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Atomic and molecular Be data in ERO for simulation of experiments at JET and PISCES-B

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Be atomic/molecular data in ERO

ATOMIC:

- Ionization, PEC
  - ➔*Metastable resolved*
- Recombination, elastic collisions with D_2

MOLECULAR:

- Be-D release from surface
  - ➔*Recent MolDyn simulations*
- BeD decay in plasma, BeD light emission (PEC)

ERO model&data benchmark:

- PISCES-B (Be target erosion)
- JET ITER-like wall (ILW solid Be limiter erosion)

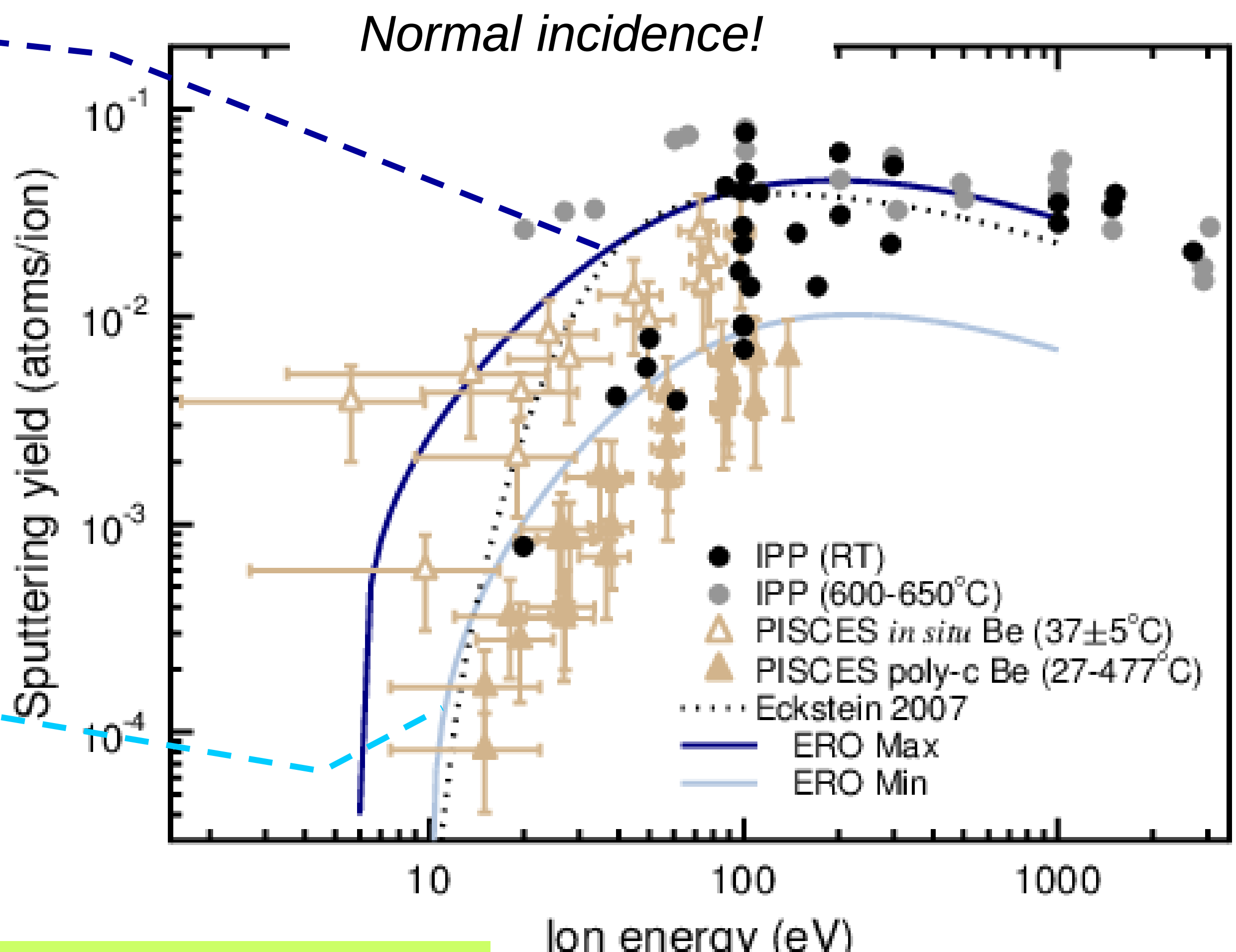
Physical sputtering
(as introduced in ERO)

Sputtering data – margin estimates

Be by D^+ sputtering

„ERO-max“
MD + SDTRIMSP
pure Be

„ERO-min“
SDTrimSP
50%Be + 50%D

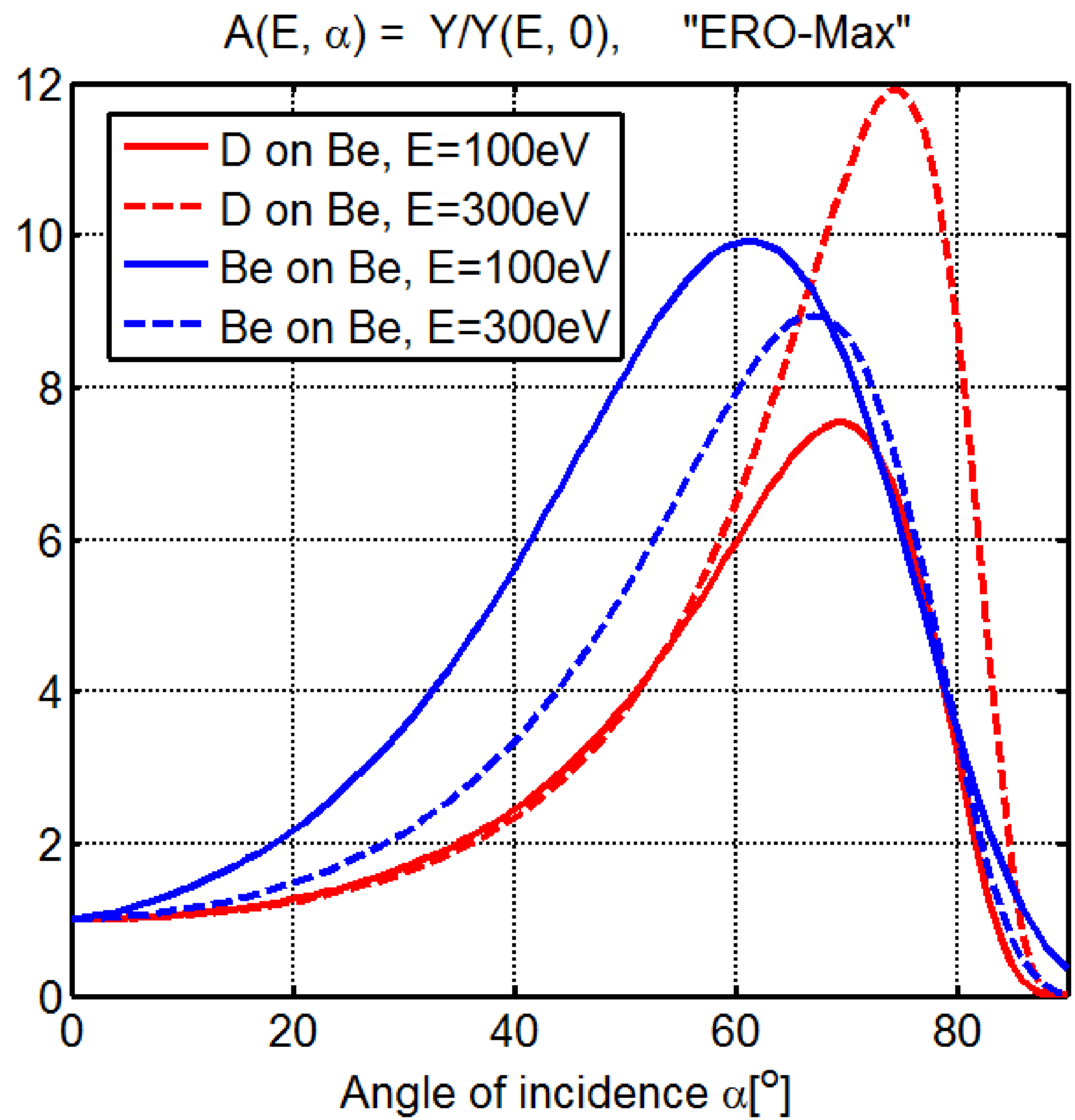


The very same limit fits are used for ITER predictive modelling and benchmark at JET.

