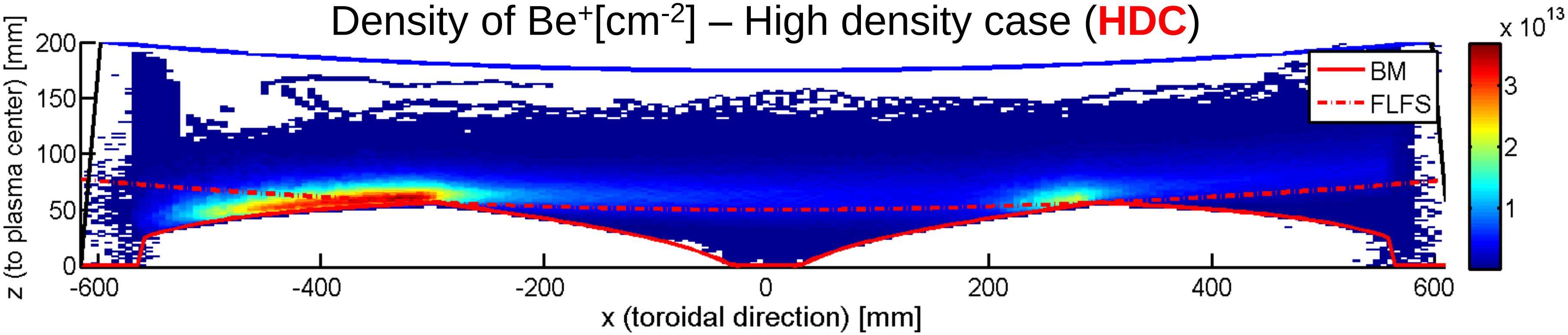
Poloidal positions of toroidal profiles



For LDC the maximal erosion point is elsewhere . . .

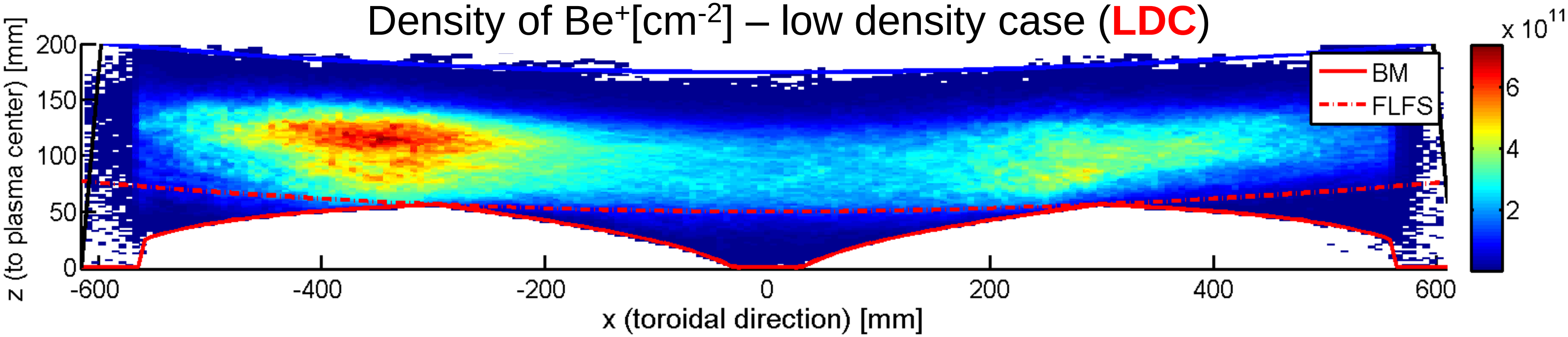
Deposition: low vs. high density plasma

Density of Be^{+}[cm^{-2}] – High density case (**HDC**)



Be is ionized close to surface . . . Large redeposition.

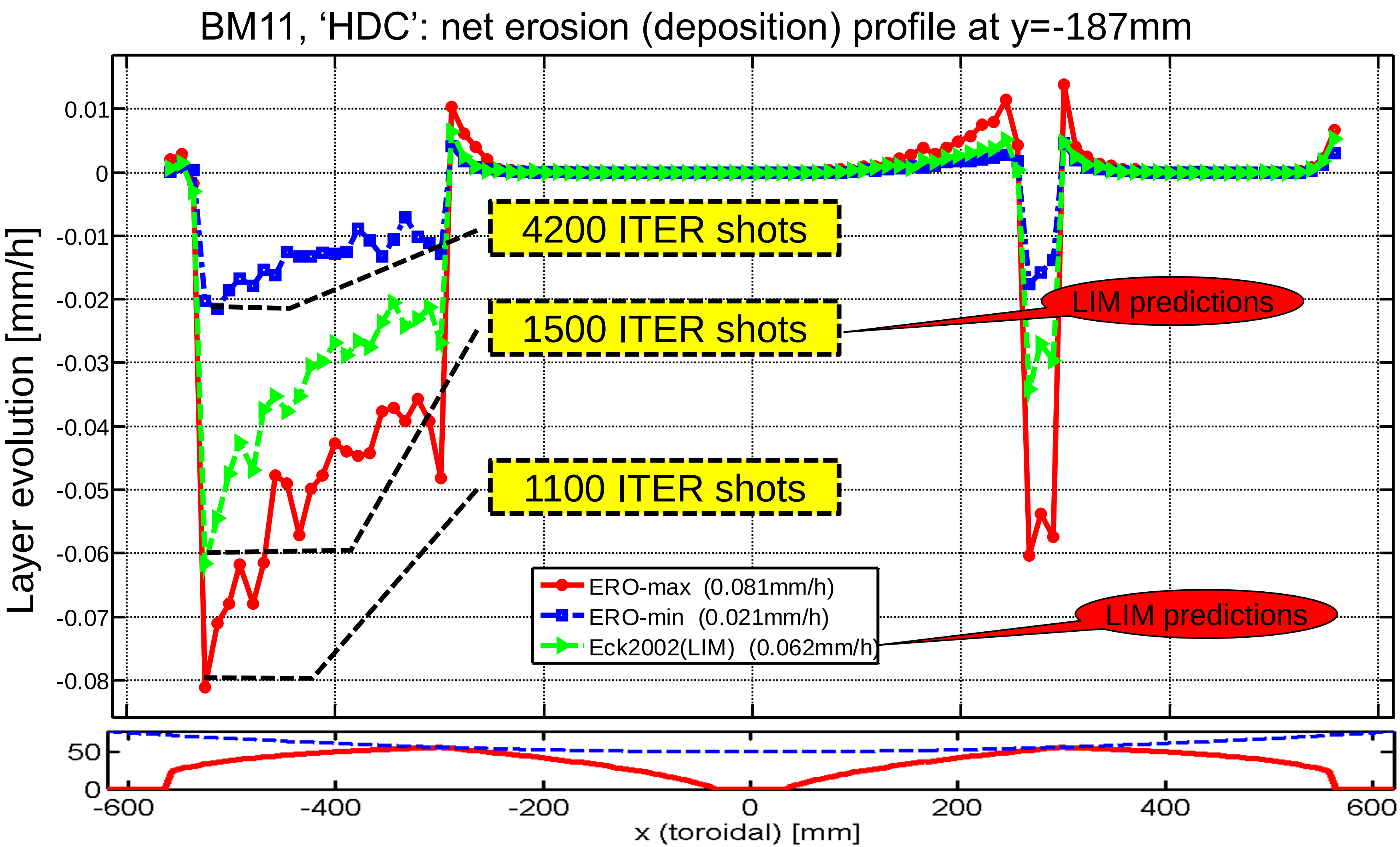
Density of Be^{+}[cm^{-2}] – low density case (**LDC**)



Be is ionized far away from surface . . . Small redeposition.

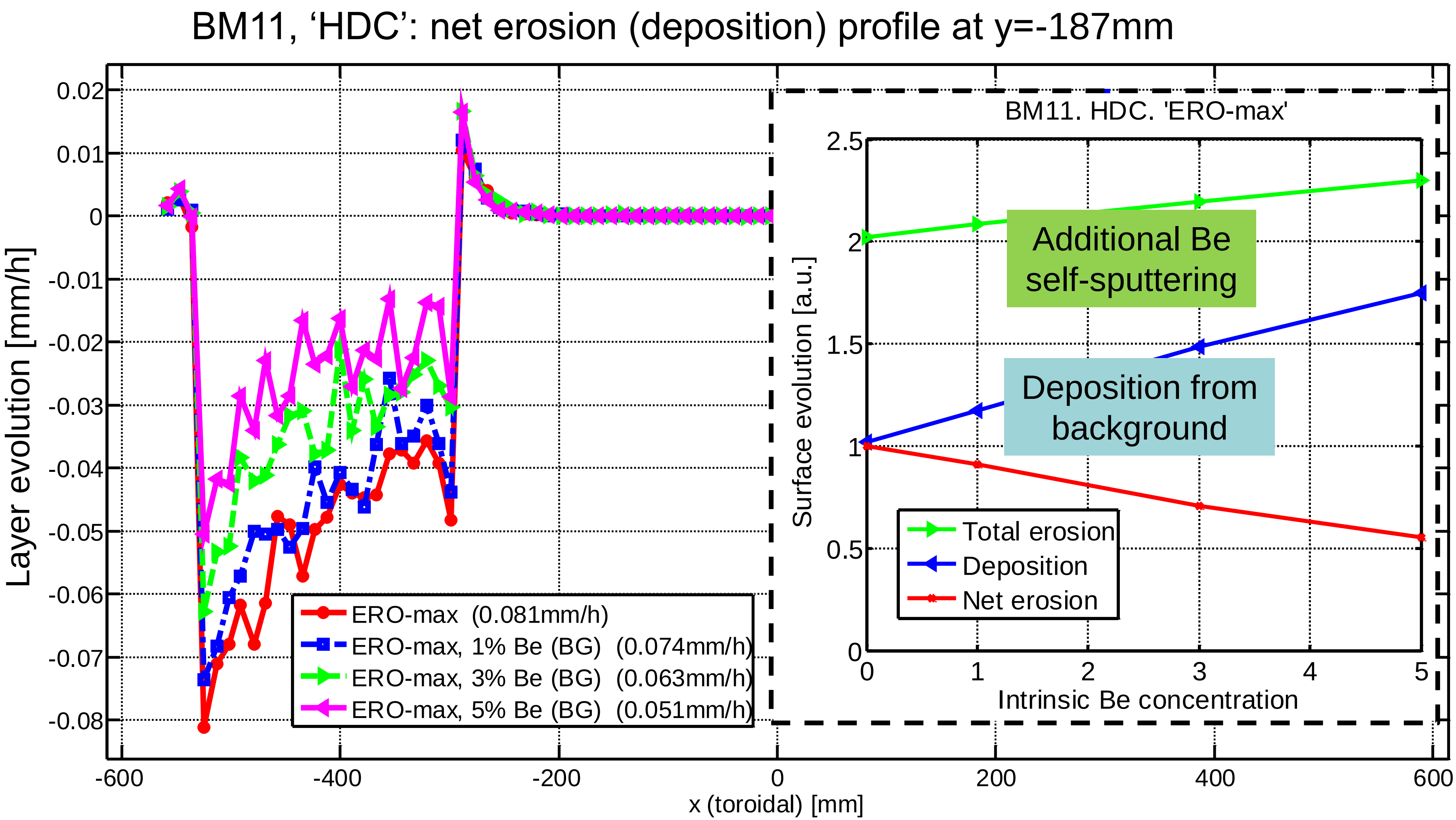
In both LIM and ERO deposition dependence on plasma parameters is feasible!

Sputter yields assumptions and net erosion



In most pessimistic case life time about 30% less than in earlier LIM predictions

Intrinsic Be impurity influence on net erosion



Deposition of Be impurity from plasma dominates over additional Be self-sputtering

Physical sputtering
(as introduced in ERO)

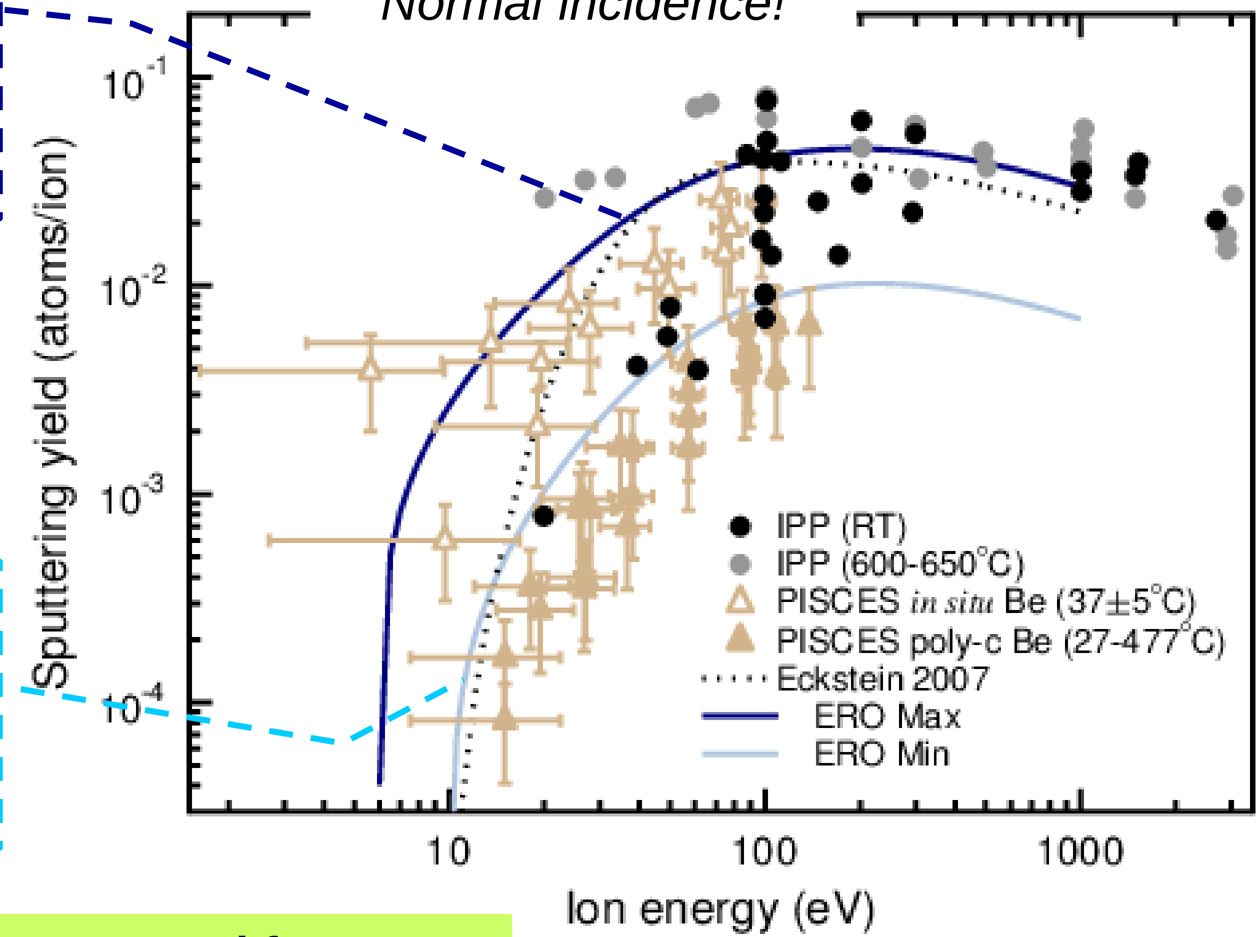
Sputtering data – margin estimates

Be by D^+ sputtering

„ERO-max“
MD + SDTRIMSP
pure Be

„ERO-min“
SDTrimSP
50%Be + 50%D

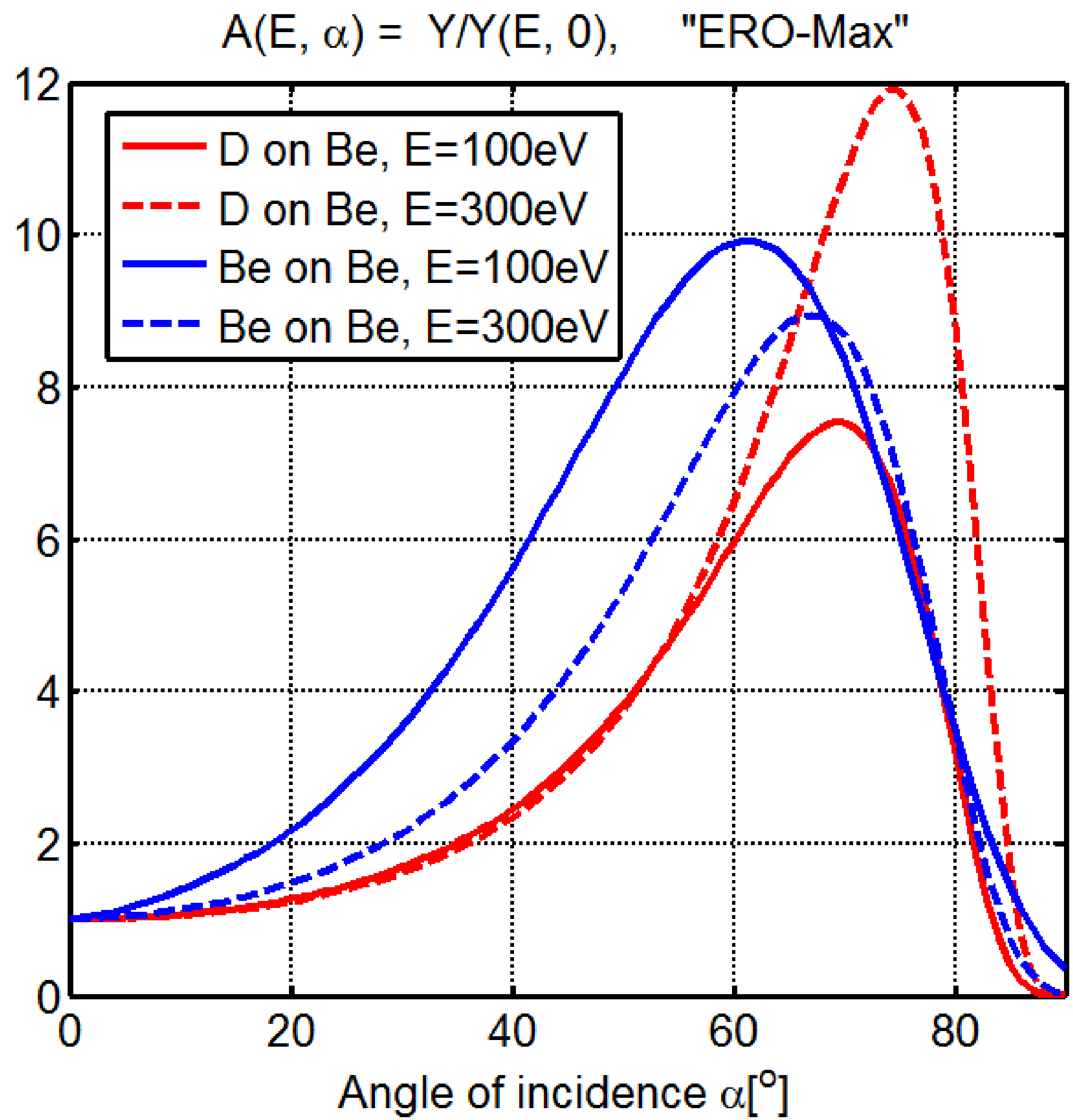
Normal incidence!