Effective sputter yield – angular part

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

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



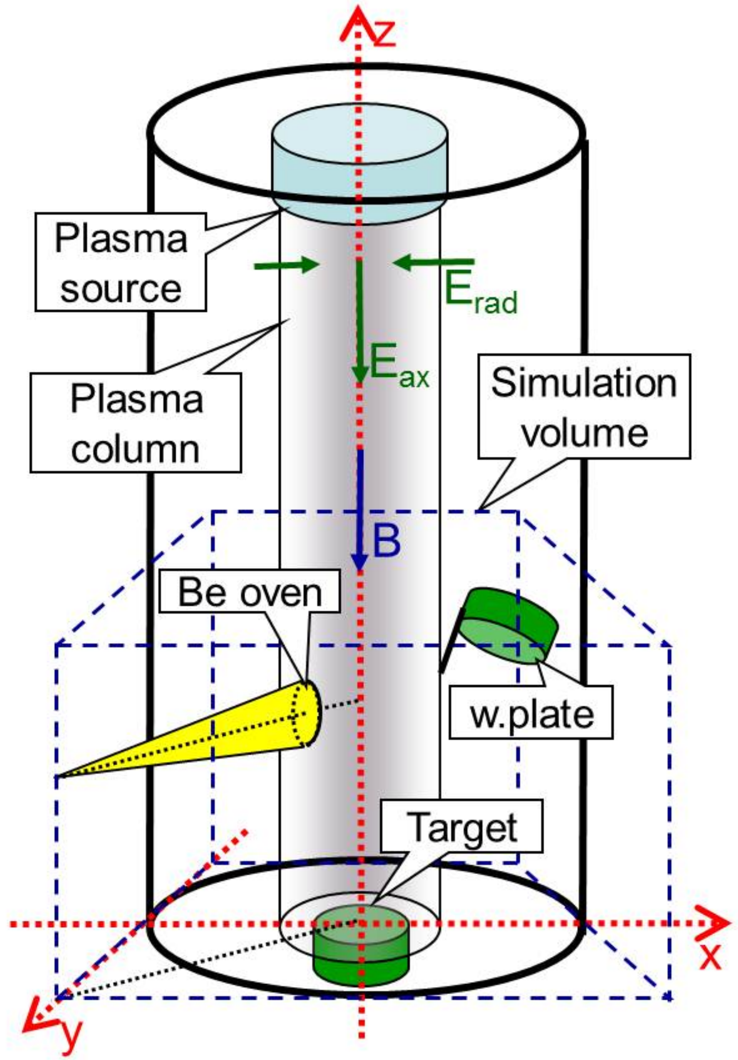
<u>PISCES-B:</u>

Spectroscopy benchmark – He plasma

Be sputtering benchmark

PISCES-B

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



Perfect for Be sputtering yields benchmark

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

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

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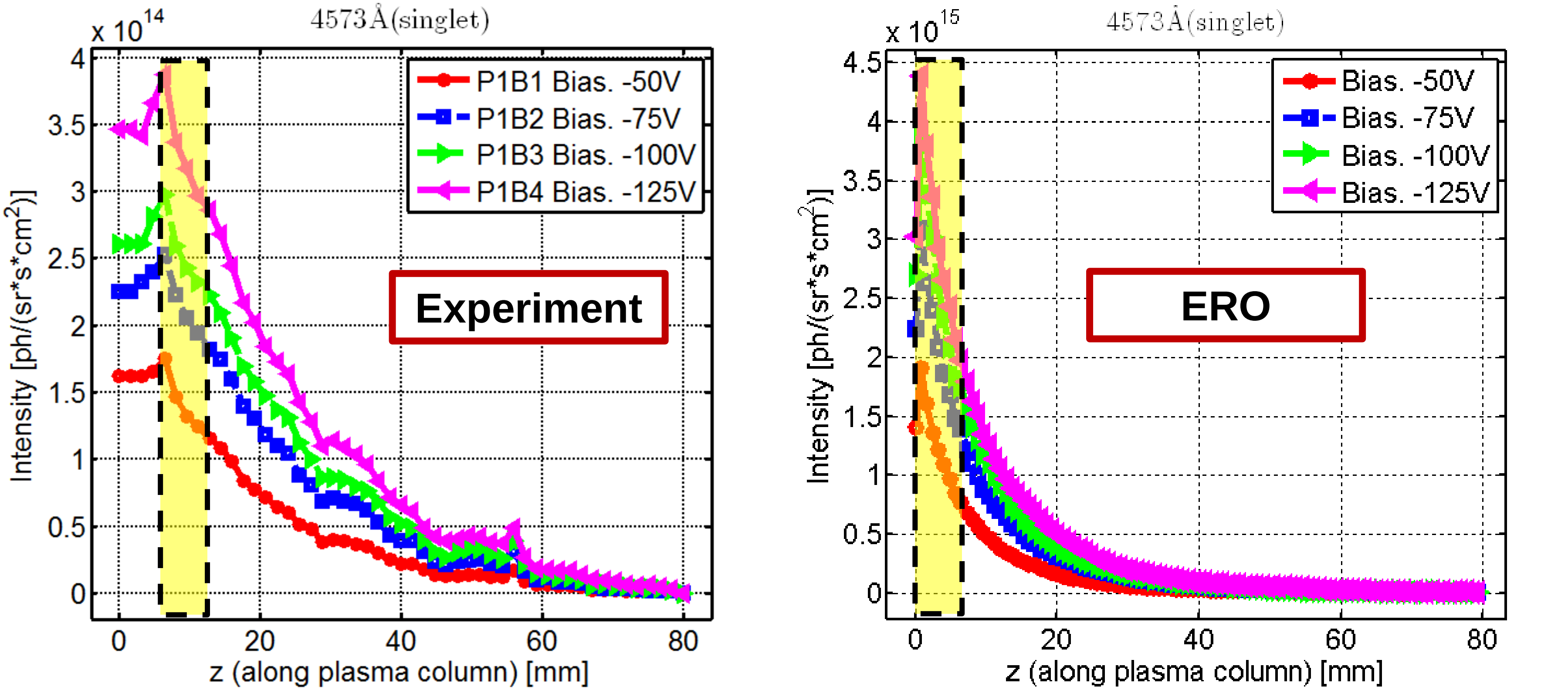
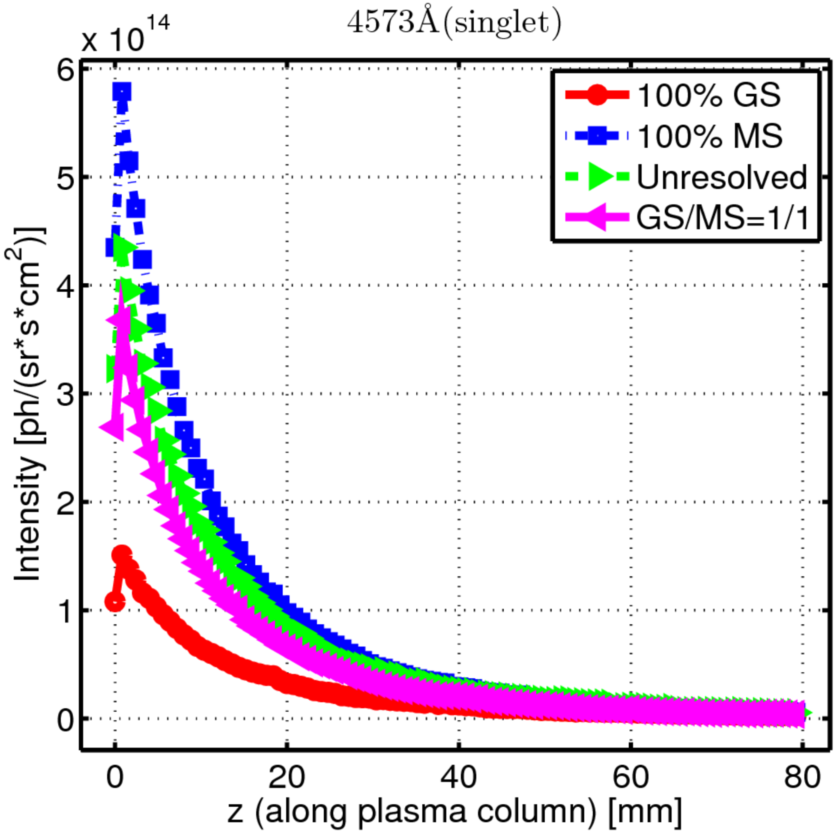
Axial BeI light intensity profiles in case of Be target erosion

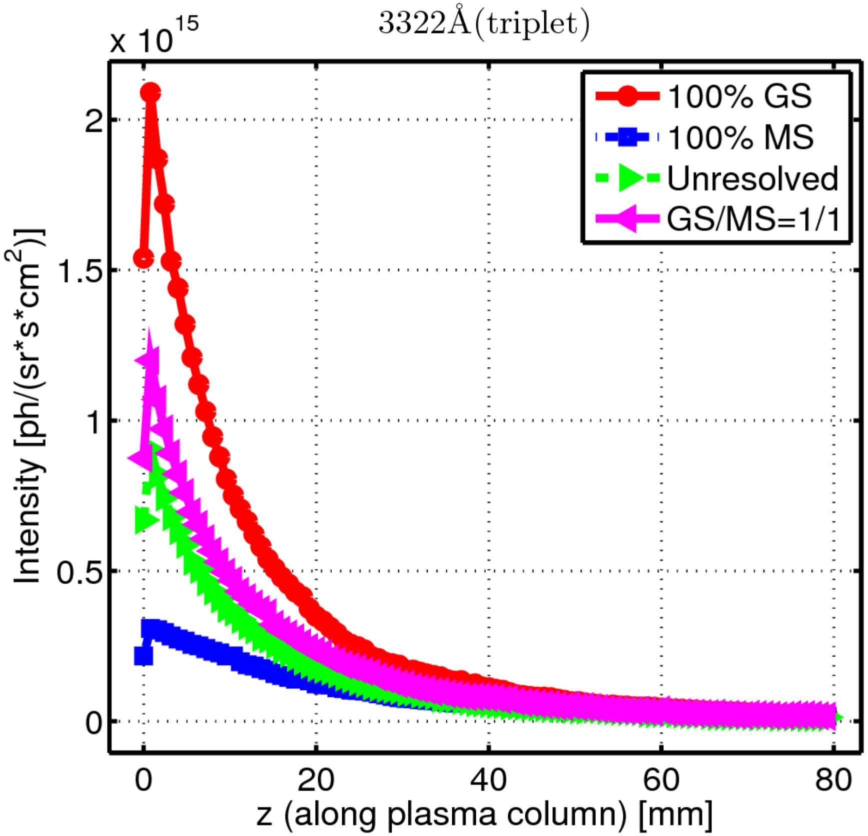


Let's try to understand first the integrated light near the target!

Initial population of MS is of importance!!!

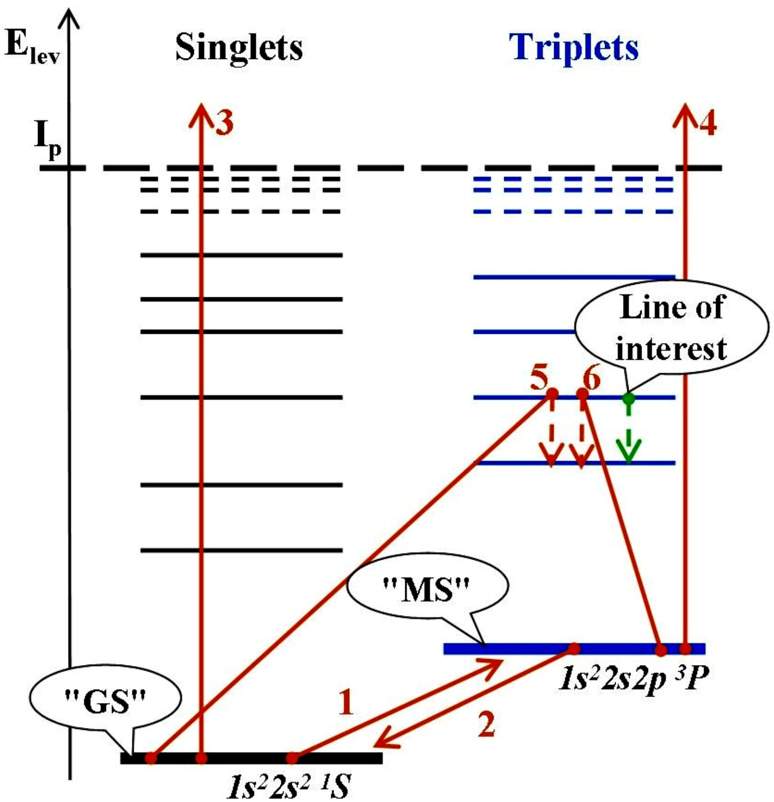
Be MS tracking in ERO: effect for PISCES-B



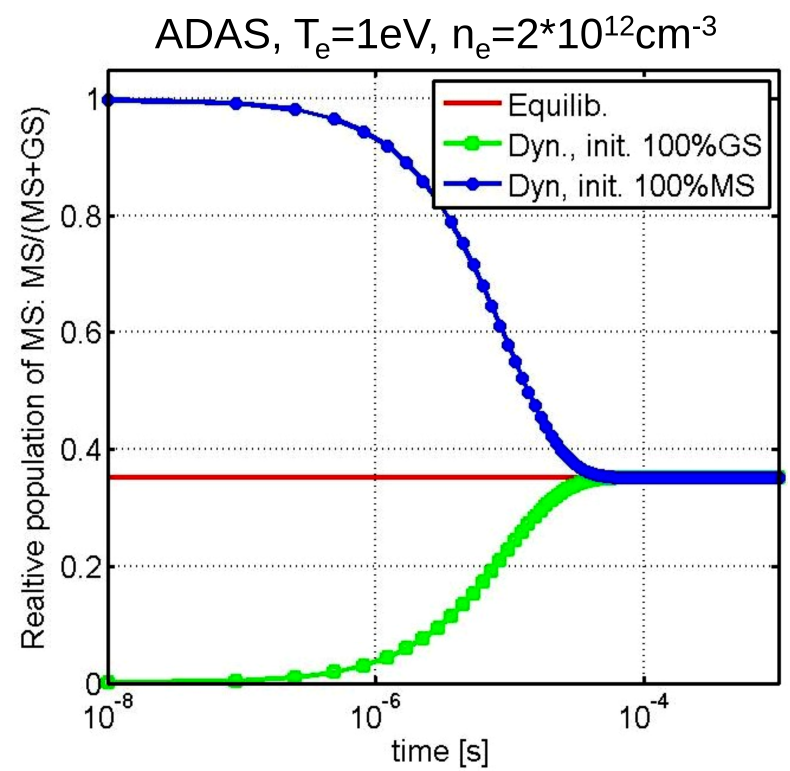


Initial MS population influences intensity near the target determines triplet to singlet ratio . . .

Be metastable state (MS) tracking in ERO



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



Effective rates:

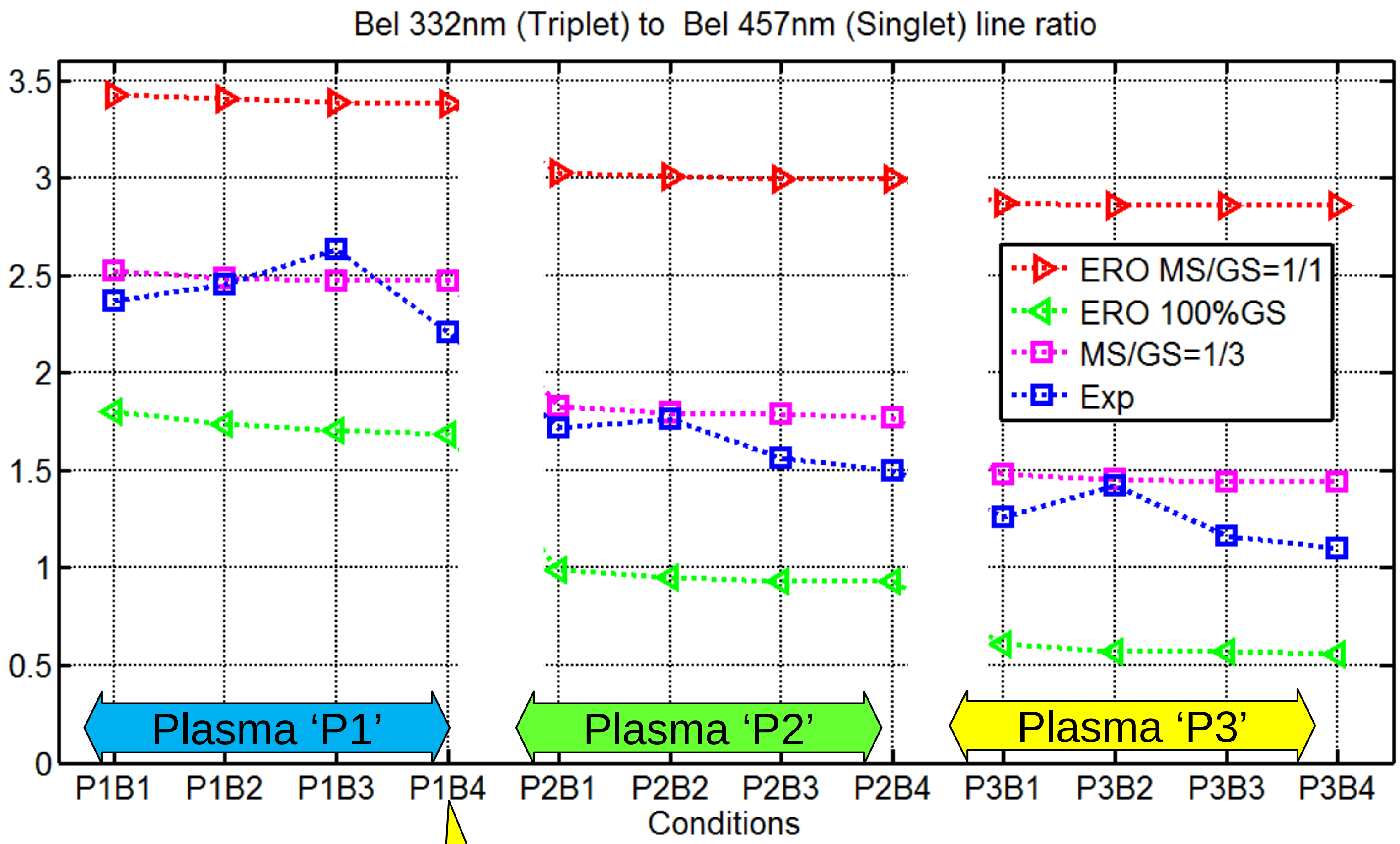
1,2) transitions between "GS" and "MS"