The very same limit fits are used for ITER predictive modelling and benchmark at JET.

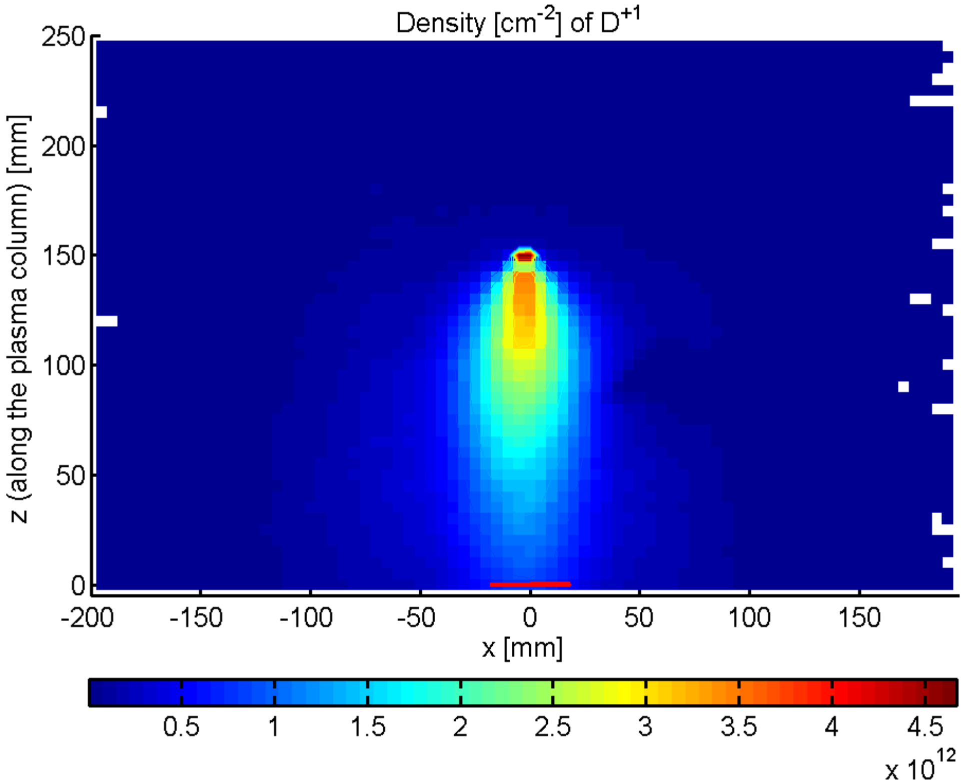
Angular part is of importance, however it is difficult to take it into account w/o modelling!

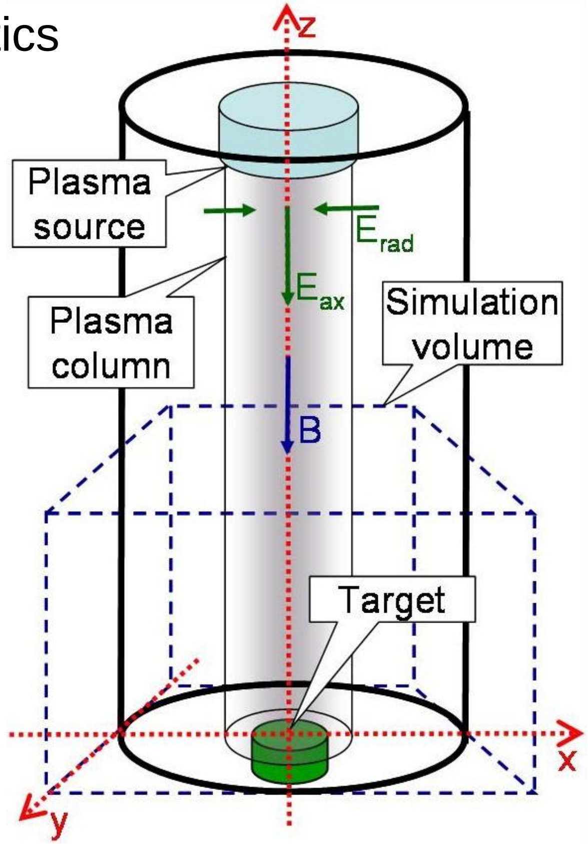
$Y(E_{in}, \alpha_{in})=$
$Y(E_{in}, 0) * A(E_{in}, \alpha_{in})$



Effective sputter yield – pre-characterization run

ERO pre-simulation for the impact angle&energy statistics





Eckstein 2007 fit:

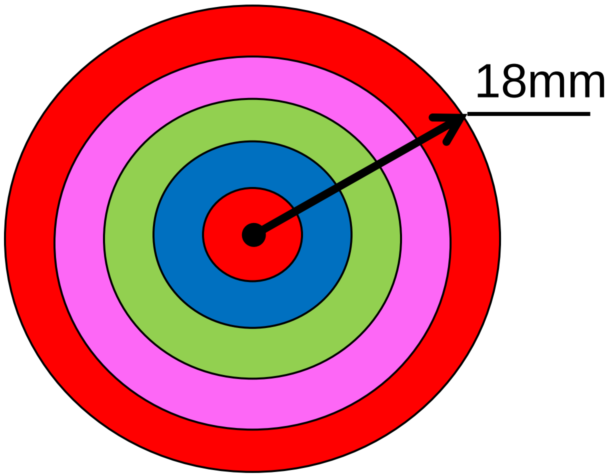
$$Y = Y(E_{in}, 0^o) * A(E_{in}, \alpha_{in})$$

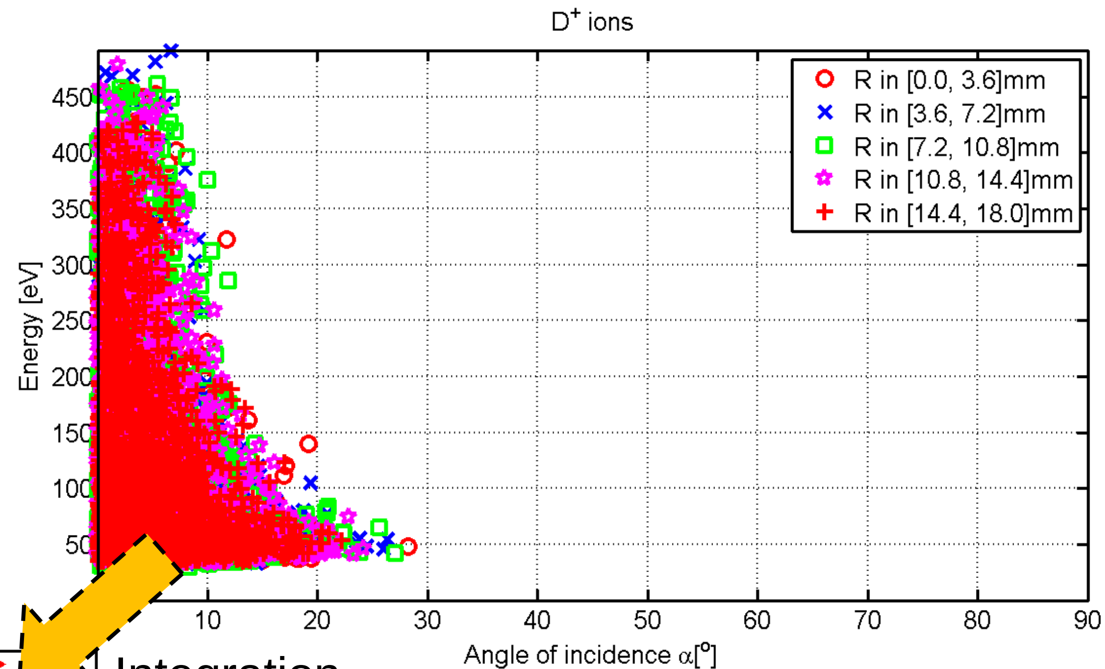
For normal incidence part we use ERO-min, ERO-max

For angular part we use SDTrimSP-based data

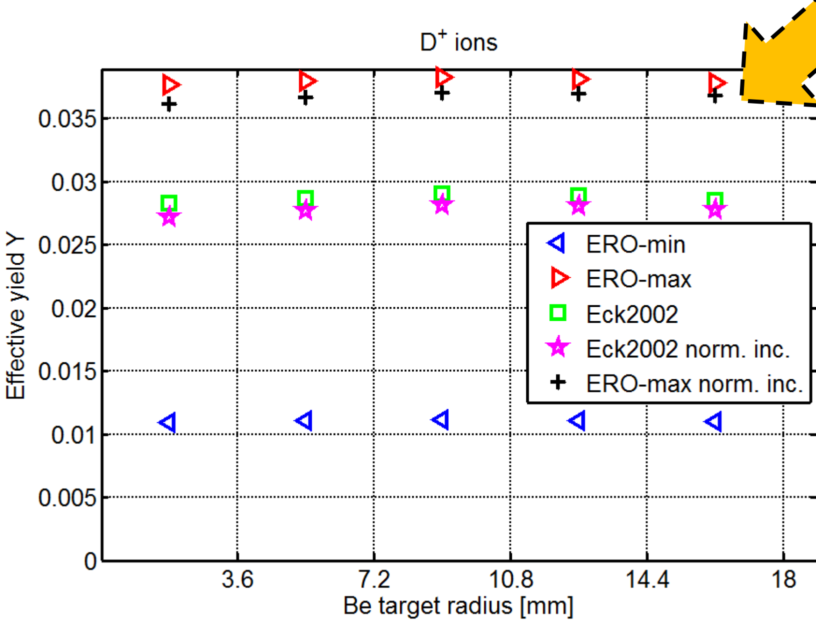
Sputter yields assumptions and net erosion

PISCES-B Be target





Integration result



No significant dependence on R!

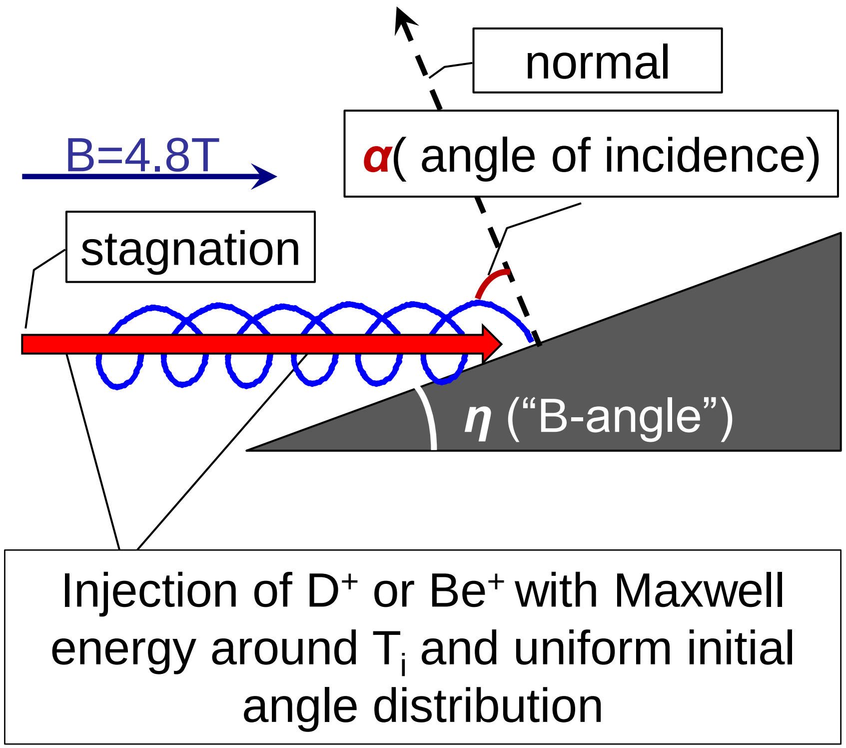
Assumption of normal incidence does not lead to essential change of result!

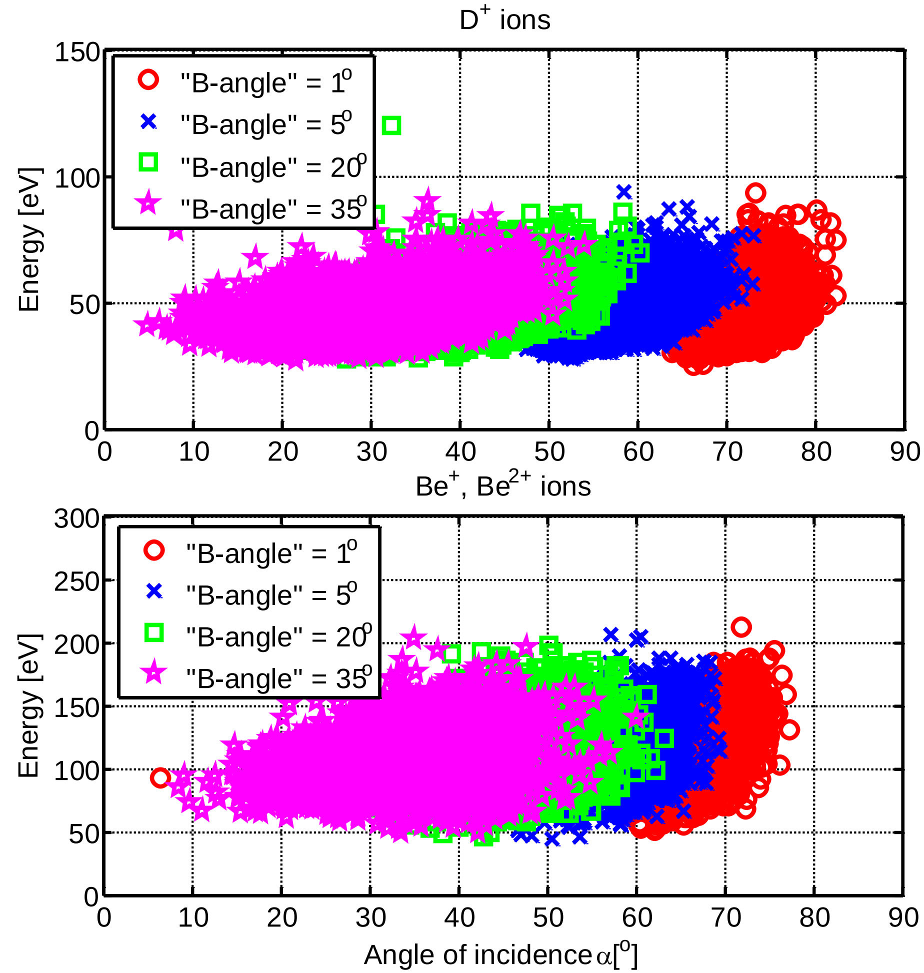
Various sputtering data lead to uncertainty by a factor of 3-4

Sputtering by BG plasma (and intrinsic Be)

- "integration" produces effective sputter yields -

ERO pre-calculation





Calculation of sputtering yield according to Eckstein's fit 2007 for Y(E, α), using angle and energy distribution as calculated by ERO (including gyration and sheath)

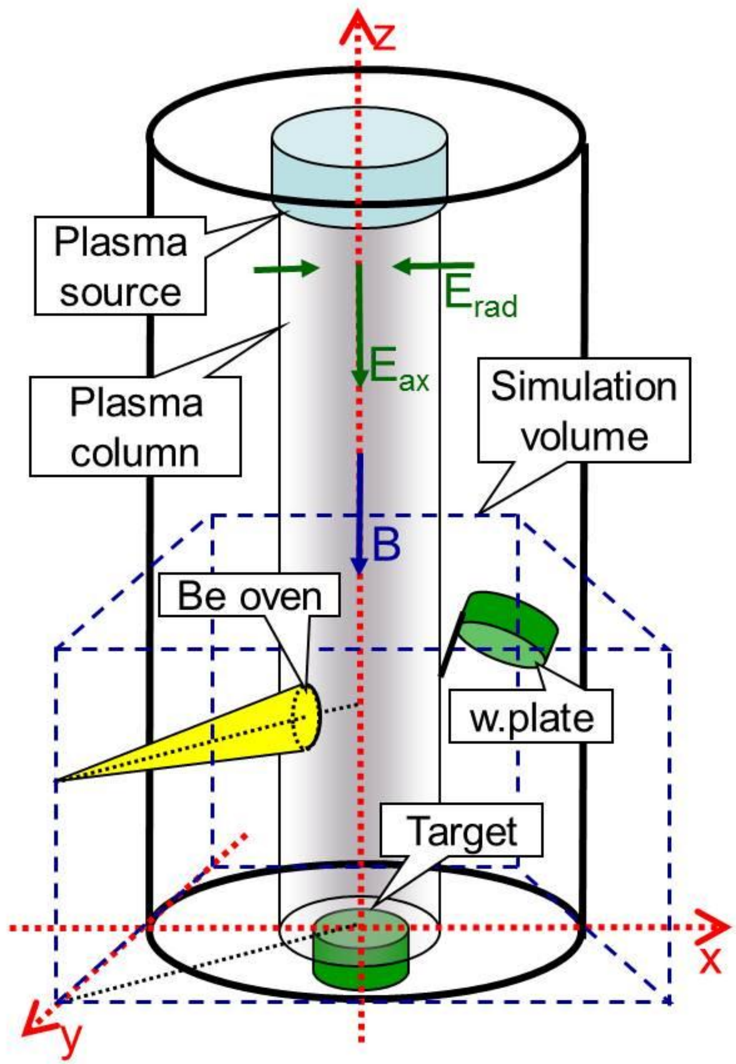
PISCES-B:

Spectroscopy benchmark – He plasma

Be sputtering benchmark

Improvement in sputtering yield uncertainty
→ model testing in PISCES-B

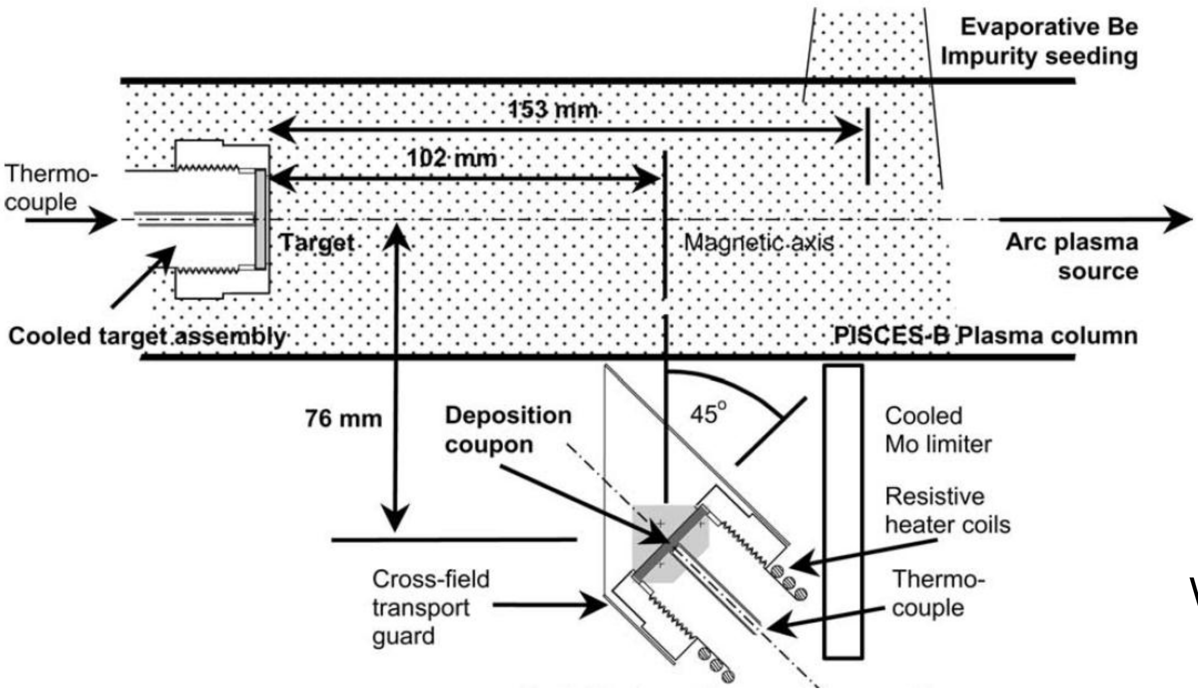
PISCES-B



Perfect for Be sputtering yields benchmark

1. *Target weight loss*
2. *Witness plate*
3. ***Spectroscopy***

Weight loss & witness plate



5000s plasma exposure

Transfer rate:

$$\frac{\text{Be target erosion } [Be/cm^2/s]}{\text{Witness plate deposit } [Be/cm^2/s]}$$

Be-D molecules . . . Chemical erosion!