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



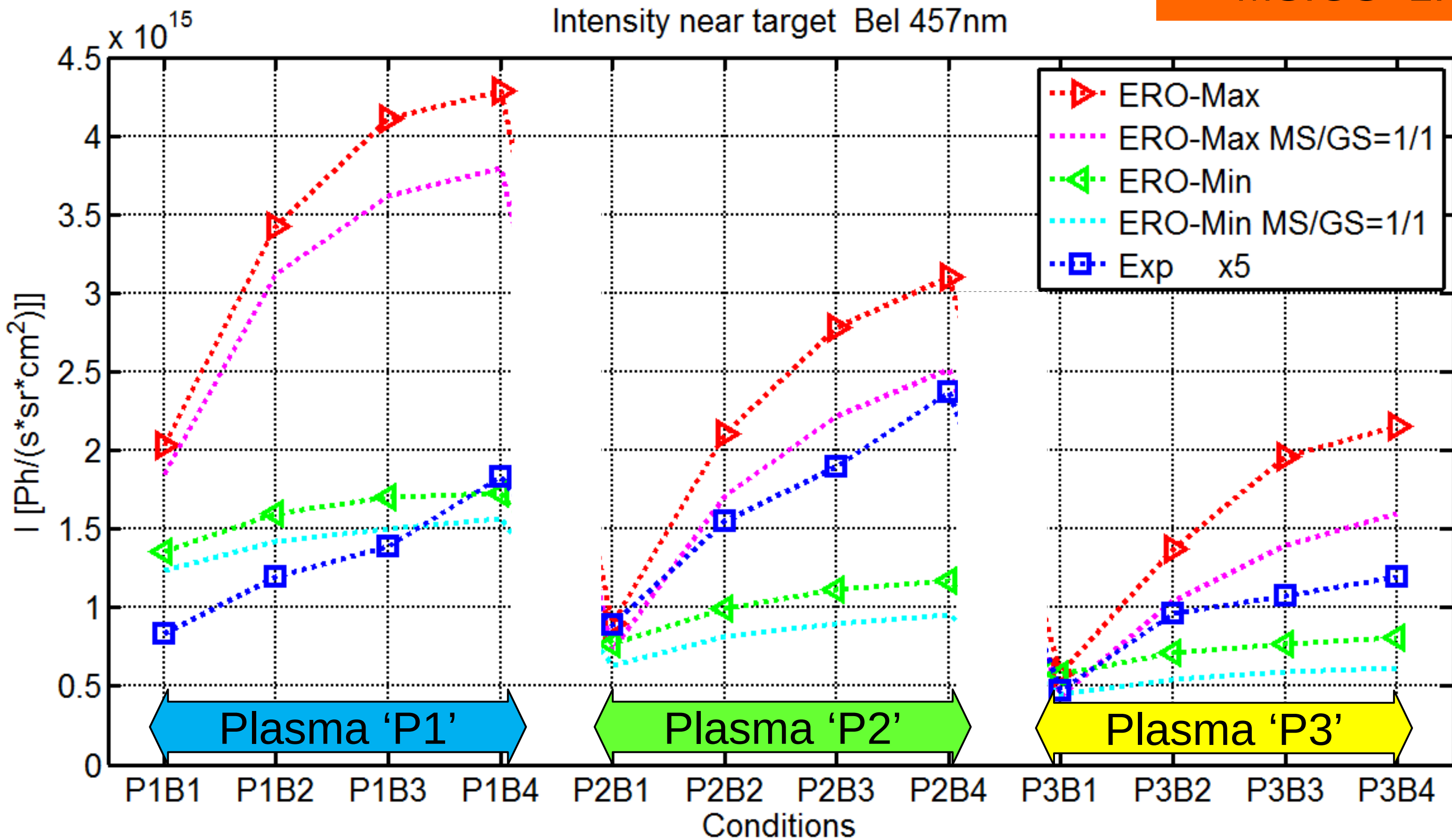
Biasing B1-B4: -50eV, -75eV, -100eV, -125eV

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!

PISCES-B:

Spectroscopy benchmark – D plasma

Spectroscopy benchmark

D plasma

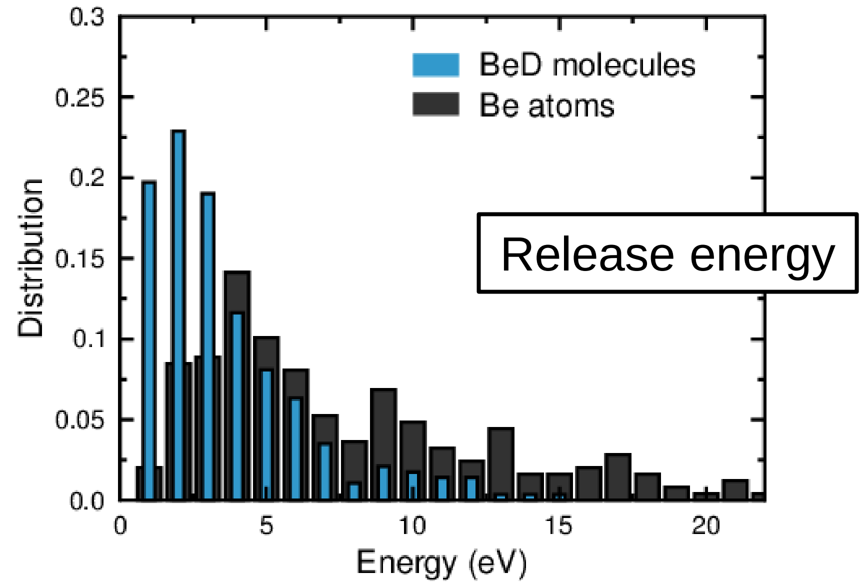
Plasma	At axis, z=150mm	Biasing	ERO 'name'
'A'	n_e=4.9*$10^{12}$$cm^{-3}$ T_e=4.6eV $P_{neutrals}$=5.4mTorr B=0.0152T P_{plasma} = -17eV	V=-140V	'A140'
		V=-120V	'A120'
		V=-80V	'A80'
		V=-60V	'A60'
'B'	n_e=2.6*$10^{12}$$cm^{-3}$ T_e=8.2eV $P_{neutrals}$=1.7mTorr B=0.0152T P_{plasma} = -12eV	V=-140V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

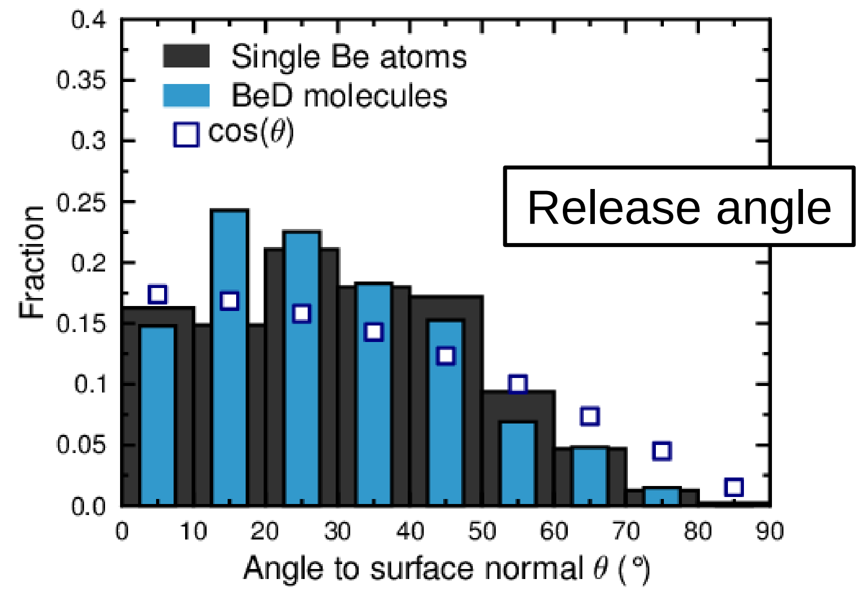
Strong influence of BeD release (recently provided in ERO)

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

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





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

Important reactions

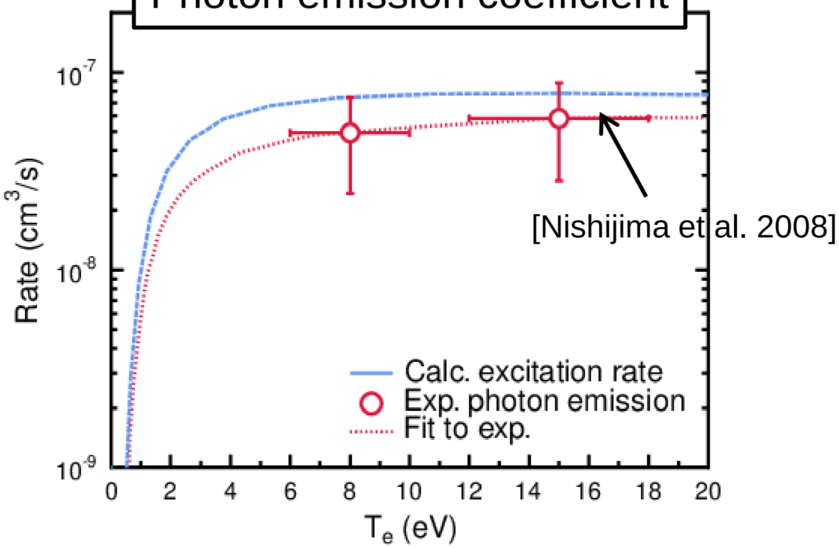
$$e + \mathrm{BeD} \rightarrow e + \mathrm{BeD}^{+}$$

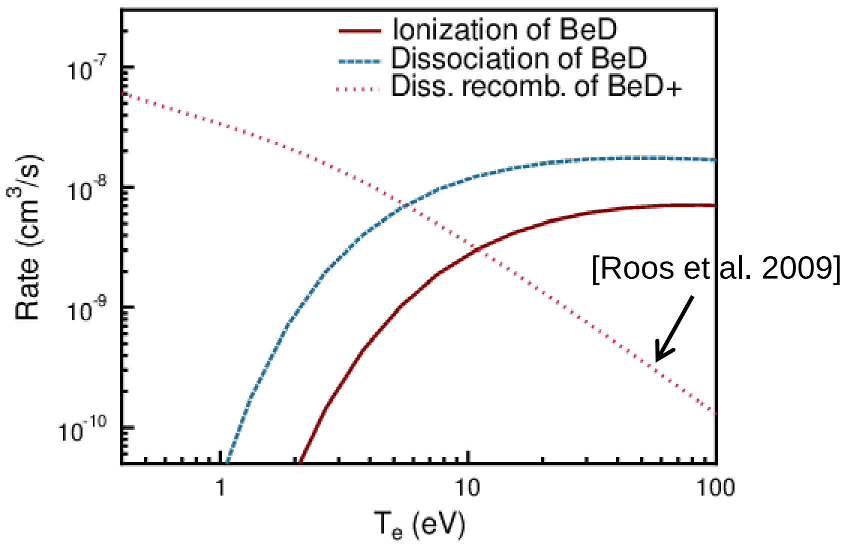
$$e + \mathrm{BeD} \rightarrow e + \mathrm{BeD}^{*}$$

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

Metastable now!

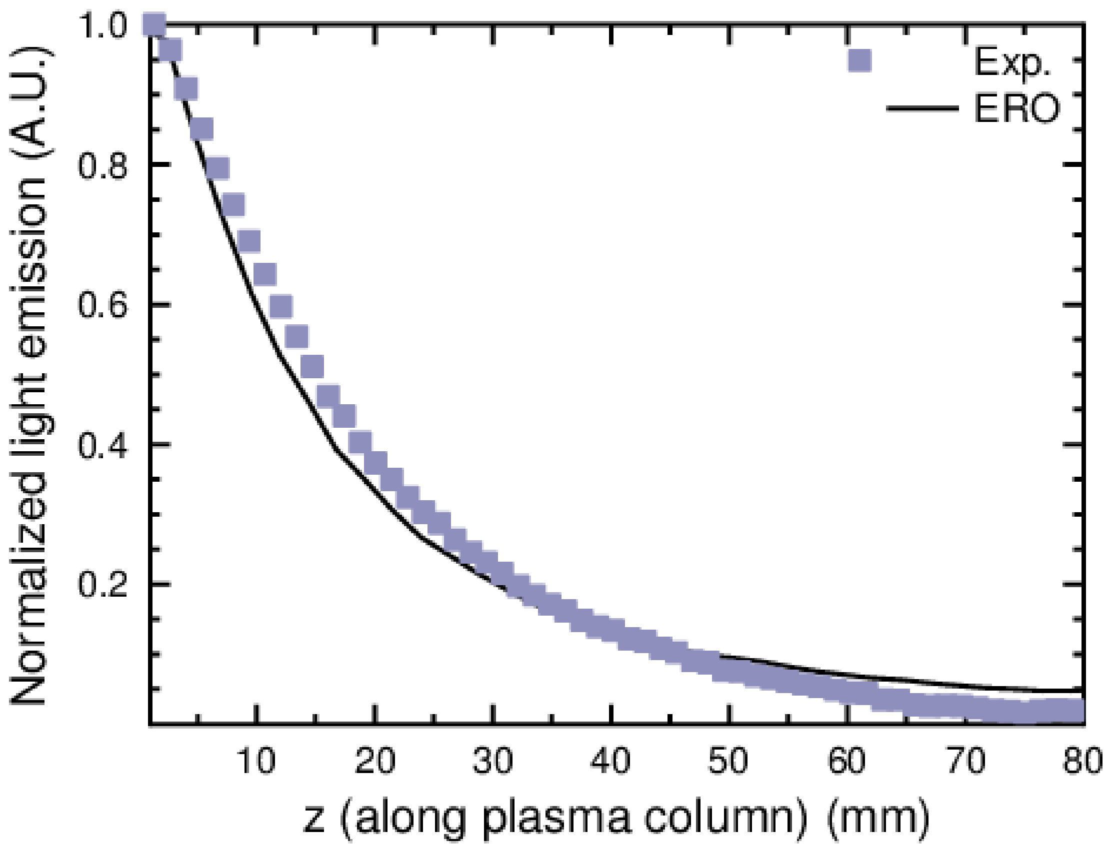
Photon emission coefficient





Comparison of BeD light

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



Comparison of BeD light

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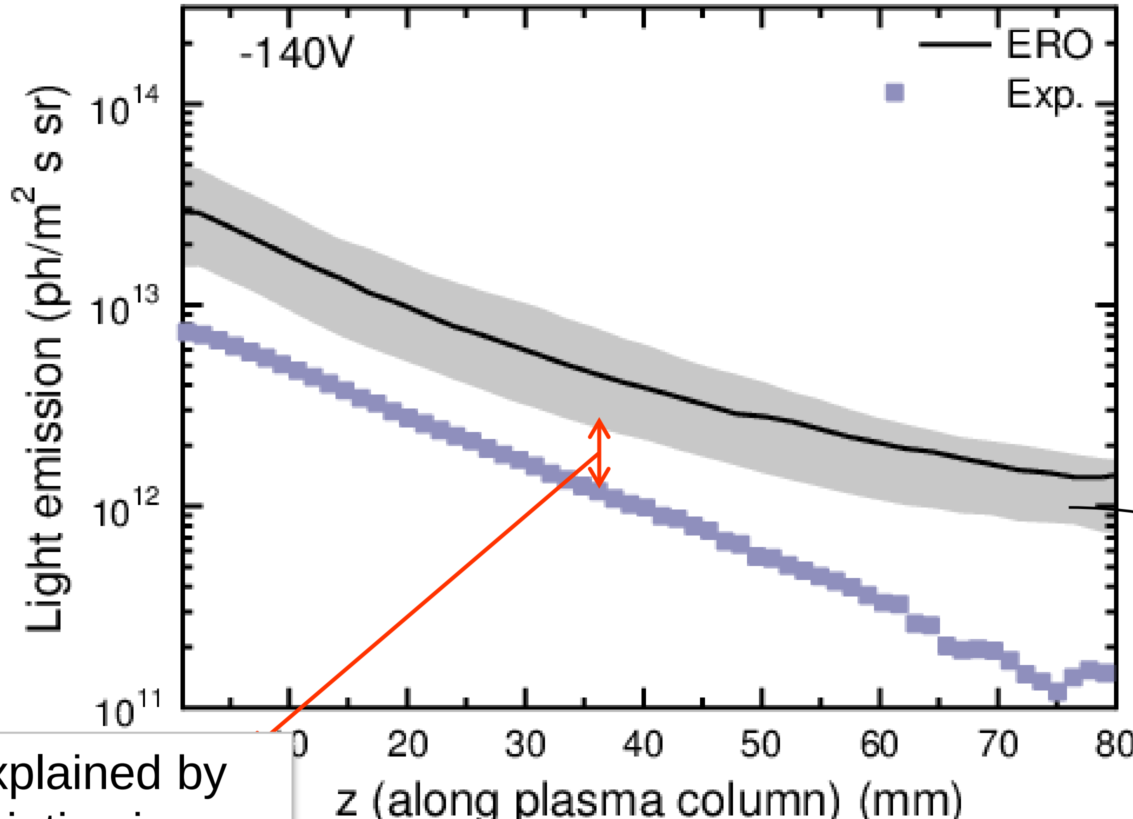
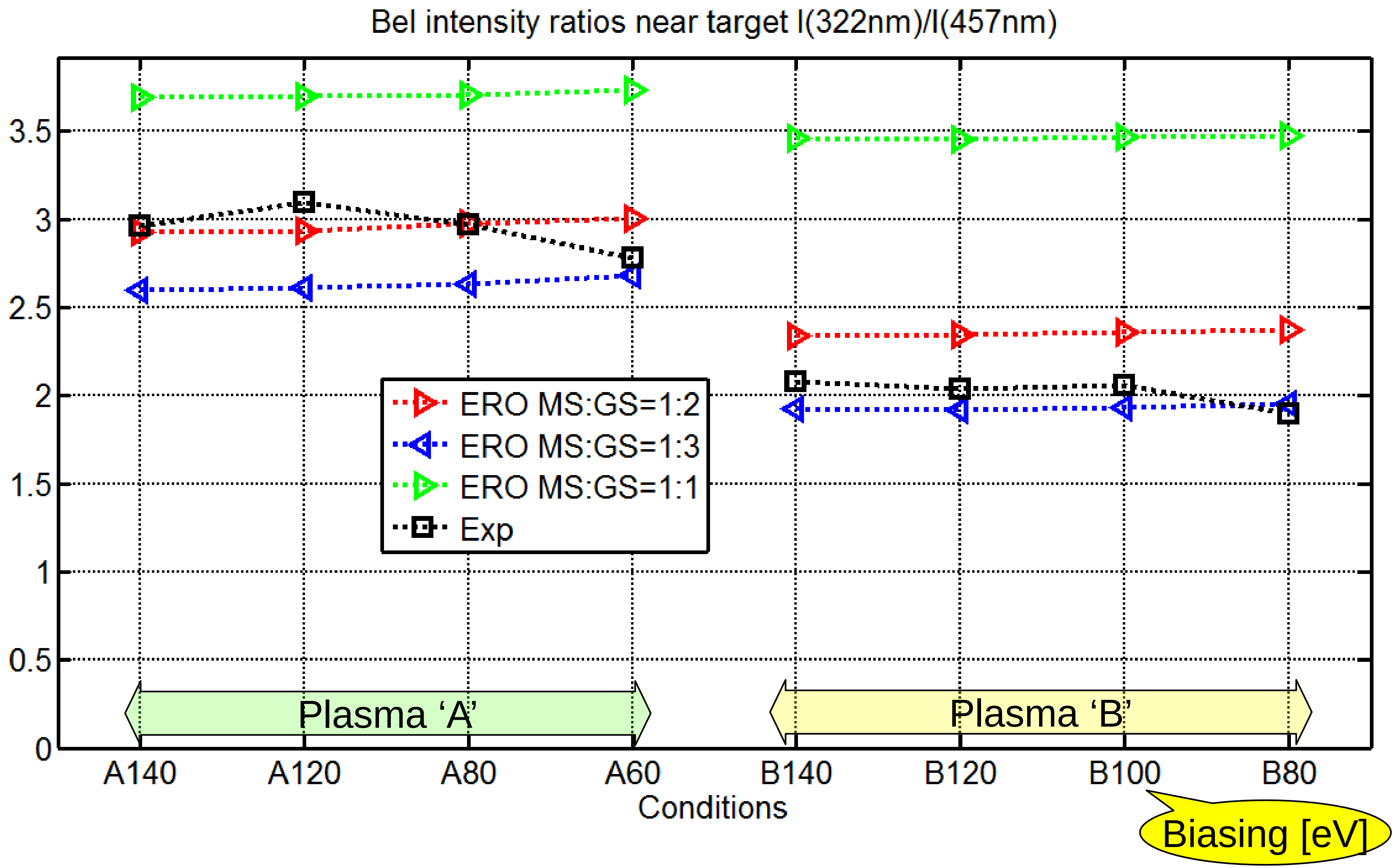