<u>Target weight loss</u>

Exp.: 20.4mg ERO-min: 20mg
ERO-max: 70mg

<u>Transfer rate TARGET→WP</u>

Exp.: $7.5 \cdot 10^{-3}$ ERO: $1.4 \cdot 10^{-2}$

Spectroscopy benchmark

He plasma – *no confusion with Be-D molecules . . .*

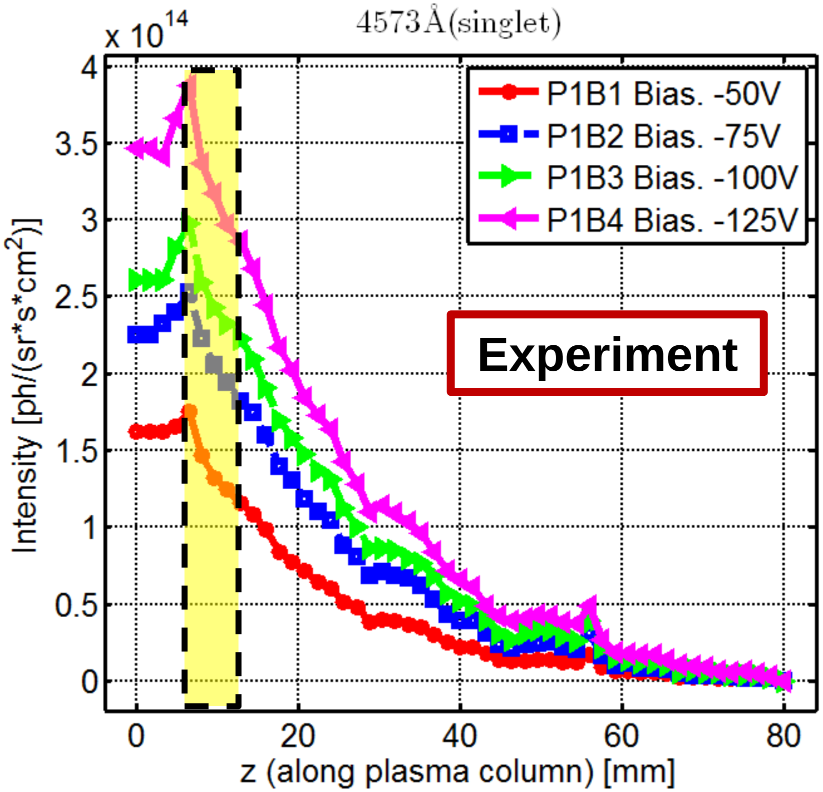
Plasma	At axis, z=150mm	Biasing	ERO 'name'
'P1'	n_e=12*10^{12}cm^{-3} T_e=4.8eV $P_{neutrals}$=7.3mTorr B=0.0152T	'B1' V=-50V	'P1B1'
		'B2' V=-75V	'P1B2'
		'B3' V=-100V	'P1B3'
		'B4' V=-125V	'P1B4'
'P2'	n_e=6.5*10^{12}cm^{-3} T_e=7.7eV $P_{neutrals}$=3.8mTorr B=0.0152T	'B1' V=-50V	'P2B1'
		'B2' V=-75V	'P2B2'
		'B3' V=-100V	'P2B3'
		'B4' V=-125V	'P2B4'
'P3'	n_e=4.0*10^{12}cm^{-3} T_e=11.5eV $P_{neutrals}$=2.5mTorr B=0.0152T	'B1' V=-50V	'P3B1'
		'B2' V=-75V	'P3B2'
		'B3' V=-100V	'P3B3'
		'B4' V=-125V	'P3B4'

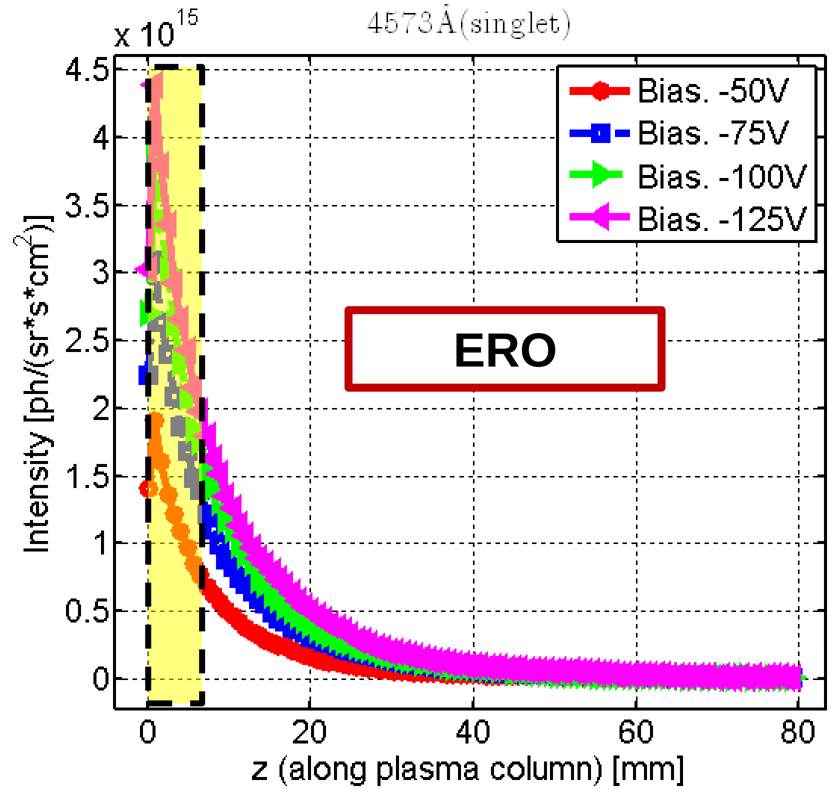
Vast material for benchmark!

(3 plasma conditions) x (4 biasing) x (BeI singlet and triplet + BeII profiles)

Spectroscopy as benchmark

Axial BeI light intensity profiles in case of Be target erosion

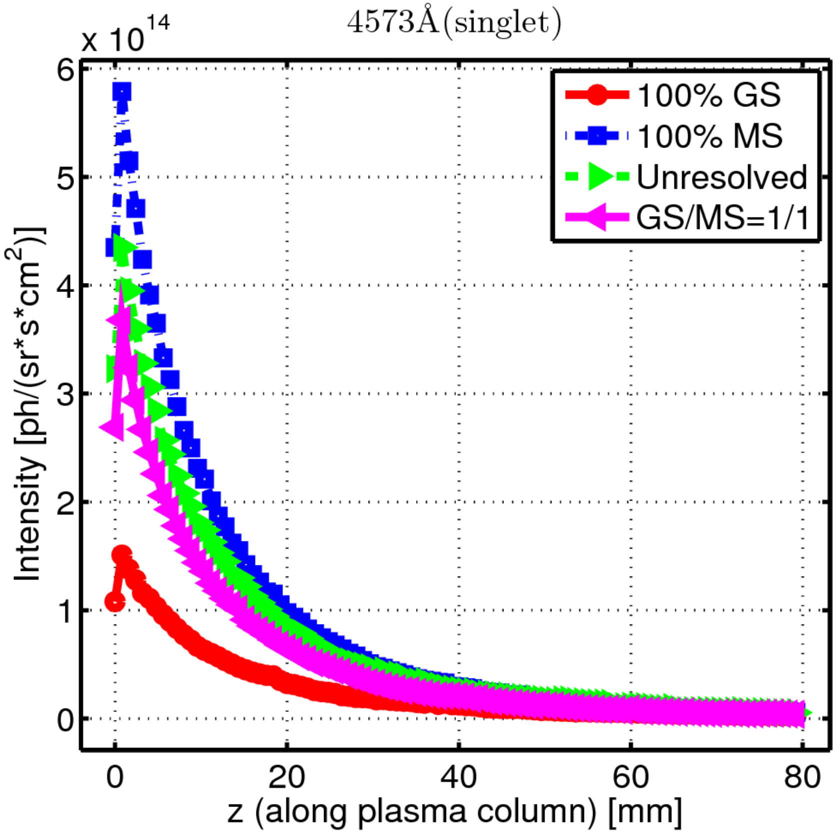


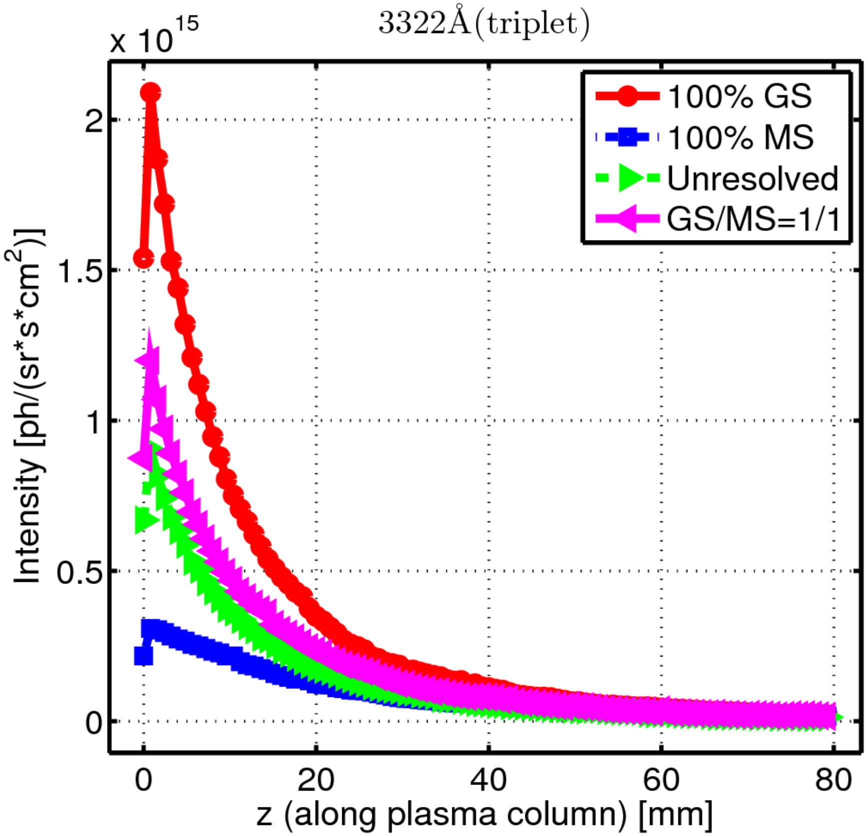


Let's try to understand first the integrated light near the target!

Initial population of MS is of importance!!!

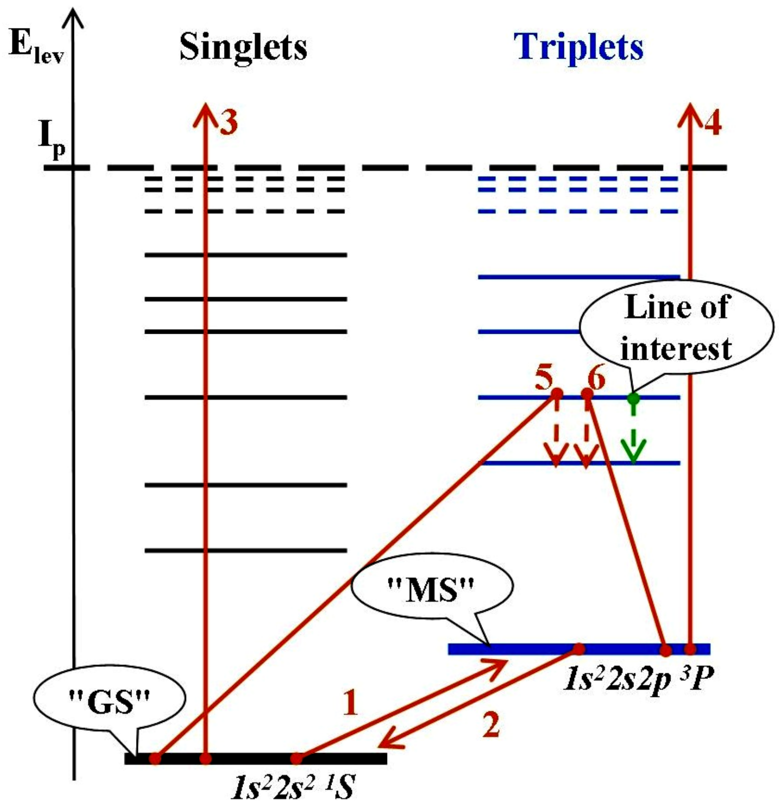
Be MS tracking in ERO: effect for PISCES-B



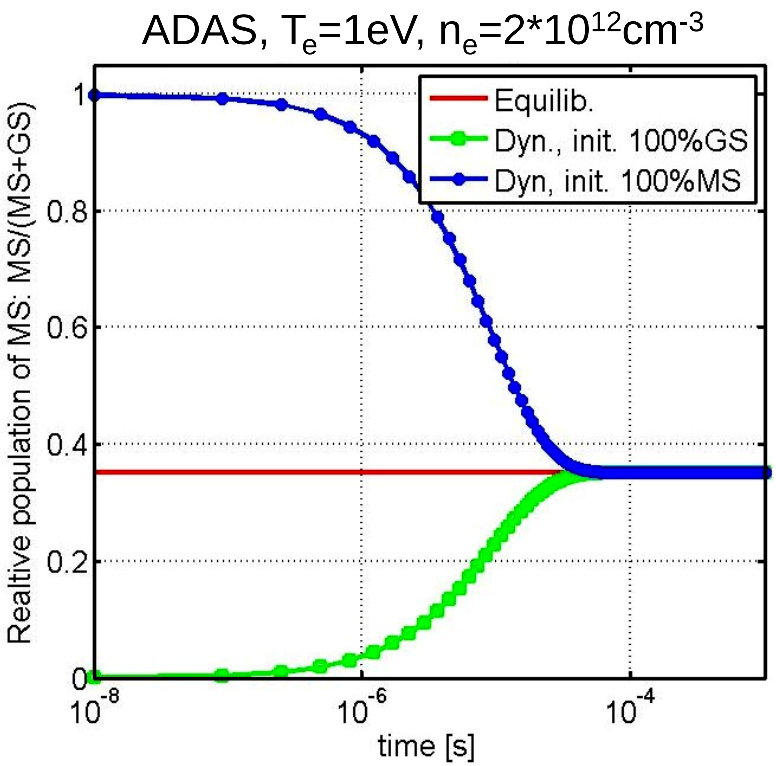


Initial MS population influences intensity near the target determines triplet to singlet ratio . . .

Be metastable state (MS) tracking in ERO



The system of 2 balance equations can be solved analytically . . .