Range including uncertainties in n_e and T_e

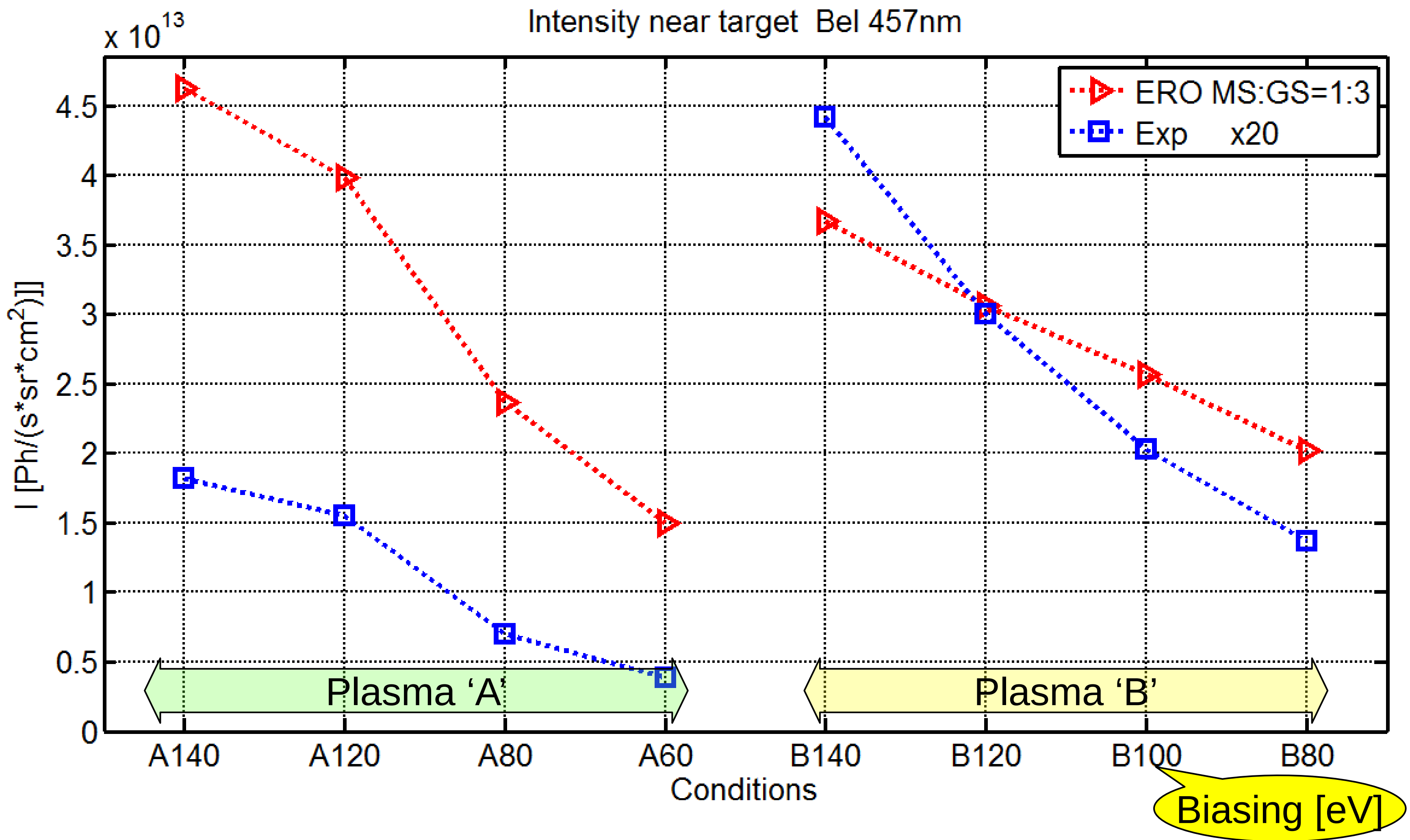
Can be explained by uncertainties in sputtering yields or spectroscopic data