Effective rates:

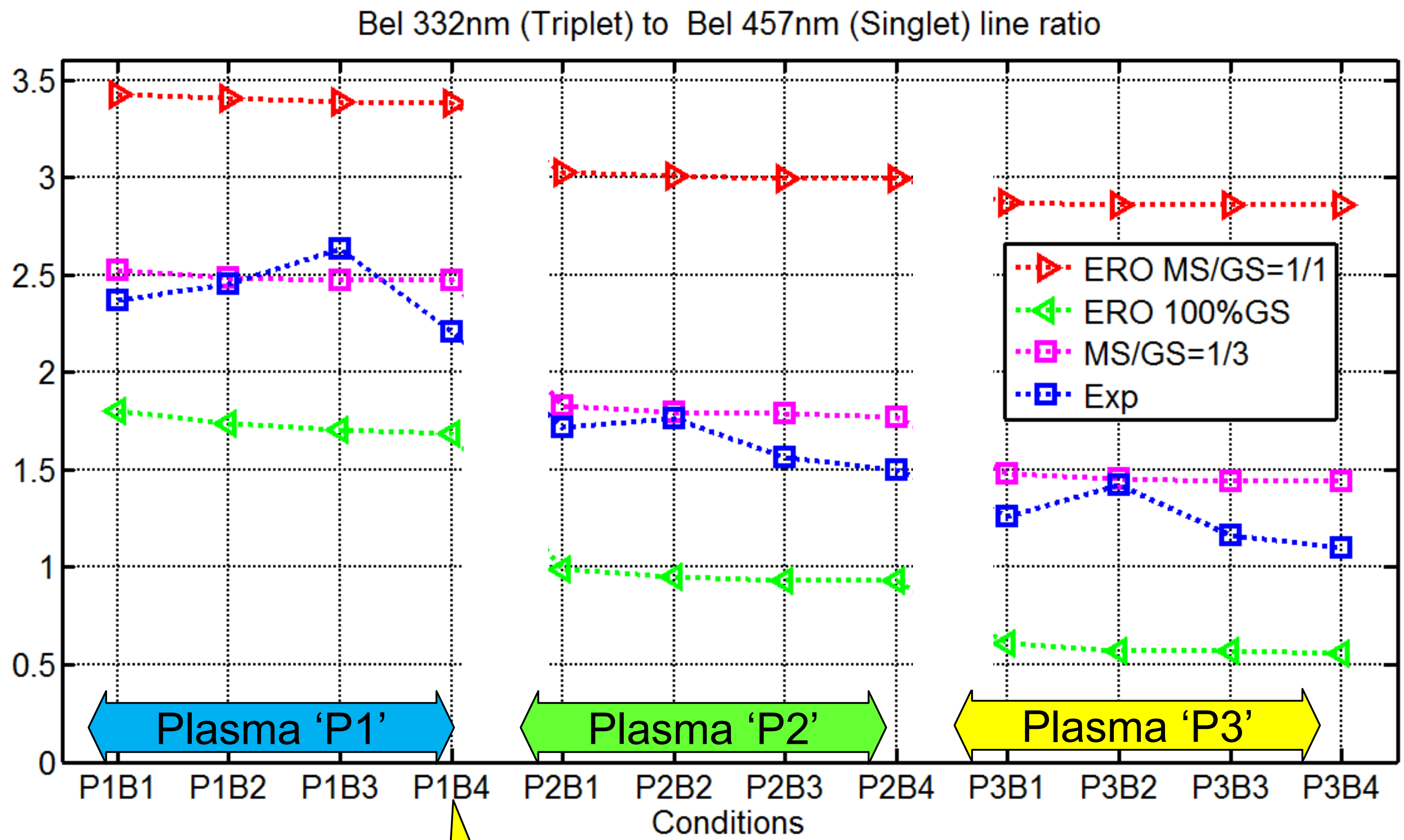
1,2) transitions between "GS" and "MS"

3,4) ionization from "GS" and "MS"

5,6) line intensity (PEC – photon emission coefficient), contributions from "GS" and "MS"

MS resolved approach allows to treat in ERO effectively the slow relaxation between triplet and singlet levels – important if MS population affected by extra processes and at high plasma parameter gradients

He plasma: determination of initial MS population



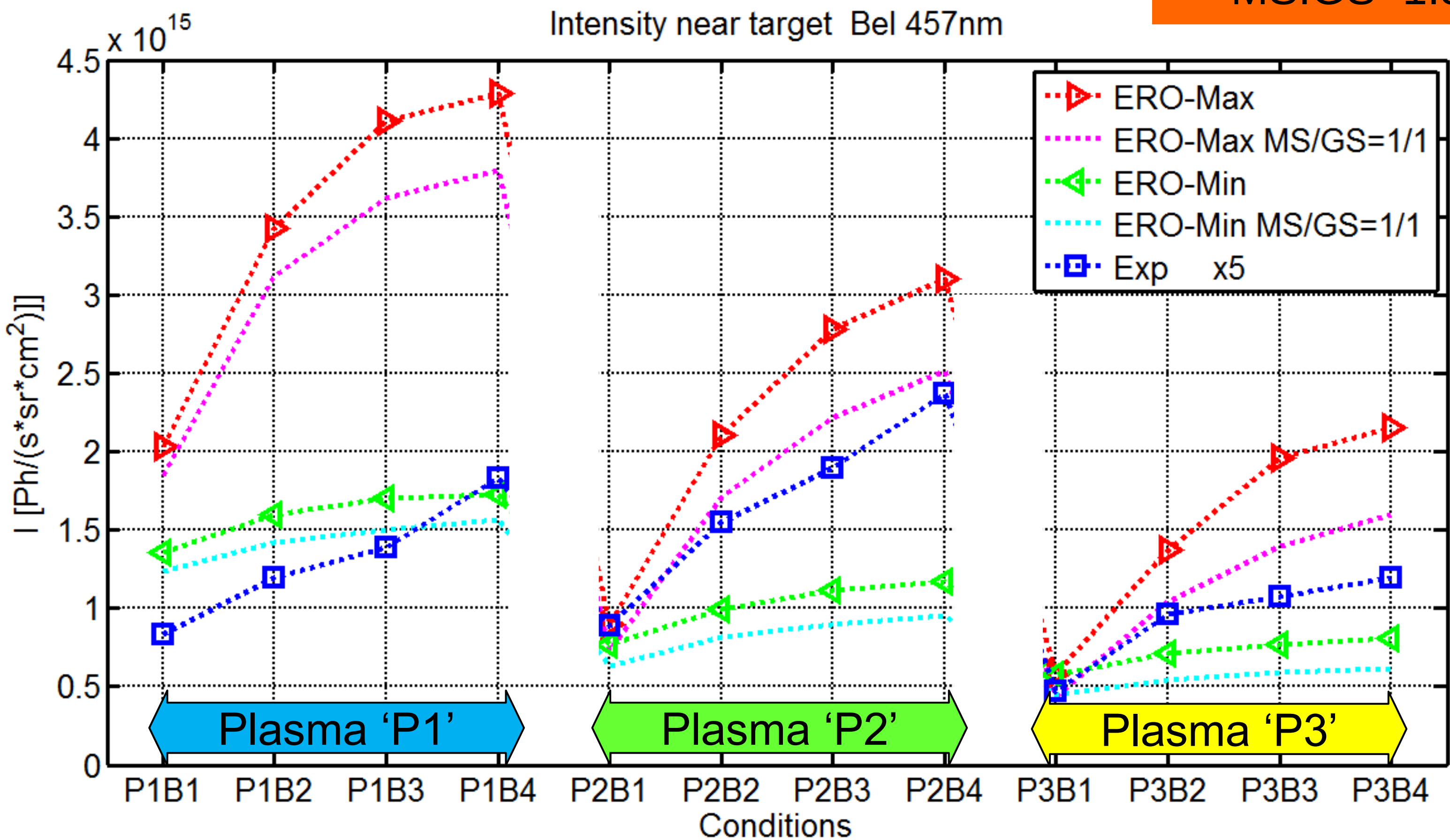
Biasing B1-B4: -50eV, -75eV, -100eV, -125eV

MS populations should be adjusted! **MS:GS=1:3**

Intensities near the target: Experiment vs. ERO

Singlet line, but agreement for triplet is similar!

MS:GS=1:3



Biasing B1-B4: -50eV, -75eV, -100eV, -125eV

Biasing effect well reproduced!

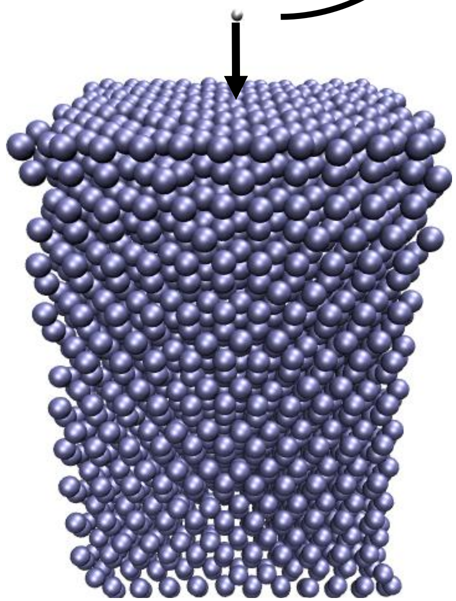
C.Björkas et al, PSI-2012, J.Nucl.Mater., in press

Be-D molecules in ERO:

Release and further tracing in plasma

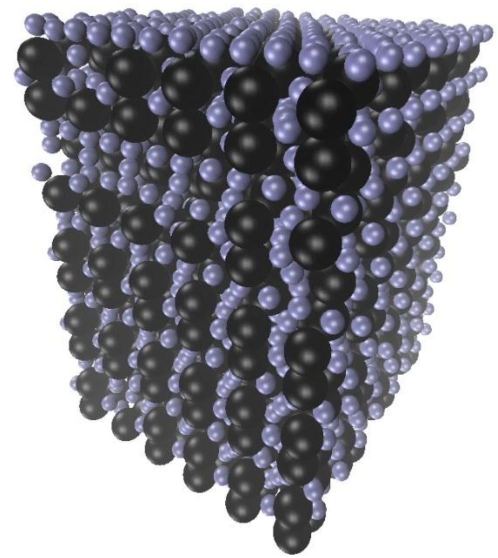
MD simulations of D bombardment

7-200eV D ions at
normal incidence



Be simulation cell

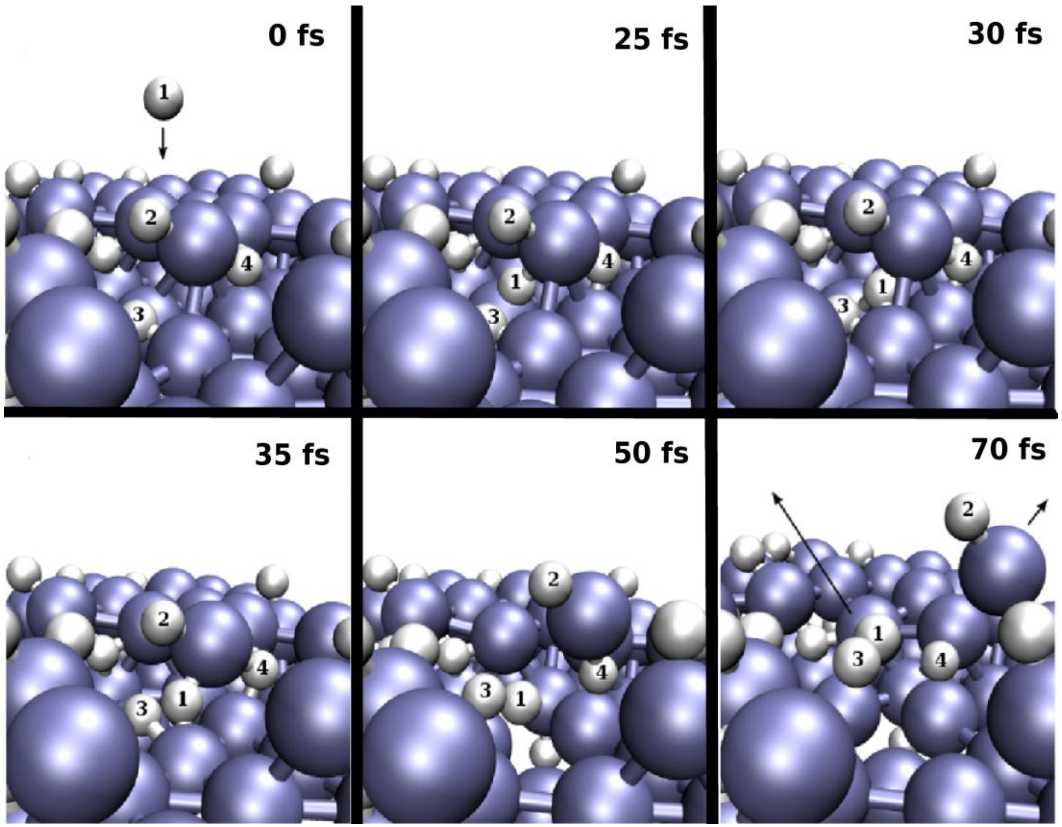
- Cell of ~3000 atoms
- D flux ~$2 \cdot 10^{28}$ $m^{-2}s^{-1}$
- 3000 cumulative bombardments
- Temperature control at borders
- Fixed bottommost layers



Be_2W simulation cell

W terminated or Be teminated
surfaces bombarded

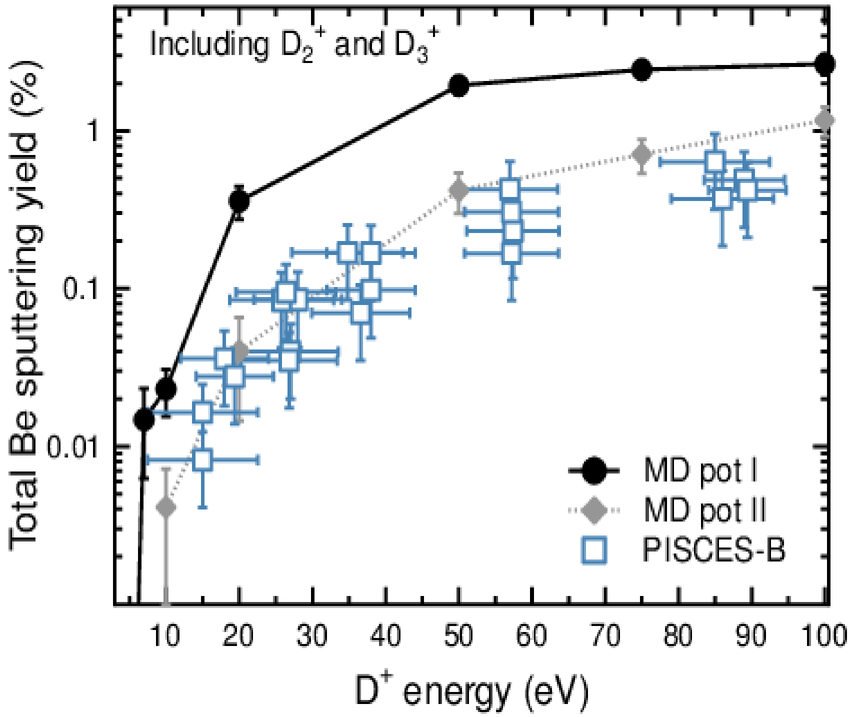
Swift chemical sputtering



- Snapshots of a similar event
- The D ion breaks all four of the Be-Be bonds
- Ideally a surface Be has nine bonds
- „Roughnening“ of the surface is needed

ERO input: sputtering yields

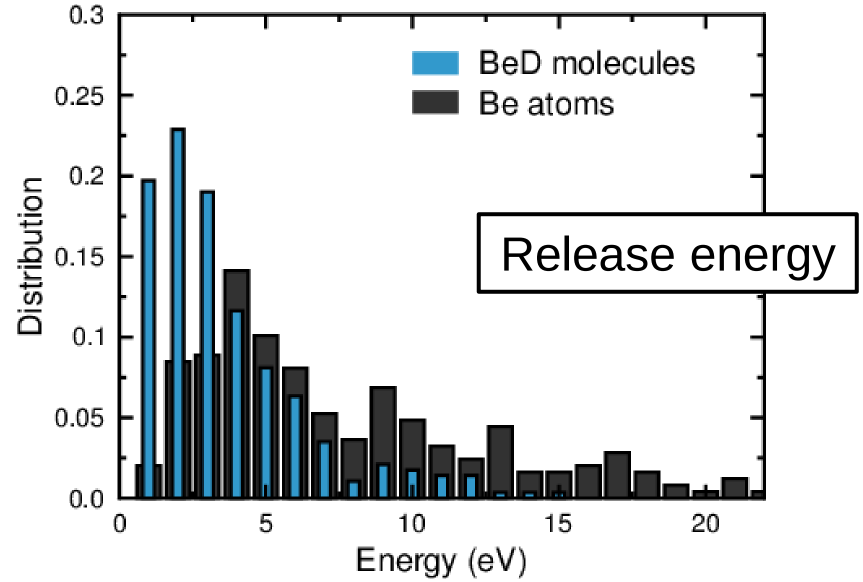
- Comparisons to previous yield measurements in PISCES-B with a similar target shows a better agreement with **pot II**
- Important to account for D_2 and D_3 ions
- 17% of total yield estimated to be BeD at all biases
  - No control of target temperature → no bias dependency

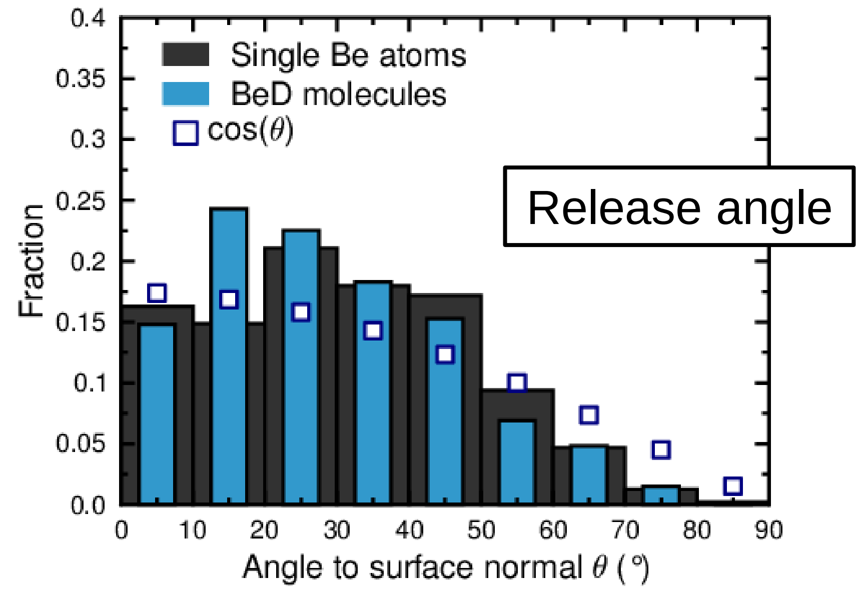


[D. Nishijima et al. 2009]

BeD implementation in ERO

- BeD yield:
  - 17% of total Be sputtering yield in current experiment
  - If surface T controlled, BeD fraction is ion energy dependent
- Sputtering and reflection:
  - MD: BeD sputters as single Be and has a low sticking
- Reactions in plasma:
  - BeD + e⁻ collision rates calculated





ERO input: BeD reactions in plasma

- BeD + e⁻ collision rates depend on T_e and vibrational state v
  - Assume v=1 and transitions Δv=0

Thanks for consultation to R.Janev

Important reactions

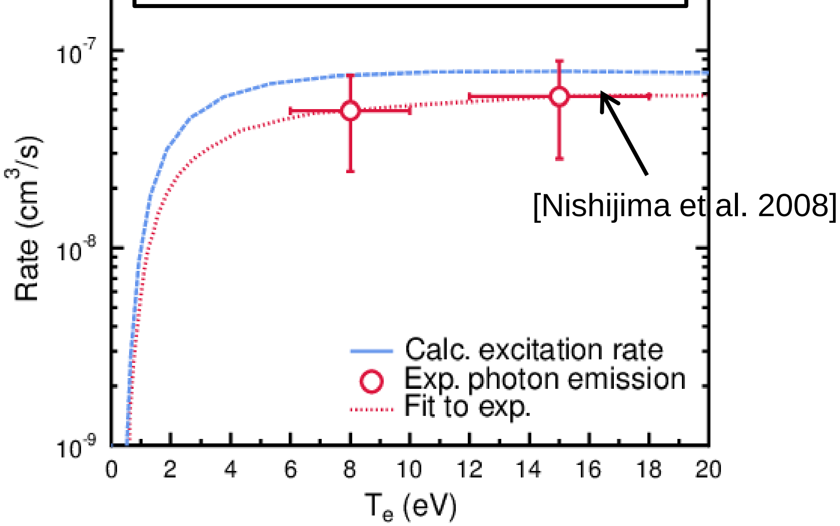
$$e + \mathrm{BeD} \rightarrow e + \mathrm{BeD}^{+}$$

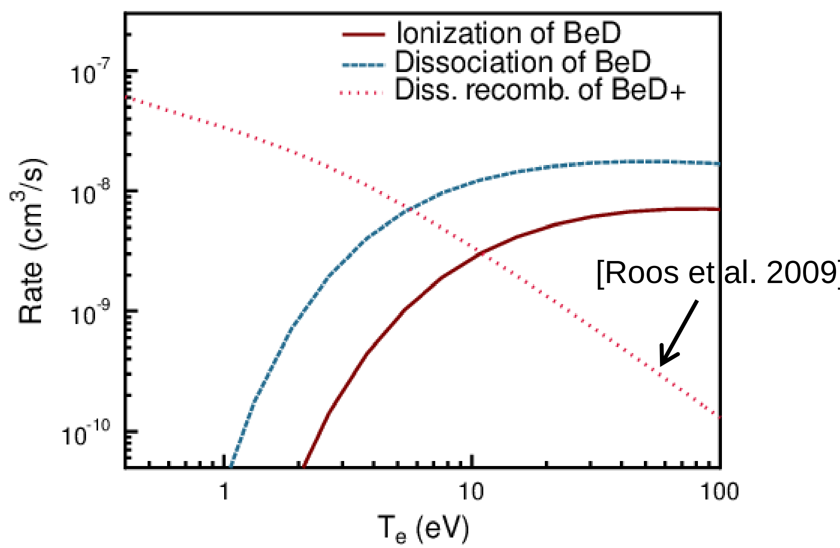
$$e + \mathrm{BeD} \rightarrow e + \mathrm{BeD}^{*}$$

$$e + \mathrm{BeD} \rightarrow e + \mathrm{BeD}^{*} \rightarrow e + \mathrm{Be}(3_P) + \mathrm{D}(1_S)$$

Metastable now!