D plasma: line ratios→ MS population



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

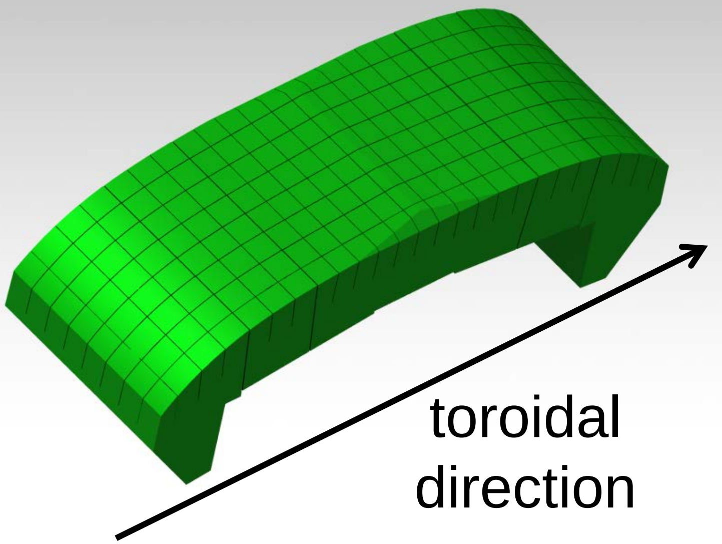
D plasma: intensities at target

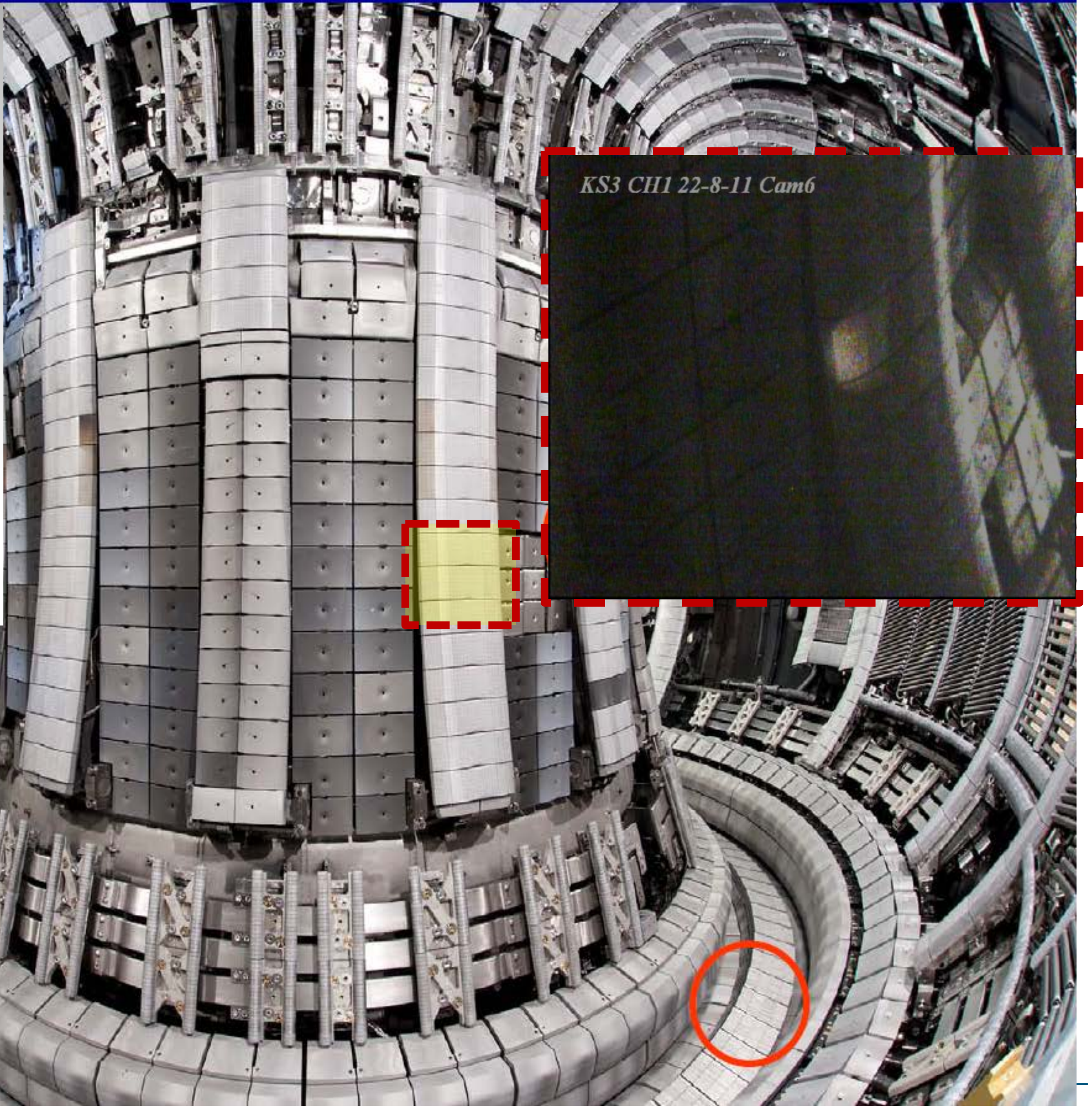


- *Be-D molecules are 17% of total Be release*
- *All Be from dissociation goes to MS level*

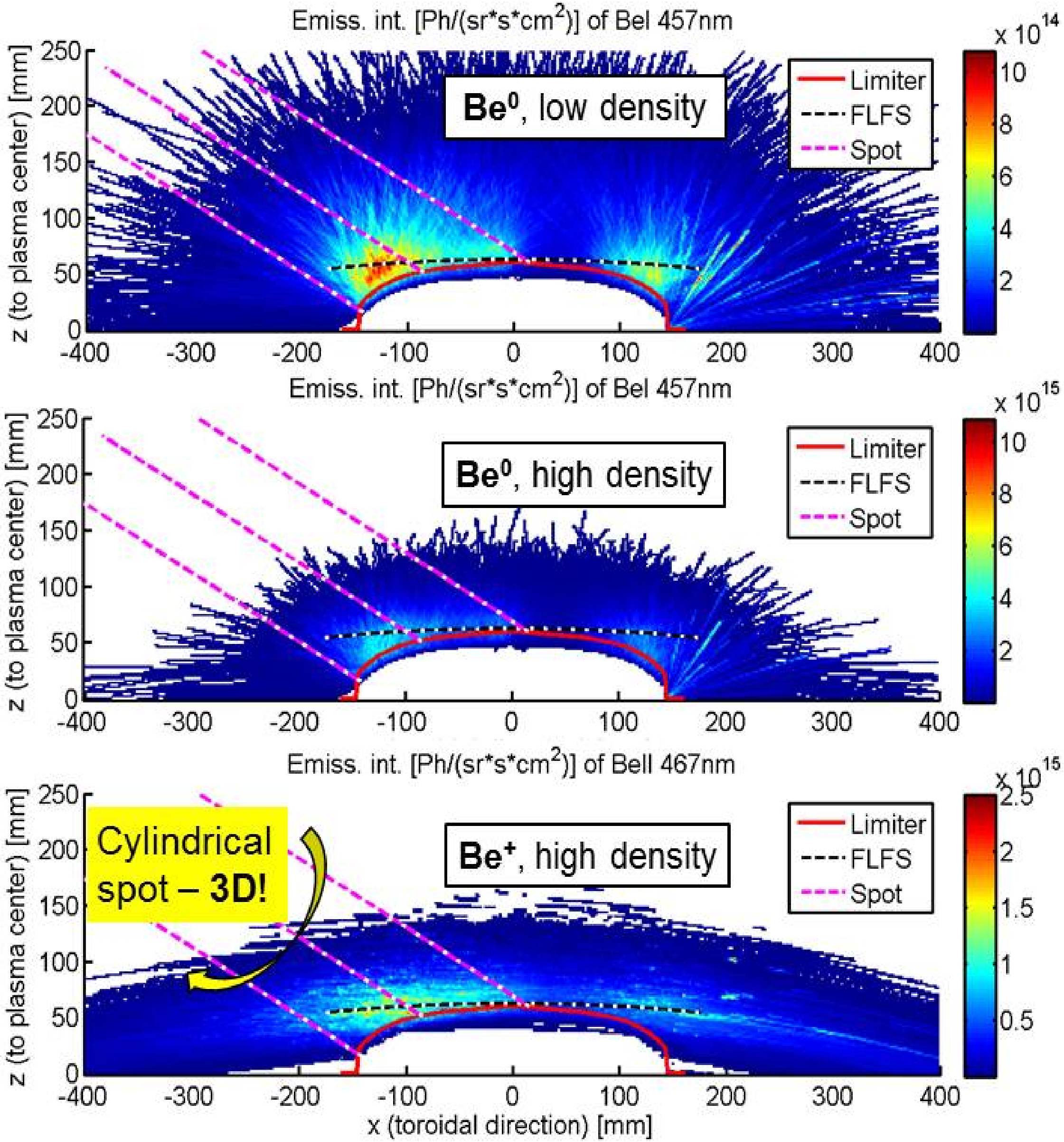
Spectroscopy benchmark at JET ILW (plasma density scan)

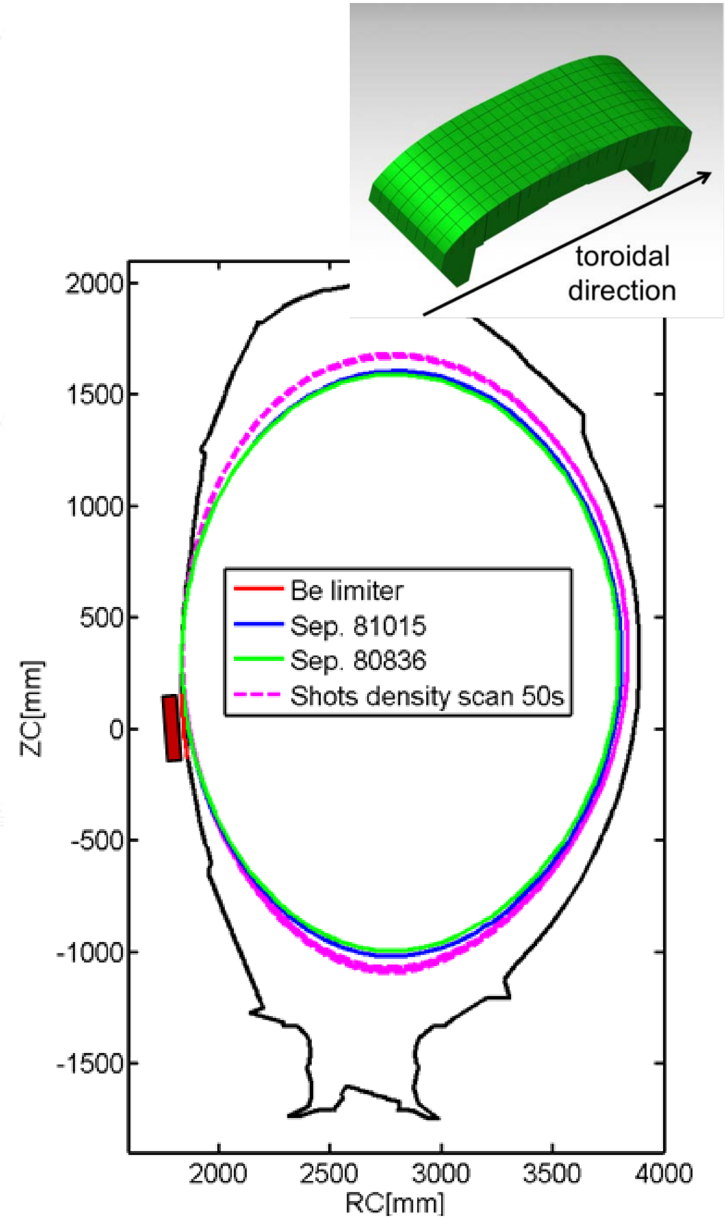
1. JET-ILW Be/W ITER-like Wall completed - 8th May 2011