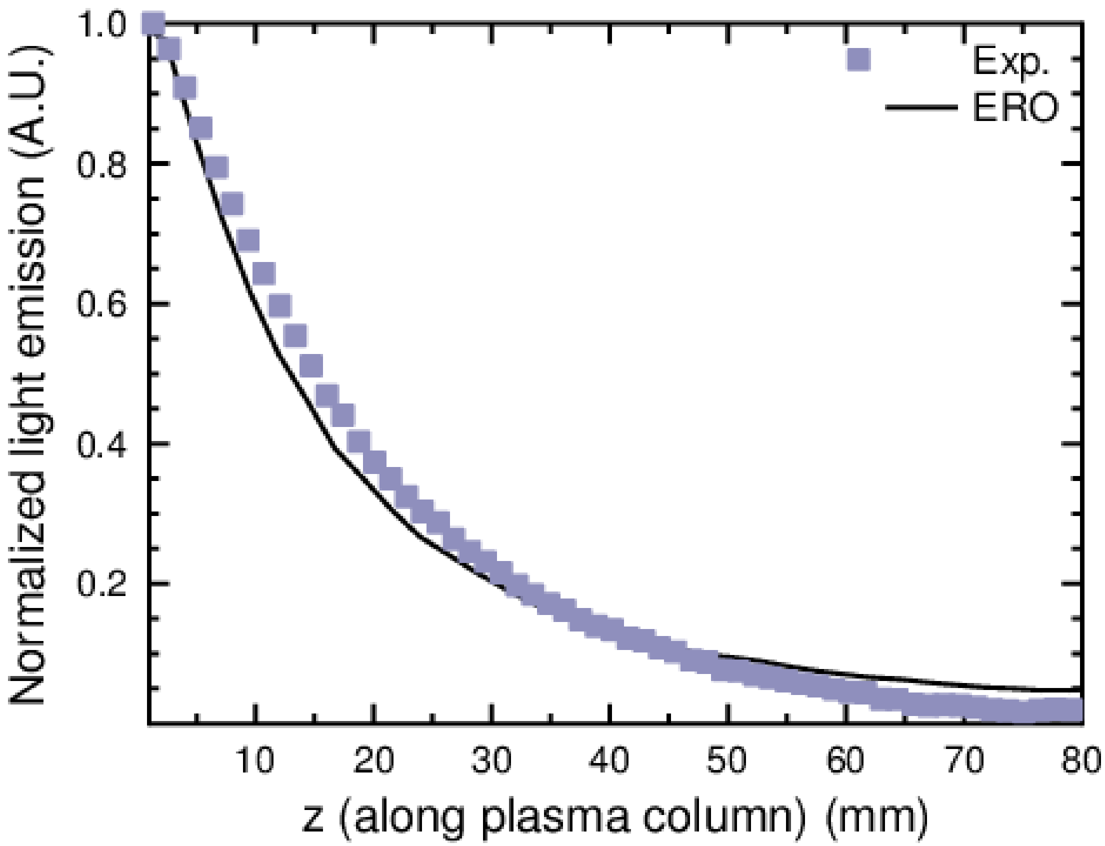
Photon emission coefficient



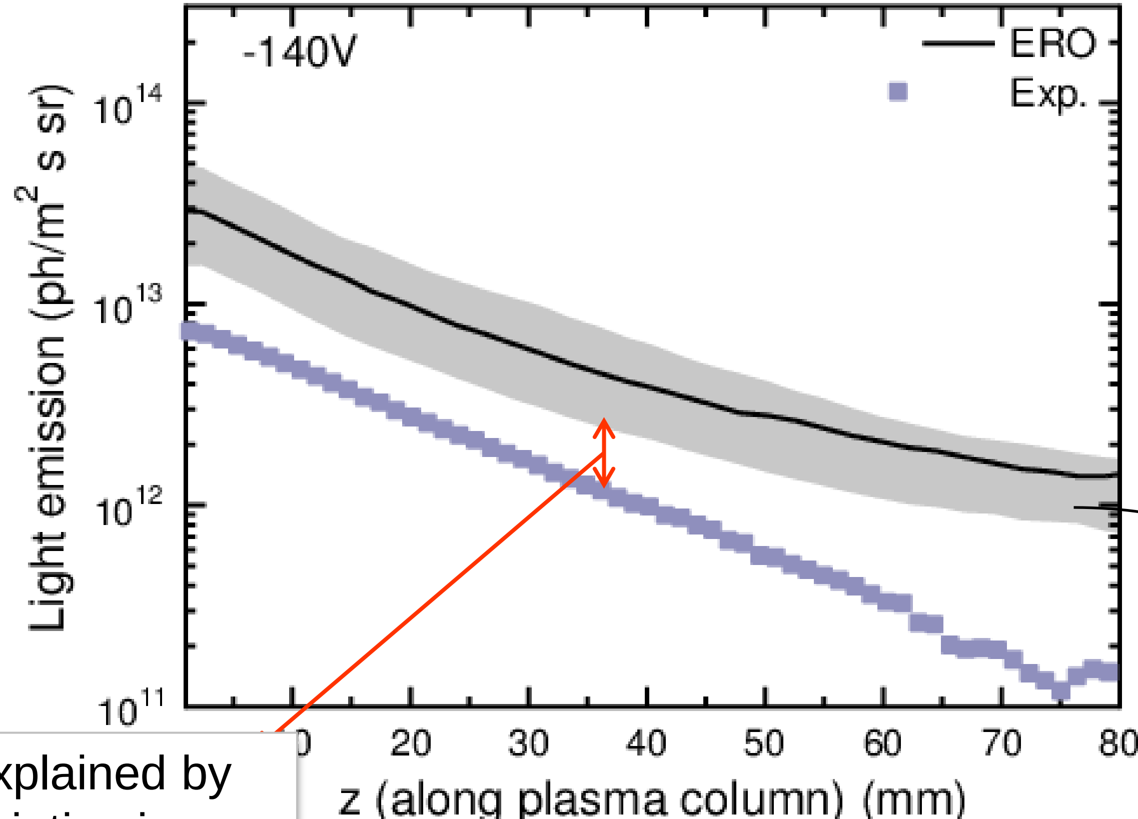


Comparison of BeD light

- BeD (497.3 - 499.2nm) light emission profiles agree well with experiments



- BeD (497.3 - 499.2nm) light emission profiles agree well with experiments



Range including uncertainties in n_e and T_e

Can be explained by uncertainties in sputtering yields or spectroscopic data

PISCES-B:

Spectroscopy benchmark – D plasma

Spectroscopy benchmark

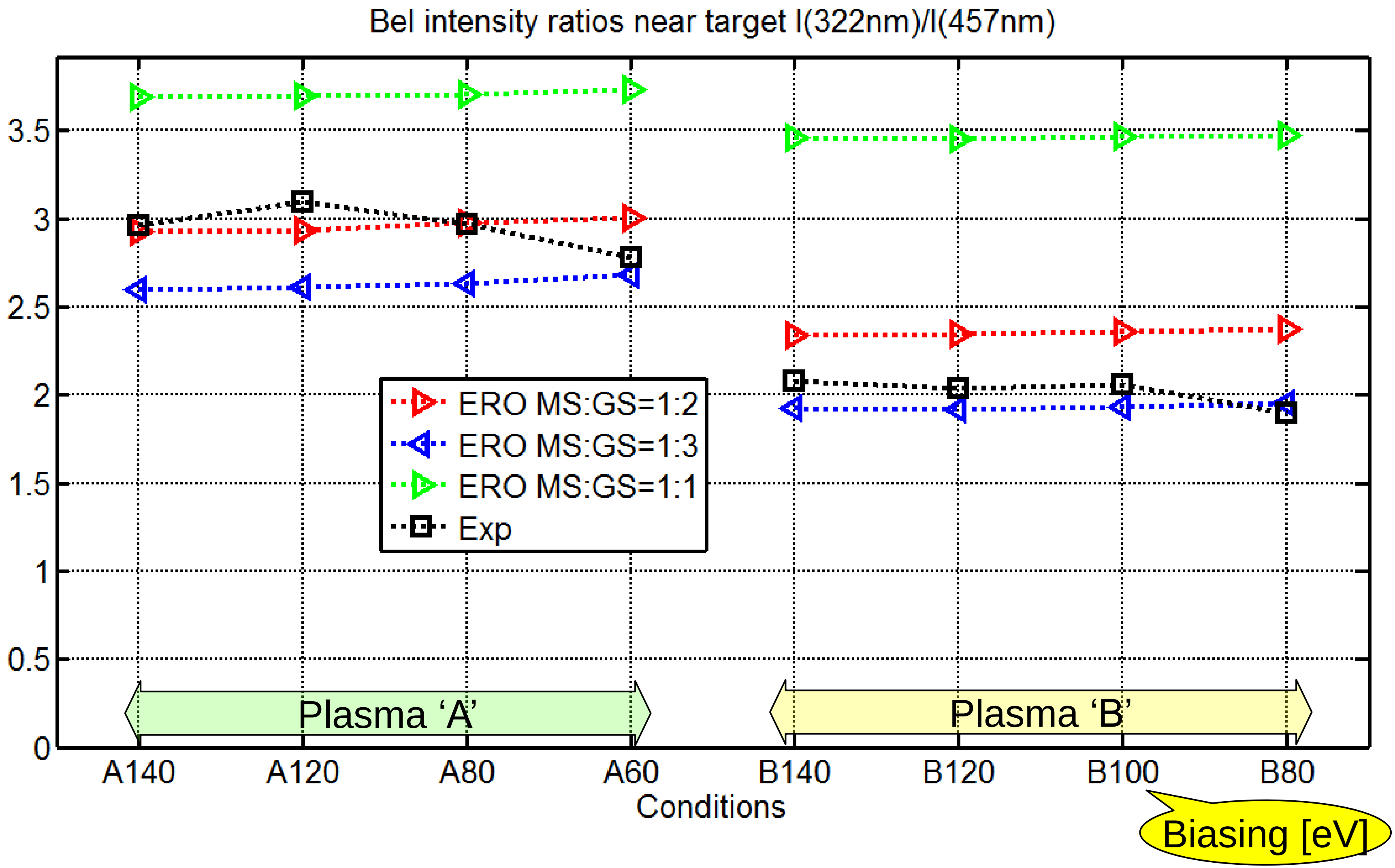
D plasma

Plasma	At axis, z=150mm	Biasing	ERO 'name'
'A'	n_e=4.9*$10^{12}$$cm^{-3}$ T_e=4.6eV $P_{neutrals}$=5.4mTorr B=0.0152T P_{plasma} = -17eV	V=-140V	'A140'
		V=-120V	'A120'
		V=-80V	'A80'
		V=-60V	'A60'
'B'	n_e=2.6*$10^{12}$$cm^{-3}$ T_e=8.2eV $P_{neutrals}$=1.7mTorr B=0.0152T P_{plasma} = -12eV	V=-140V	'B140'
		V=-120V	'B120'
		V=-100V	'B100'
		V=-80V	'B80'

Strong influence of BeD release (recently provided in ERO)

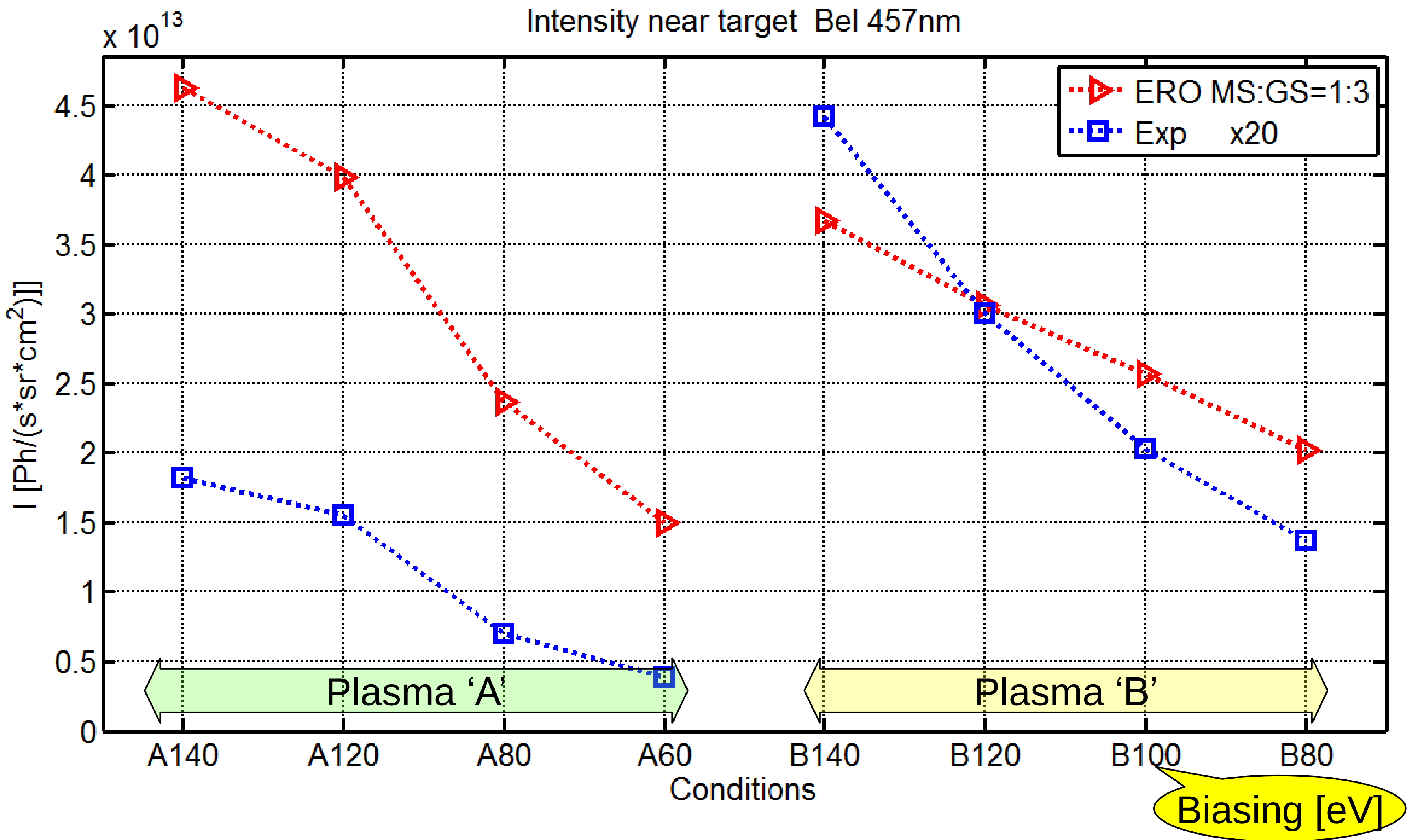
Vast material for benchmark!
(2 plasma conditions) x (4 biasing) x (BeI singlet and triplet + BeII +BeD profiles)

D plasma: line ratios→ MS population



MS populations should be adjusted! **MS:GS=1:3**

D plasma: intensities at target

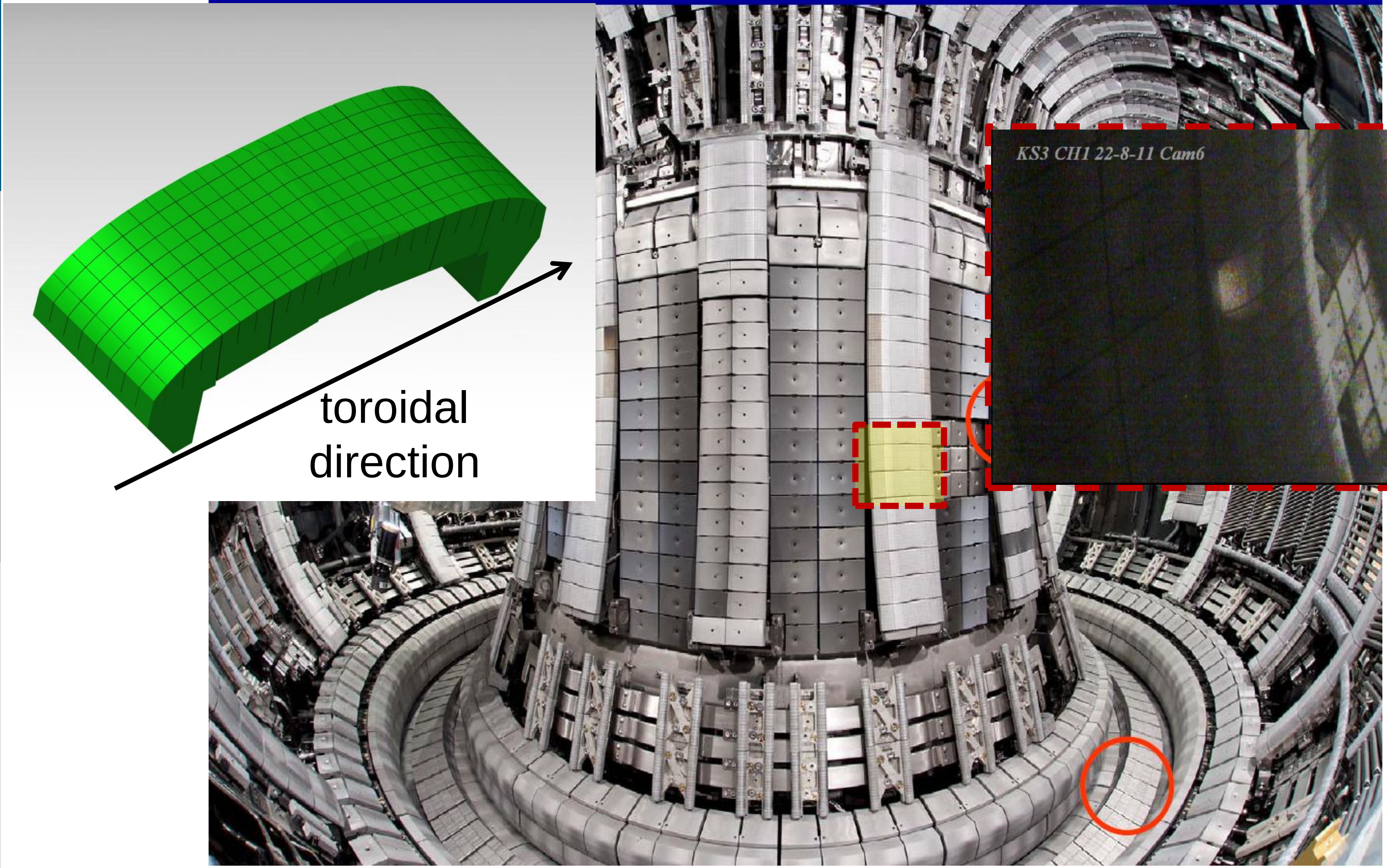


- *Be-D molecules are 17% of total Be release*
- *All Be from dissociation goes to MS level*

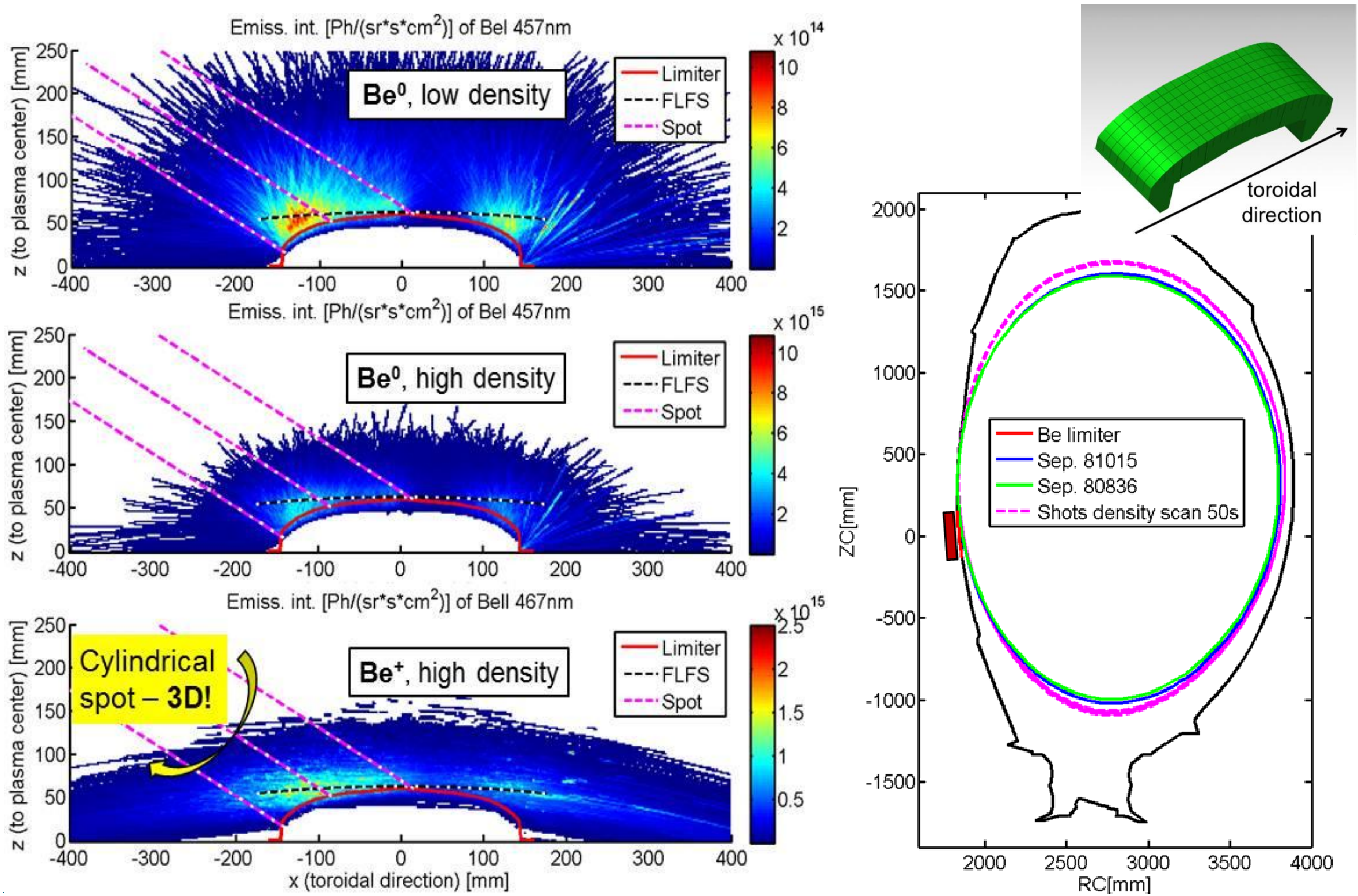
D Borodin et al, PSI-2012, J.Nucl.Mater., in press

Spectroscopy benchmark at JET ILW (plasma density scan)

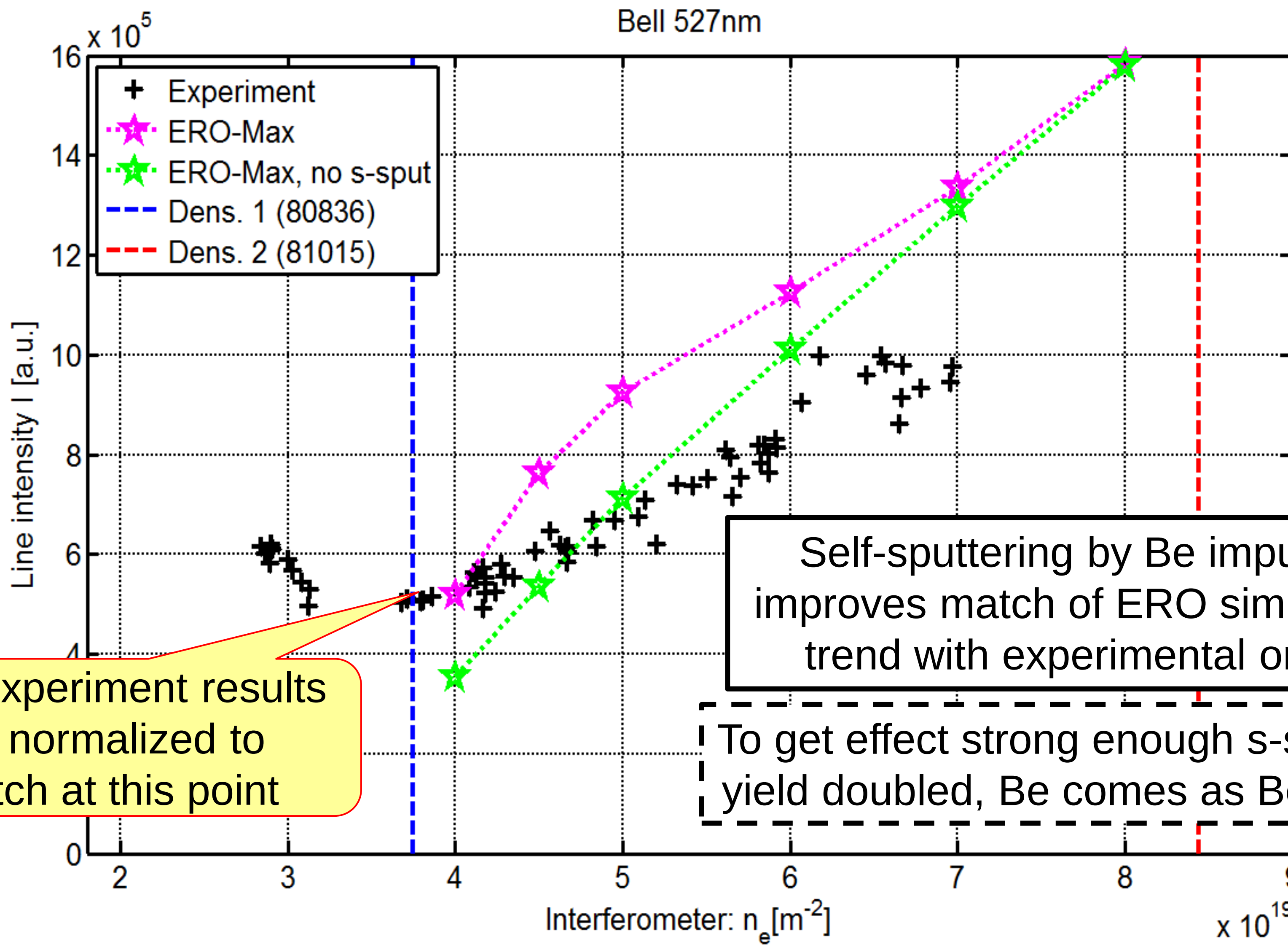
1. JET-ILW Be/W ITER-like Wall completed - 8th May 2011



Line-of-sight integration



ERO&Experiment: Bell light

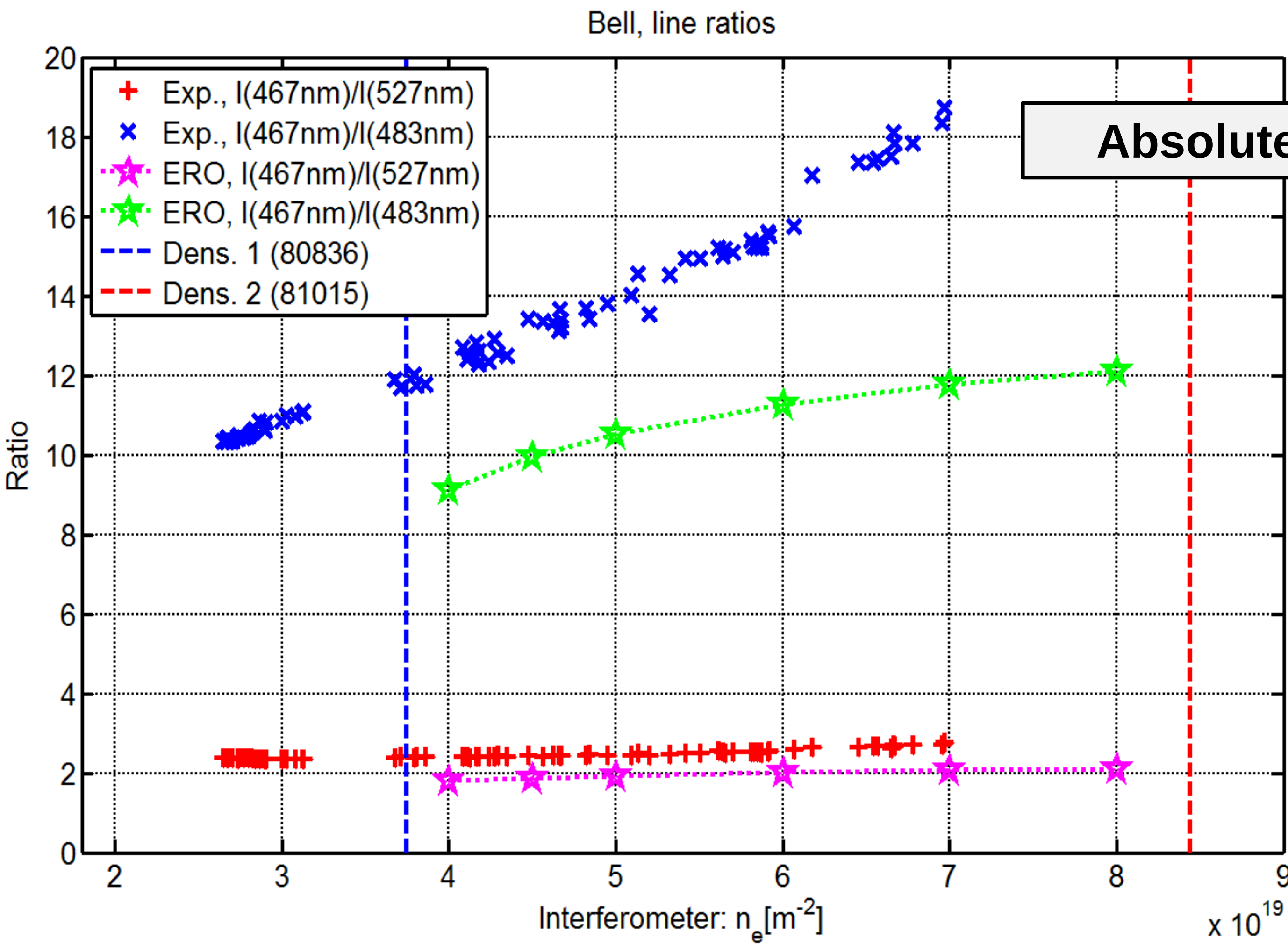


ERO/experiment results are normalized to match at this point

Self-sputtering by Be impurity improves match of ERO simulated trend with experimental ones

To get effect strong enough s-sputter yield doubled, Be comes as Be^{3+} . . .

ERO&Experiment: BeII line ratios



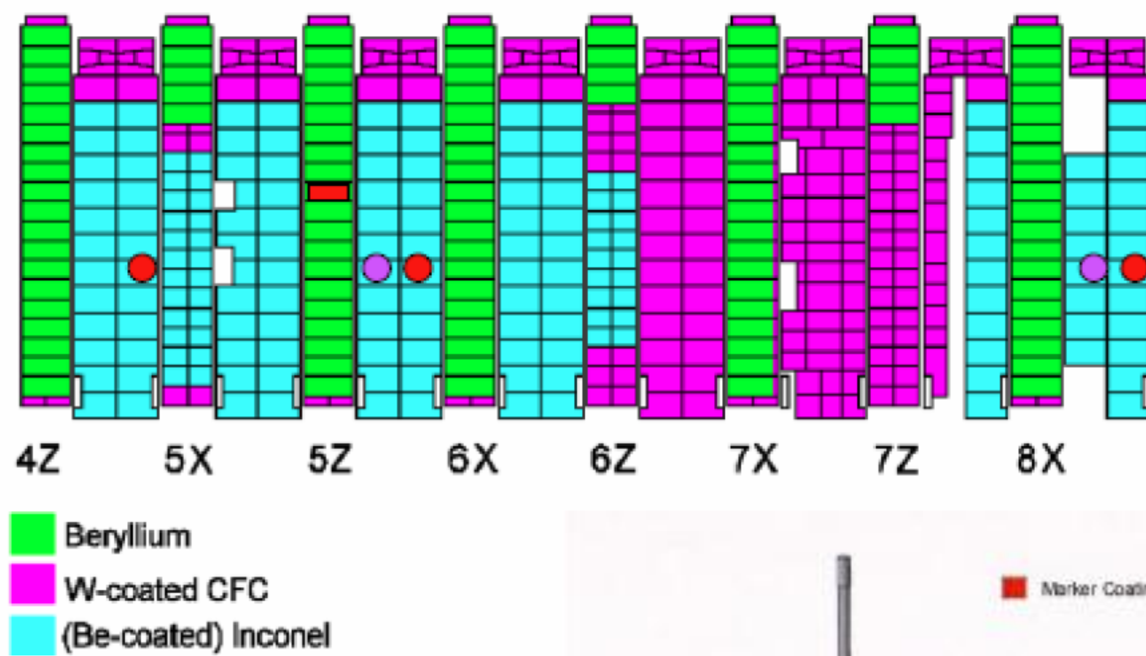
Absolute values!

Ratios inside BeI and BeI/BeII are also within factor 2!

Indicates that atomic data (ADAS '96') and simulated Be transport (3D density pattern) are reasonable!

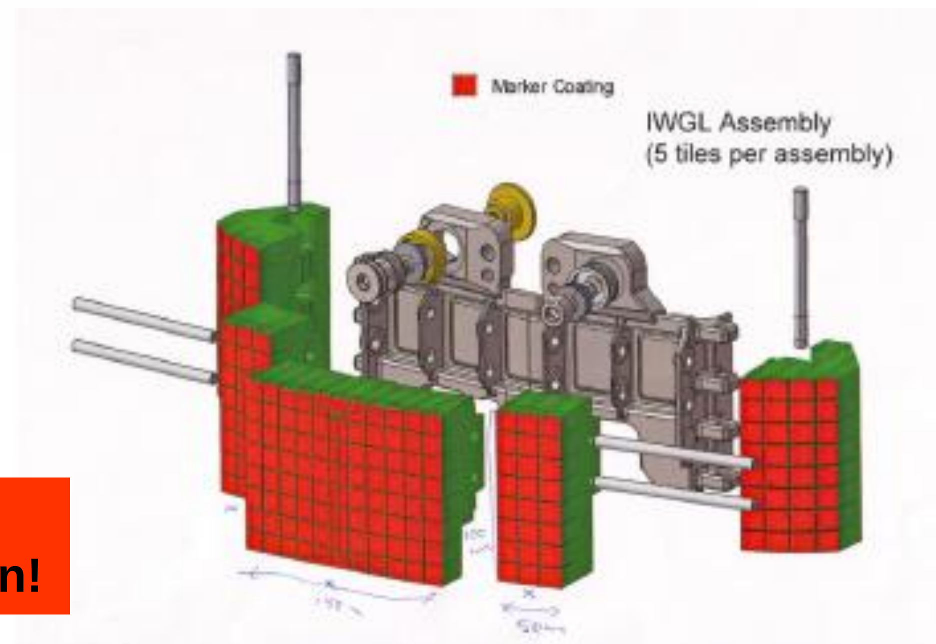
Further ERO applications for Be experiments at JET

^{10}Be experiment – local transport study

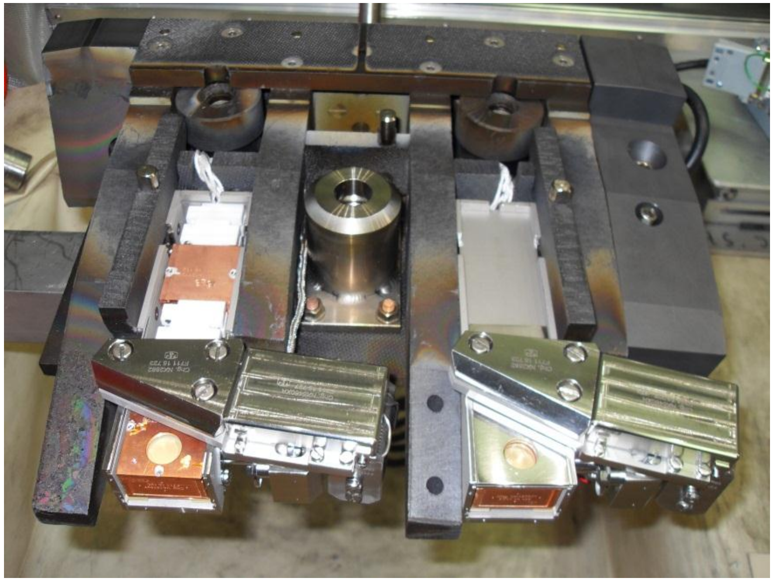


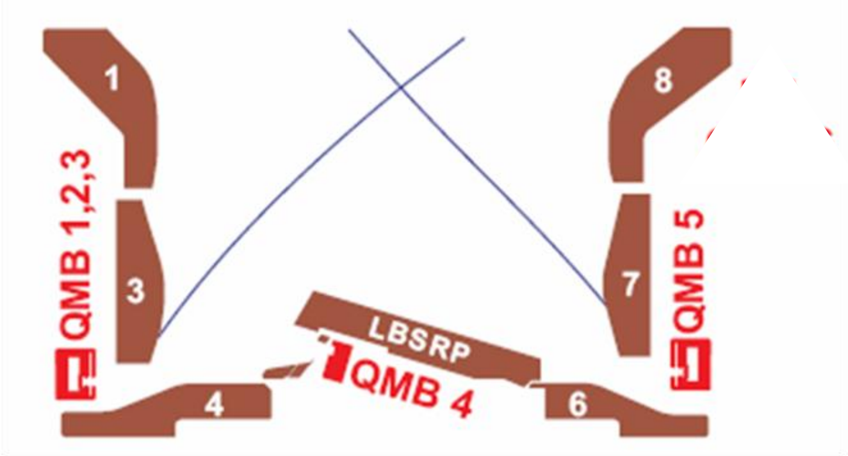
Redeposition on the „wings“
Benchmark for ERO (similar geometry, plasma conditions, etc.)