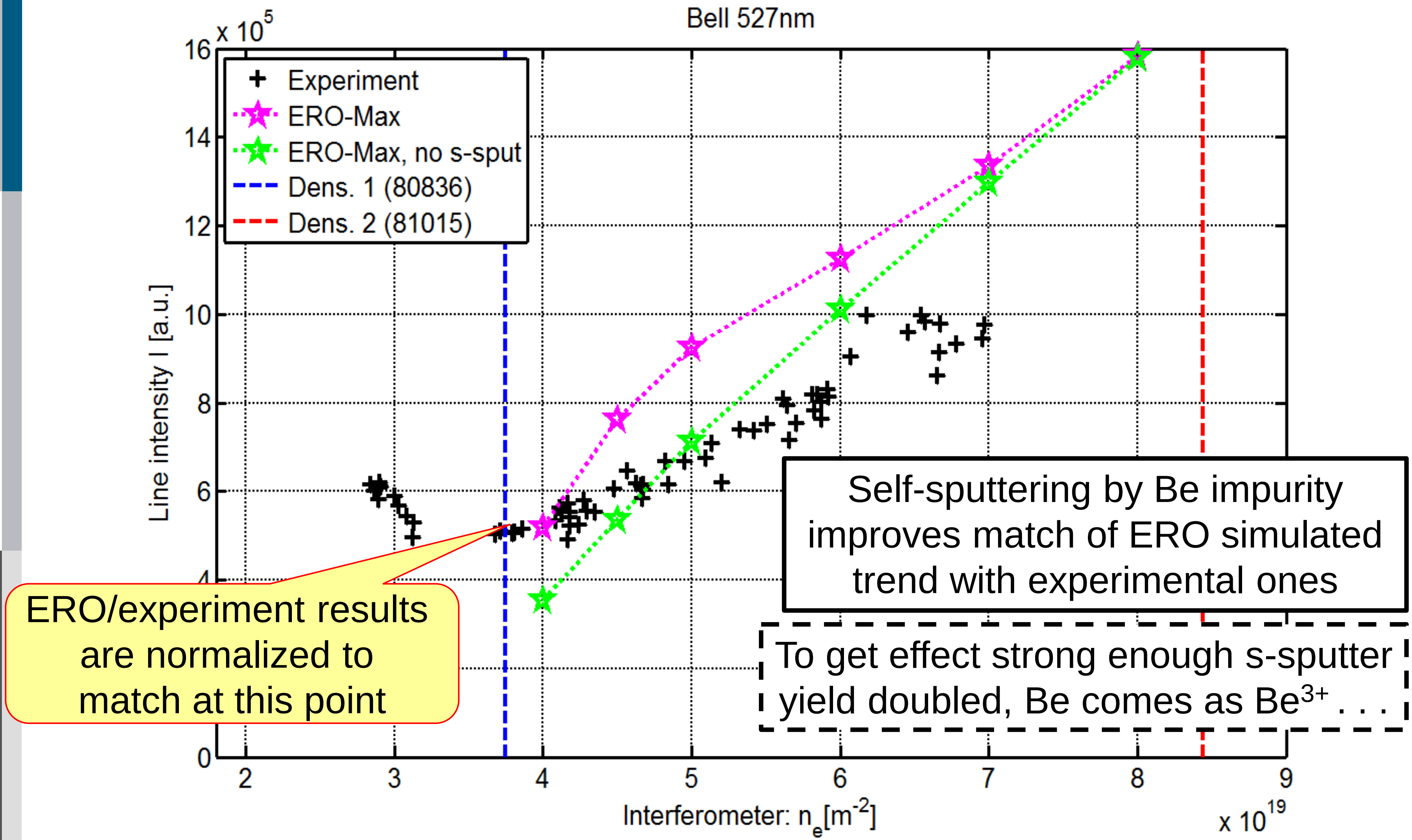


Line-of-sight integration

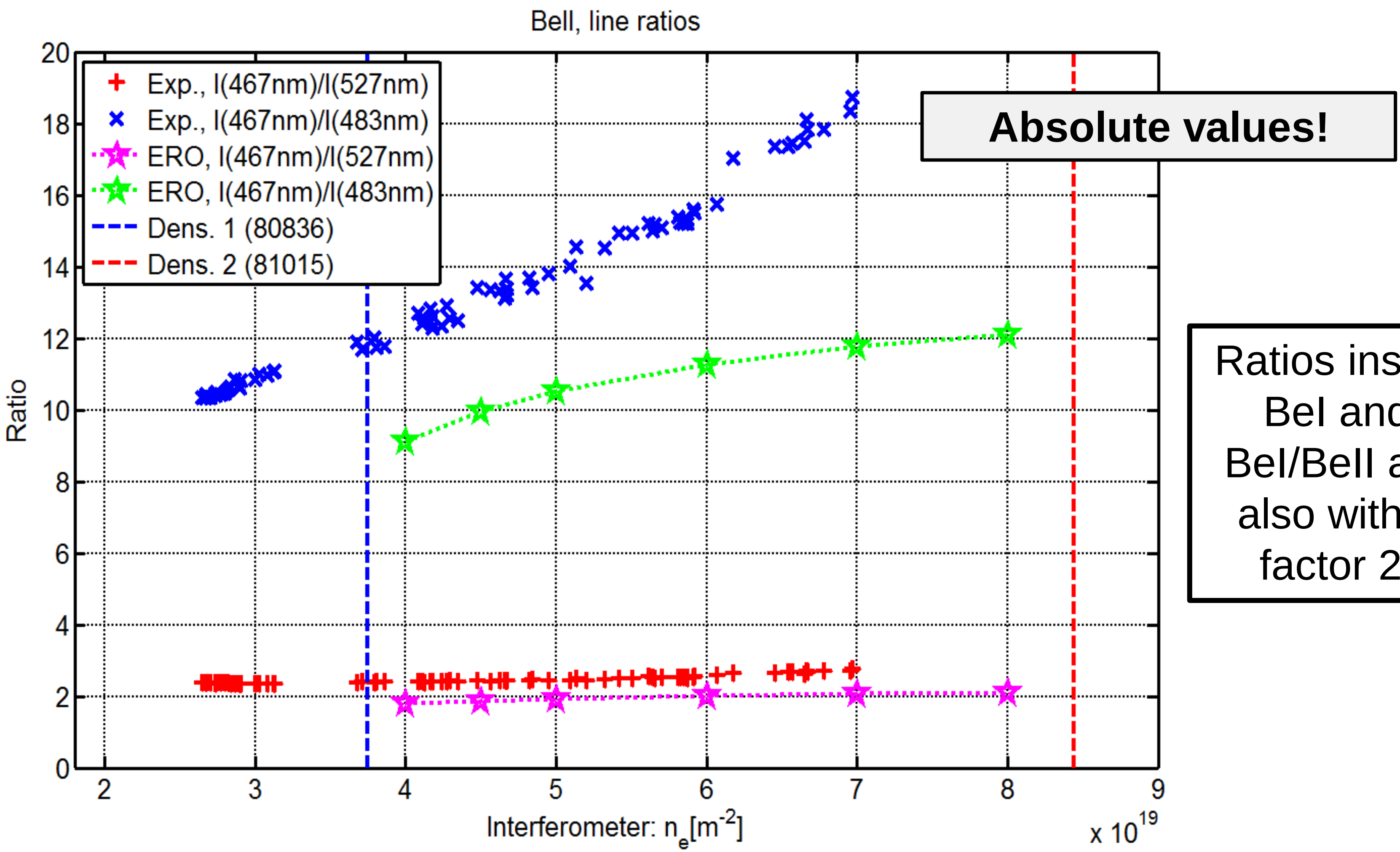




ERO&Experiment: Bell light



ERO&Experiment: BeII line ratios



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!

Summary

- The ADAS MS-resolved atomic data for Be is implemented in ERO and being validated with experiments.
  - *Benchmark at PISCES-B and JET*
  - *MS-effect is demonstrated to be of importance*
  - *MS population just after sputtering determined*

- The Be-D molecules release, transport in plasma and light emission are introduced in ERO.
  - *Benchmark on PISCES-B goes on succesfully*
  - *Benchmark at JET expected*
  - *Still missing: BeD_2 release, Be-D formation in plasma . . .*

ADAS:

- *It would be very useful to have a molecular extension . . .*
- *ERO can surve as a useful bridge for ADAS data benchmark with experiments*

The End