Long-term exposure to various plasmas . . . uneasy interpretation!



QMB JET installations 2011 and 2012





Schematic showing location of QMBs in the divertor

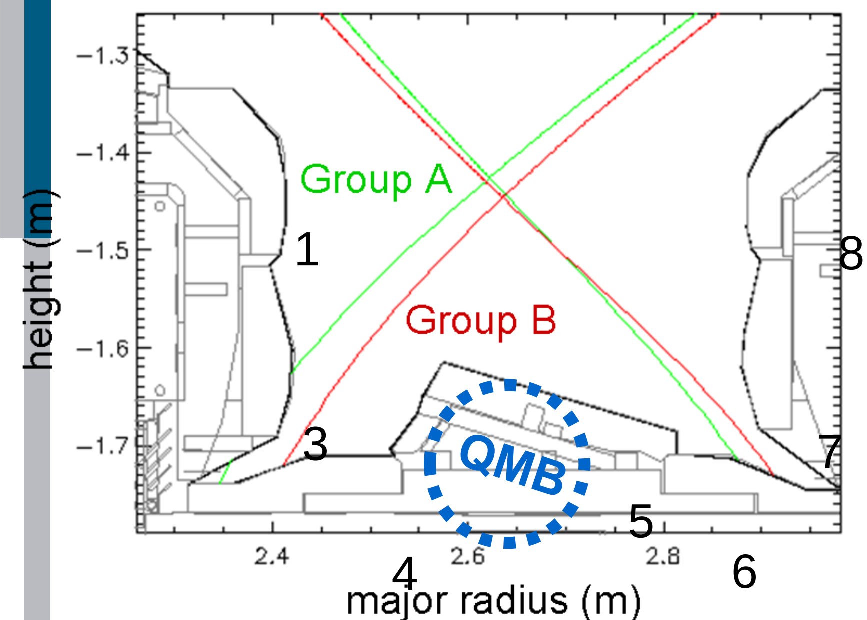
QMB systems on divertor carrier, tiles removed

replacement during present shutdown in BeH facility in November supported by FZJ

QMB 1 Module 13 inner
QMB 2 Module 2 inner
QMB 3 Module 2 inner
QMB 5 Module 2 inner

QMB 4 under LBSRP

QMB below LBSRP (restart 2005)



Carbon wall

Erosion/deposition behaviour on QMB

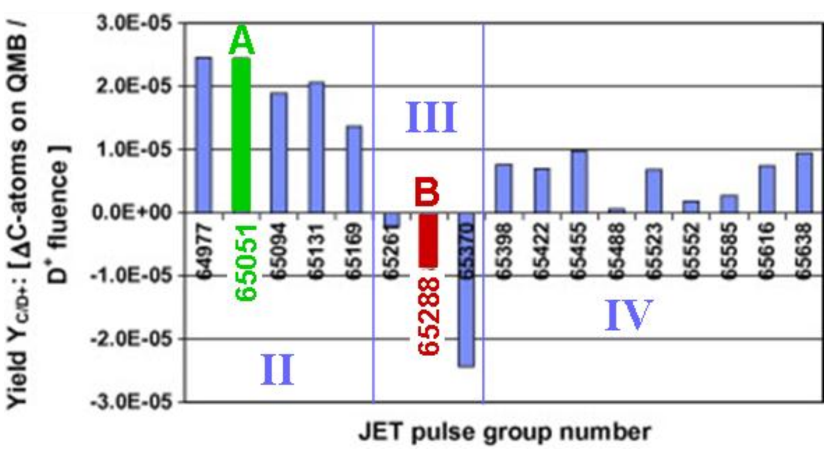
Group A: - SP on tile 3

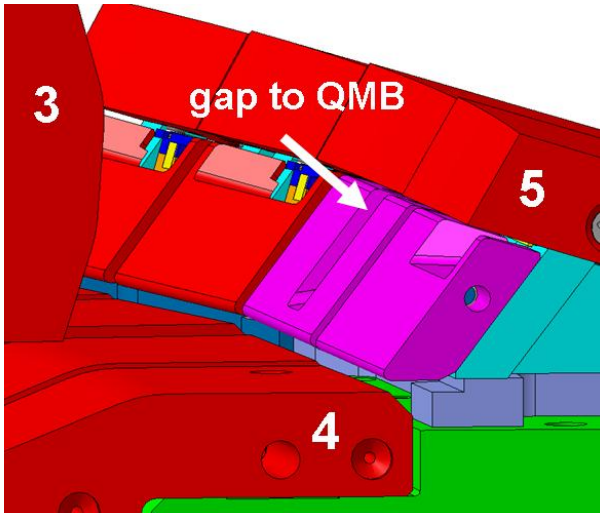
- deposition on QMB

Group B: - SP on tile 4

- erosion on QMB

(H.G. Esser et al., PSI 2008)





New linear devices in FZ Juelich

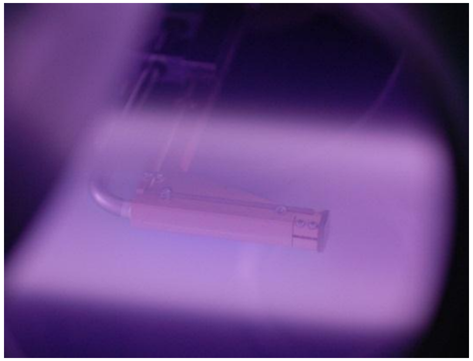
New research programme at FZJ: PMI in nuclear environment

e-beam for high heat loads

Integrated concept to test neutron irradiated and toxic plasma-facing materials under high heat loads and plasma exposure in Jülich

- ***Electron beams JUDITH-1/2:***
  Thermo-mechanical properties of plasma-facing materials (fatigue, shock resistance)
- ***Linear Plasma Device JULE-PSI:***
  PMI processes defining availability of reactor (material erosion, fuel retention and dust formation)

Linear plasma for PMI processes



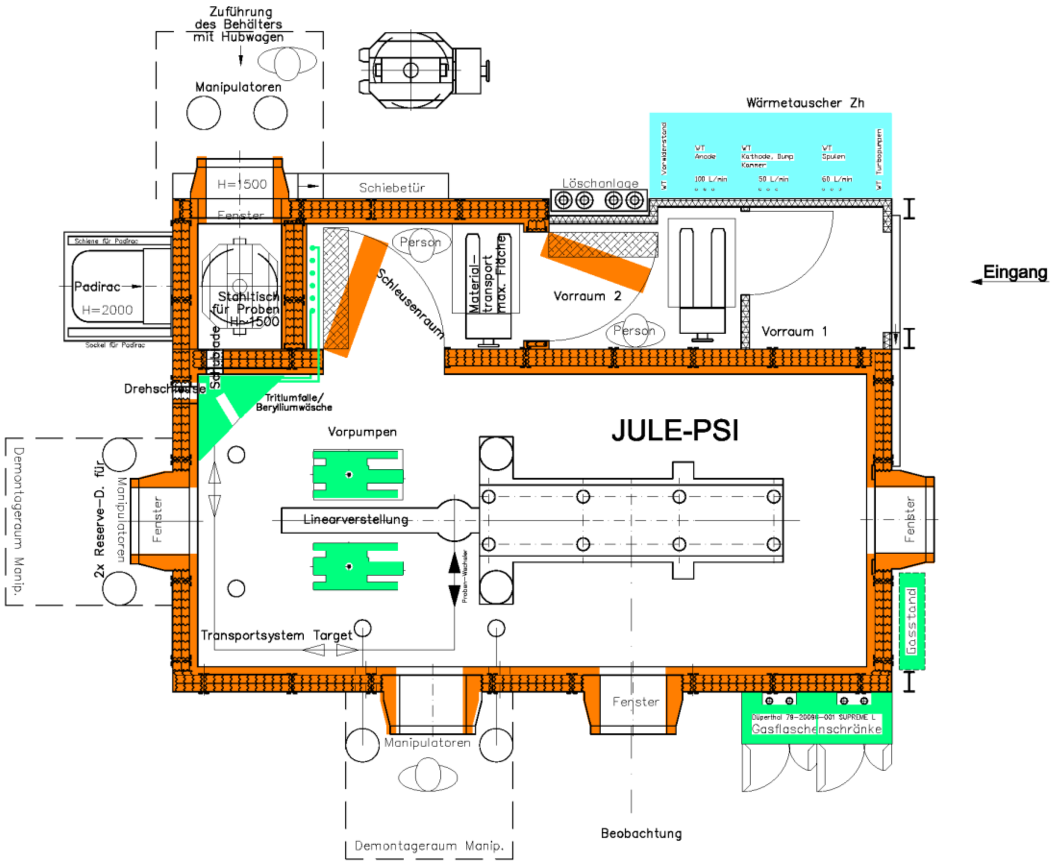
JULE-PSI: Jülich Linear Experiment for PSI studies in Hot Cell

Based on PSI-2 / PISCES type device

Installation in the Hot Cell for handling of *radioactive* and *toxic* materials

PMI studies with
- **Neutron irradiated materials**
- **All wall materials incl. beryllium**
- **Low quantities of tritium**

Envisaged installation in hot cell



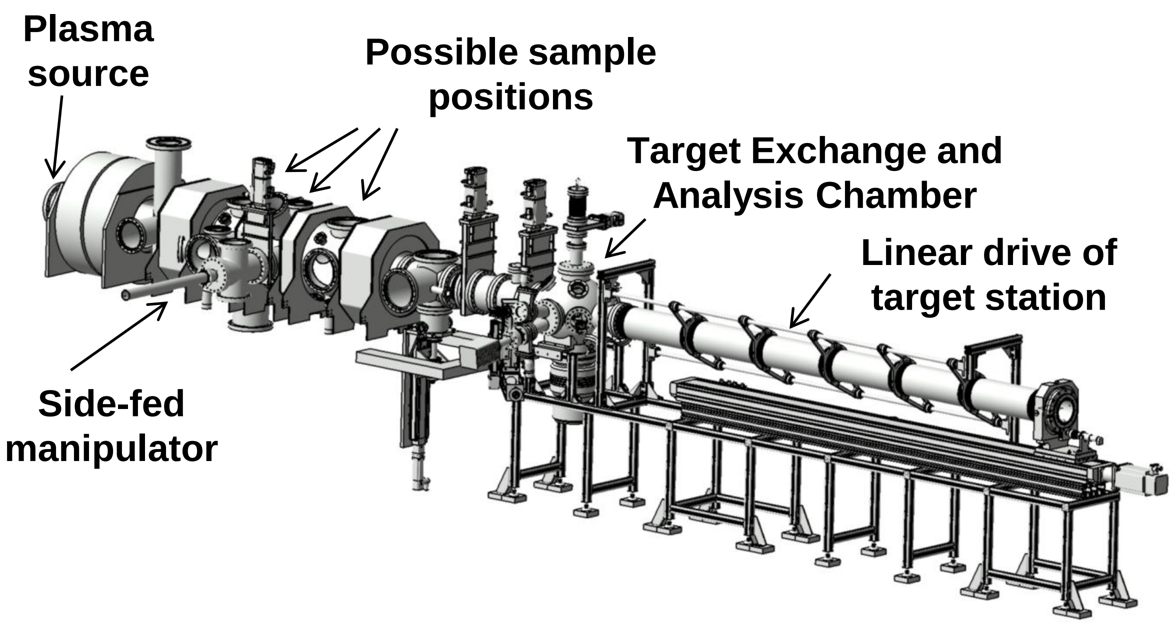
- ♦ **Planning is in advanced stage**
- ♦ **Refurbishing of Hot Material Lab is completed**
- ♦ **Infrastructure for JULE-PSI installation is being prepared**
- ♦ **Licensing procedure for hot cell installation is ongoing**

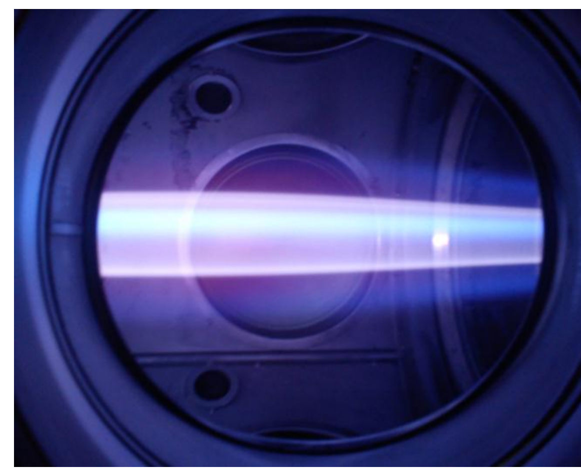
PSI-2 is the pilot experiment of the JULE-PSI project outside of hot cell

PSI-2 as the pilot experiment of the JULE-PSI project

Aims of PSI-2 as the pilot experiment

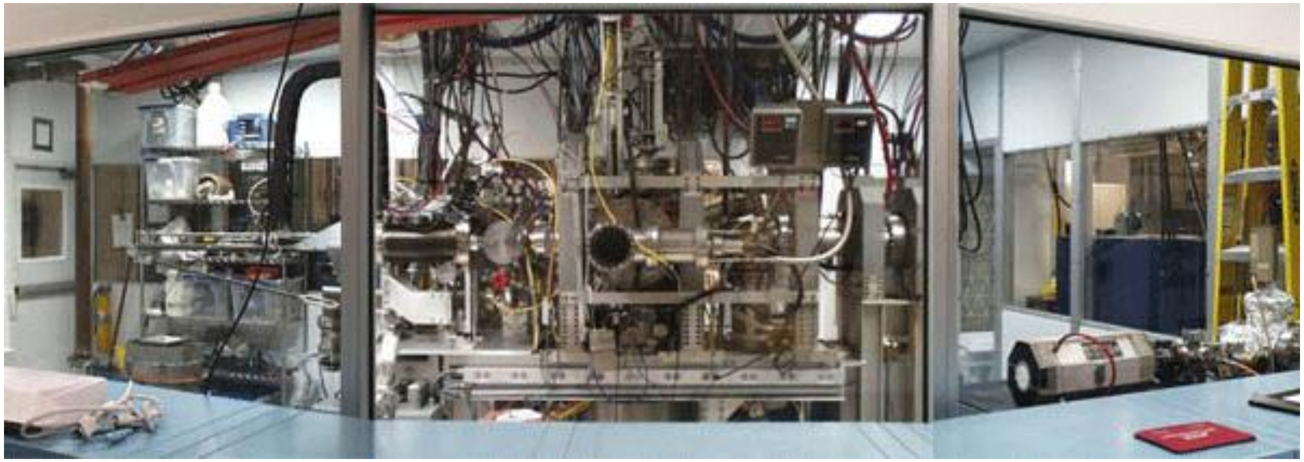
- Test-bed for components and solutions for JULE-PSI
- Train personnel operating linear plasma device
- Contribute to current PMI research topics, including studies with a Be proxy

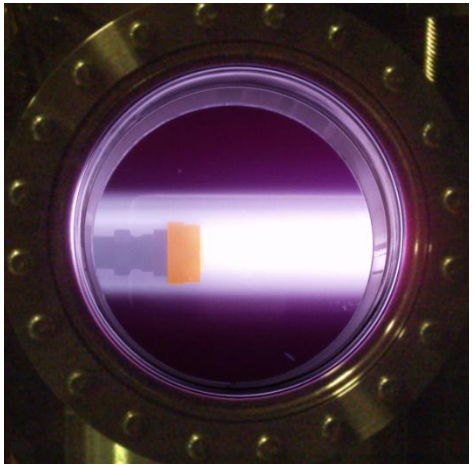




Collaboration with UCSD to qualify aluminum as beryllium proxy

PISCES-B linear plasma device





PISCES-B is contained within an isolated safety enclosure to prevent the release of Be dust

Joint experiments on PISCES-B planned for October-November 2012

- **Exposure of Be and Al samples to deuterium plasma at the same conditions under variation of incident ion energy**
- **Comparison of erosion rates by spectroscopy and mass loss**
  → Validation of spectroscopy on aluminum
- **Comparison of deuterium retention by thermal desorption spectrometry**

➢ **If the results are positive, Al can be used as Be proxy in PSI-2**

Be proxy

Mg		Al

Spectroscopy

Electronic configuration: Mg $3s^2$ Be $2s^2$ Al $3s^2 3p$ ($\rightarrow 3s3p^2$)

Mg	Al
Electronic structure very similar to Be including similar MS state. Acceptable atomic data available, improvement expected.	Electronic structure very different from Be and complicated. Atomic data in ADAS is worse than average . . .

Physical properties (atomic number, mass) compared to *Be(6, 9)*

Mg	Al
Mg(12, 24) is a bit closer to Be than Al . . . Hexagonal structure (as Be)	***Al(13, 27)*** is less close to Be . . . Cubic structure (not as Be)

Oxygen

Mg	Al
Oxygen getter as Be.	Oxide layer on surface

Melting point

Mg	Al
923 K	933K

High vapor pressure

Safety issues?.. Which ones?..

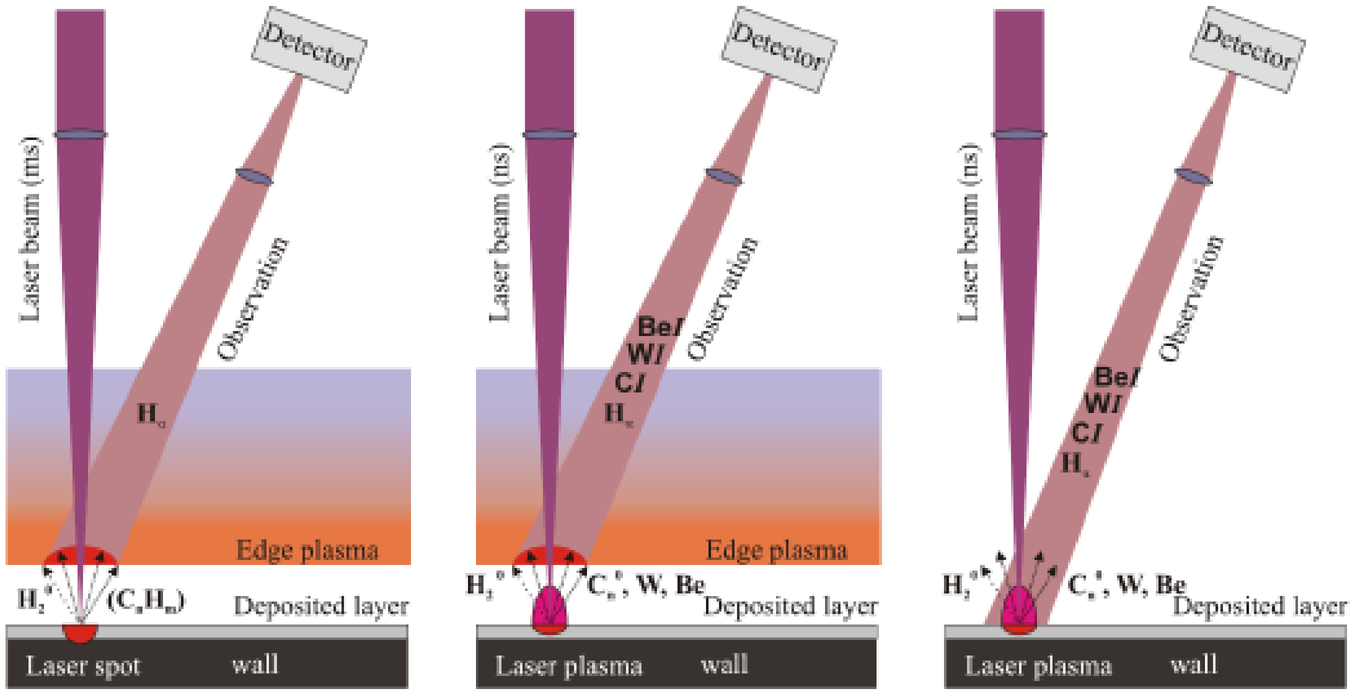
Selected by ITPA . . .

Laser techniques

Laser-based surface analysis overview

Laser-based diagnostics:

- Laser-induced desorption spectroscopy (LIDS),
- Laser-induced ablation spectroscopy (LIAS) and
- Laser-induced breakdown spectroscopy (LIBS)



a) LIDS

b) LIAS

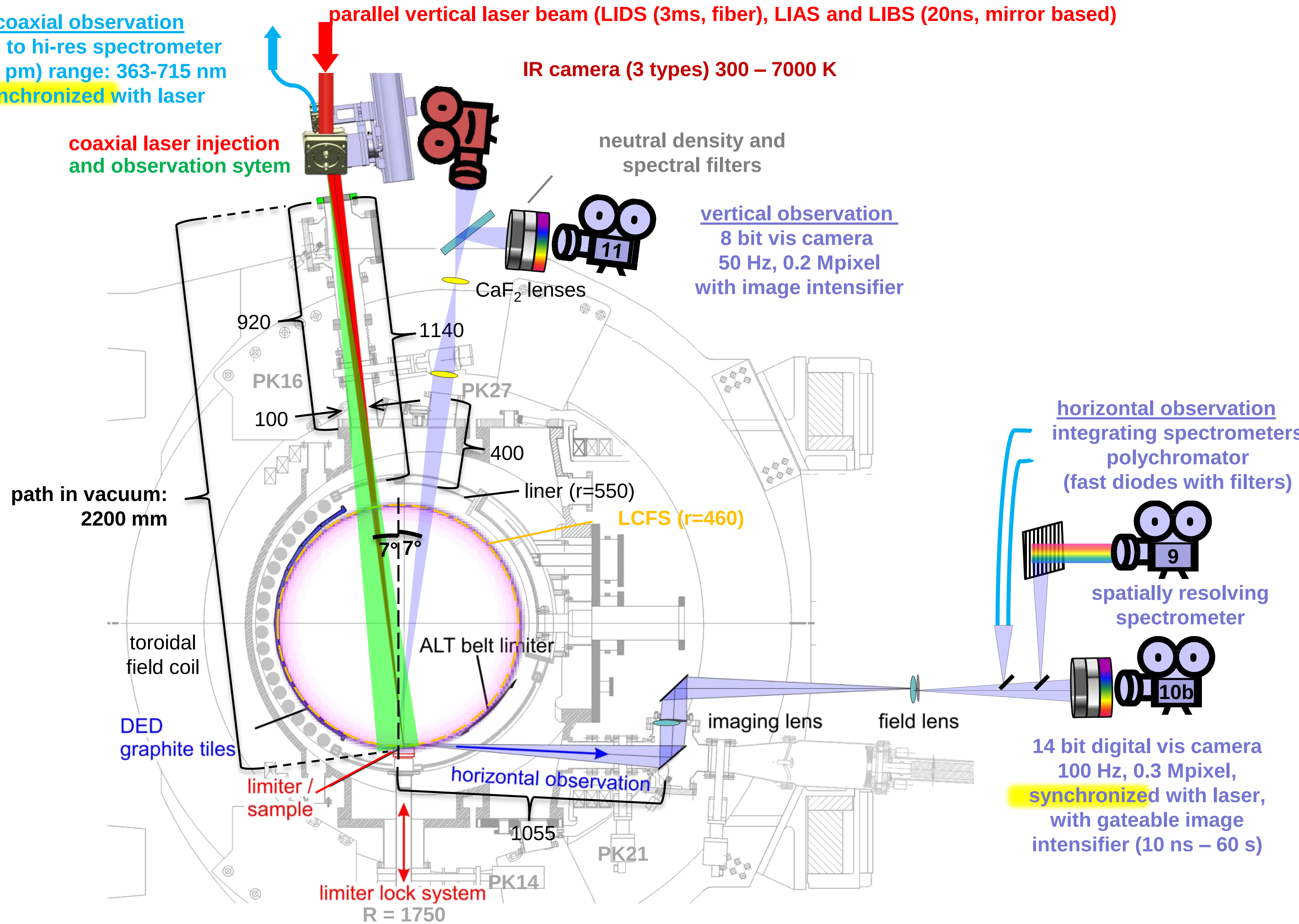
c) LIBS

Idea: only fuel desorption, no material ablation

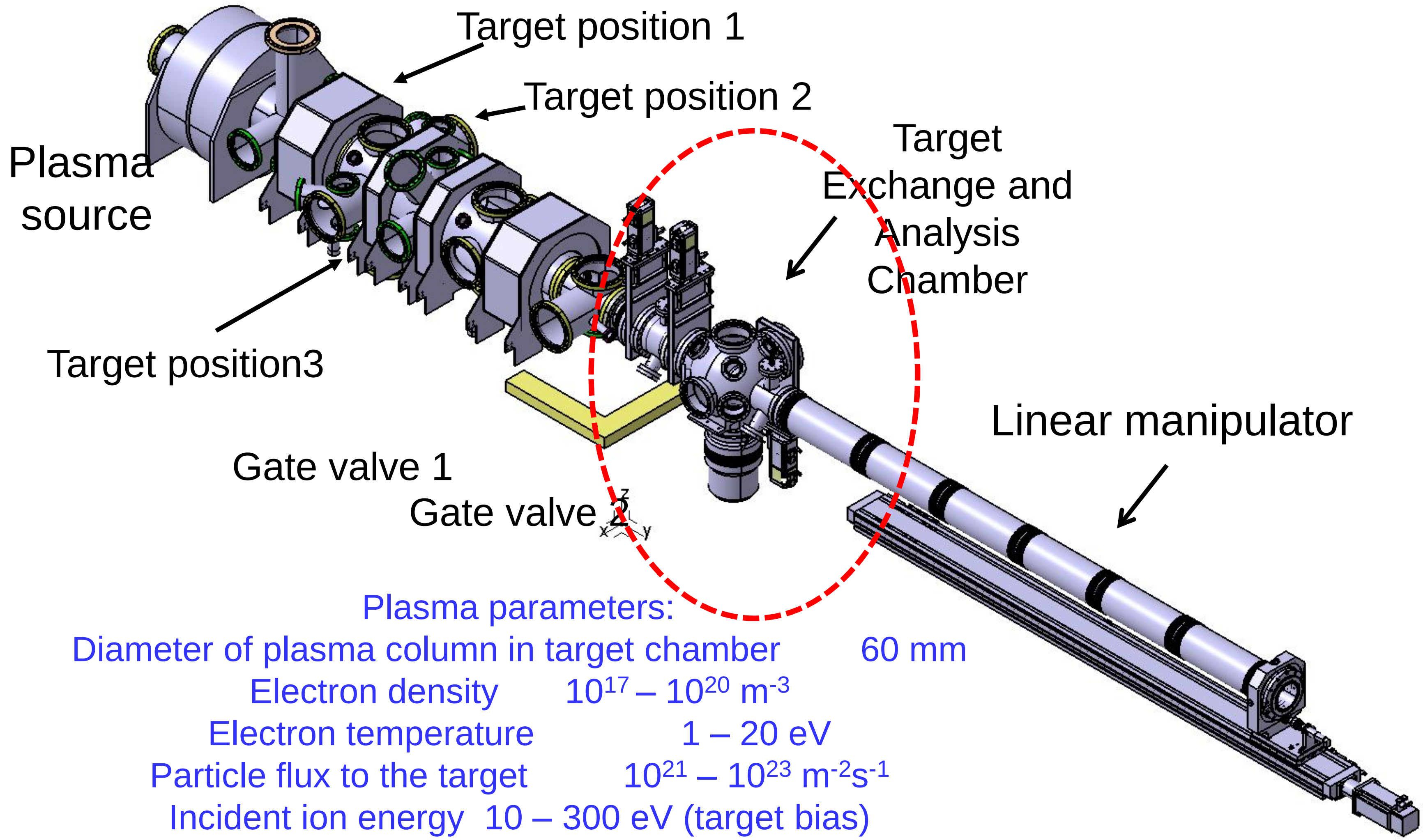
Material ablation

Material ablation

ITER- like LIDS, LIAS, LIBS system at TEXTOR



Future plans for ELM simulation Experiments in PSI-2

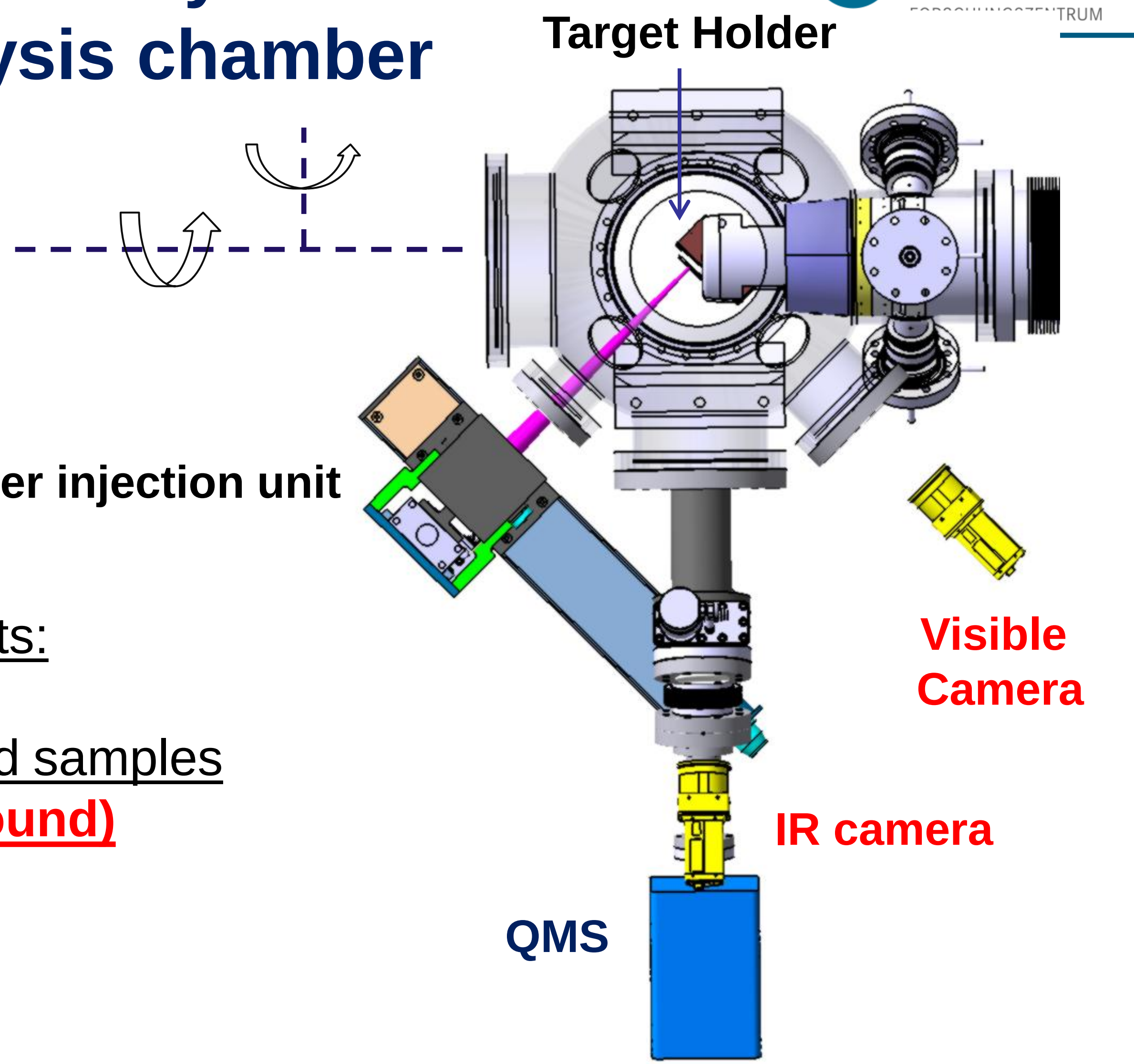


Plasma parameters:

Diameter of plasma column in target chamber	60 mm
Electron density	$10^{17} – 10^{20}$ m^{-3}
Electron temperature	1 – 20 eV
Particle flux to the target	$10^{21} – 10^{23}$ m^{-2}s^{-1}
Incident ion energy	10 – 300 eV (target bias)
Min. neutral gas pressure in target chamber	10^{-2} Pa

Laser exposure system at PSI-2 analysis chamber

Target Holder:
- rotatable
- heatable up to 600 ^{0}C
- with active cooling
- exchangeable



<u>Laser heat load experiments:</u>
- <u>Unexposed and</u>
- <u>Plasma pre-exposed samples</u>

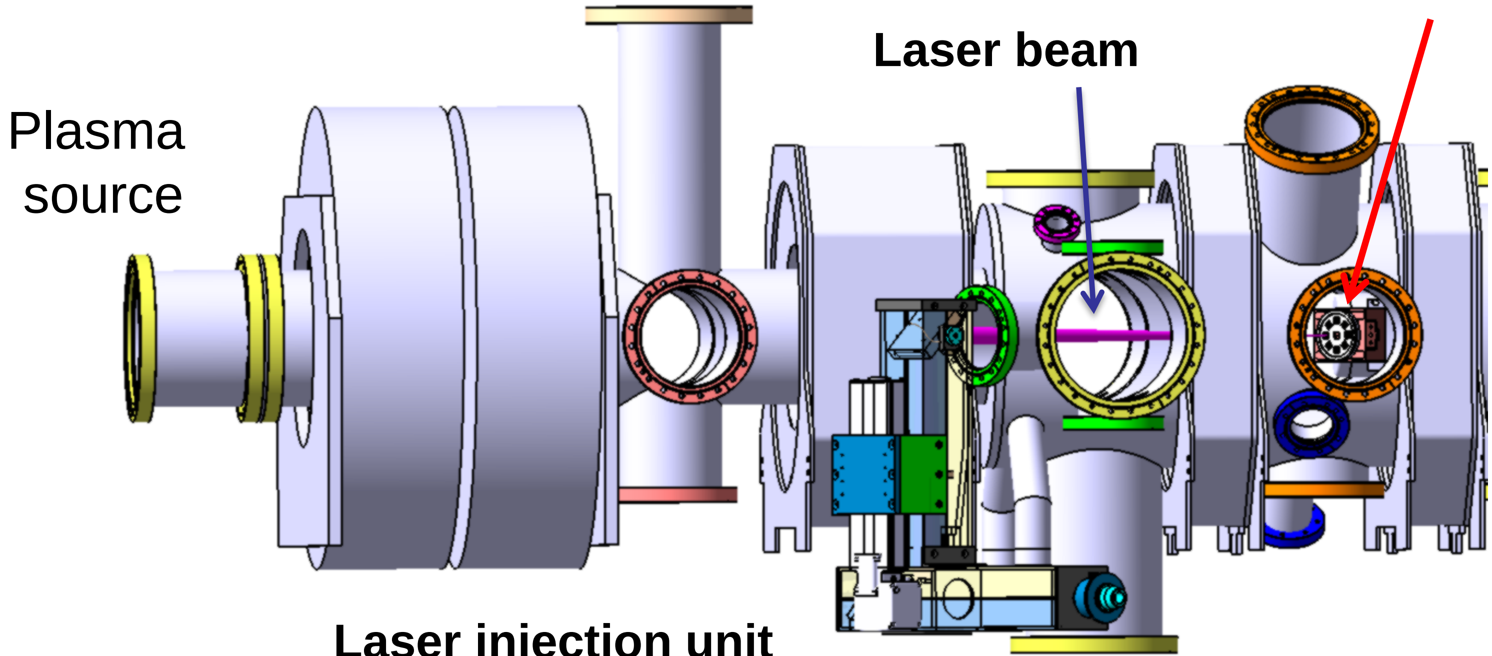
<u>**(without plasma background)**</u>

Without breaking the vacuum in the plasma chamber the probes can be removed easily for post mortem analysis.

Laser exposure system at PSI-2

Target Holder:

- rotatable
- heatable up to 1600 ^{0}C
- with active cooling
- exchangeable



- Transient heat load experiments in the PSI-2 facility simultaneously to a steady state plasma exposure **(with plasma background)**.

Summary

- The ERO code is a useful bridge allowing to benchmark various PSI-relevant Be data (erosion, atomic and molecular processes, etc.) with plasma experiments, most of which are difficult for an interpretation
  - *Benchmarks at PISCES-B and JET*
  - *MS-effect is demonstrated to be of importance*
  - *Be-D molecules tracing instroduced; benchmark ongoing*
  - *ITER predictive modelling; sensibility analysis*

- FZJ developes further experimental techniques relevant for Be research
  - *New linear devices (hot cell JULE-PSI operation not earlier than 2015!)*
  - *Laser techniques for TEXTOR/ITER and linear devices*

The End