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JÜLICH FORSCHUNGSZENTRUM

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

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and many other FZJ, UCSD, ITER, TEKES, MEPhI, ADAS, JET and EUROfusion contributors

Outline

ERO simulations:

- Be erosion in PISCES-B (He plasma)
- JET ITER-like wall, IW solid Be limiter erosion
  - *Density scan experiment*
  - *Surface temperature scan experiment*
  - *MAPES (EAST) benchmark – connection lengths*
- JET OW: ICRH Antenna effect
- Be deposition in JET divertor

New model:

- Kinetic model for D retention in Be and thermodesorption experiments (based on DFT data)

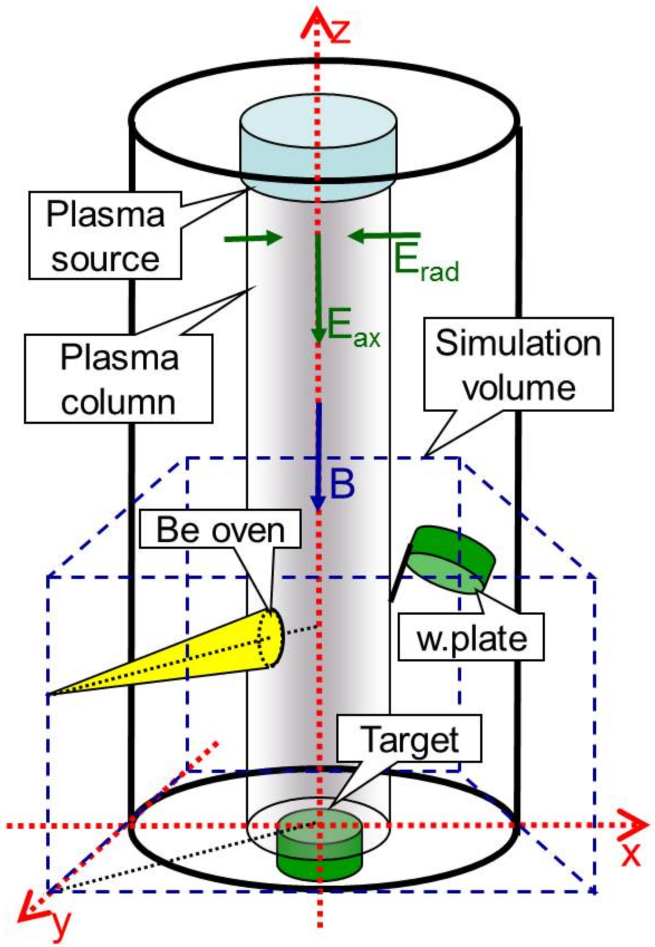
I would live off reported things (e.g. ITER predictions) and concetrate on the recent progress.

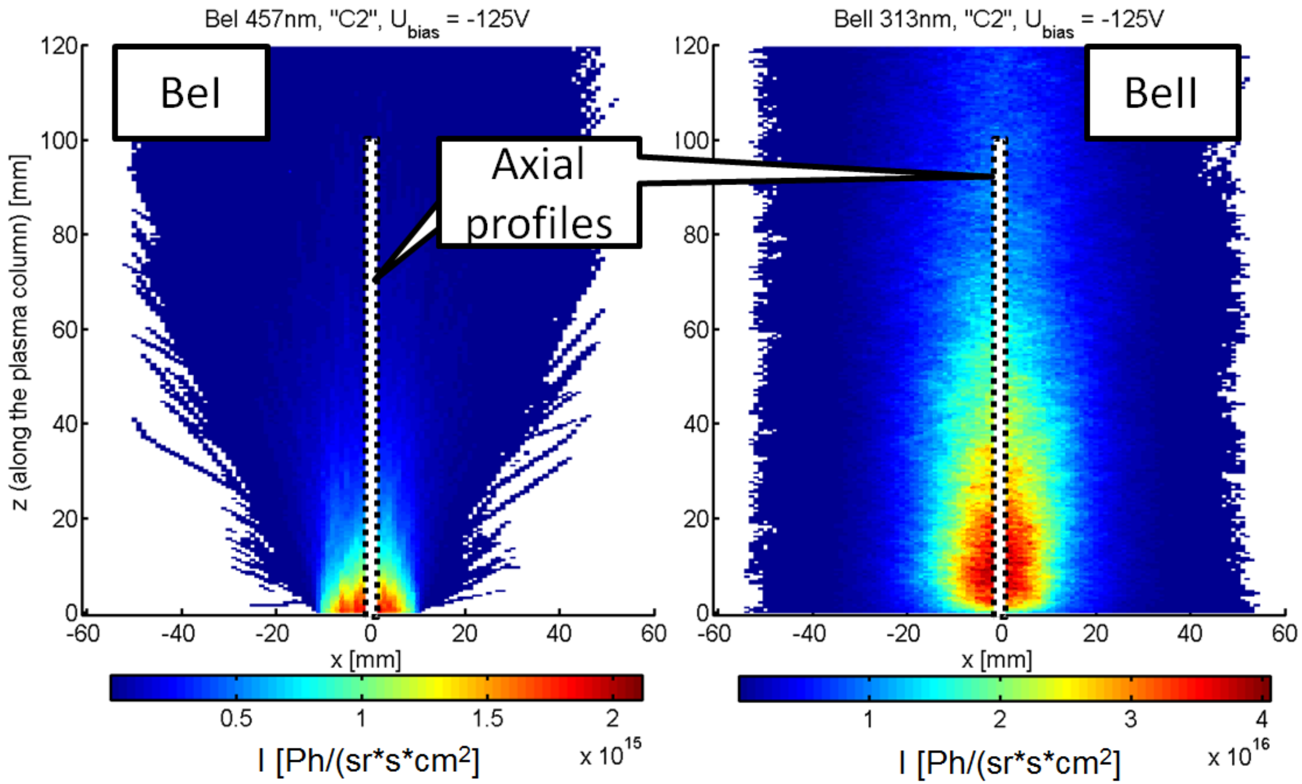
Erosion yields: Be exposure to He plasma in PISCES-B

Please, don't warry! Many slides need just 10 seconds like this one.

D.Borodin, D.Nishijima, R.Doerner et al., PSI-2016

Simulation of axial profiles

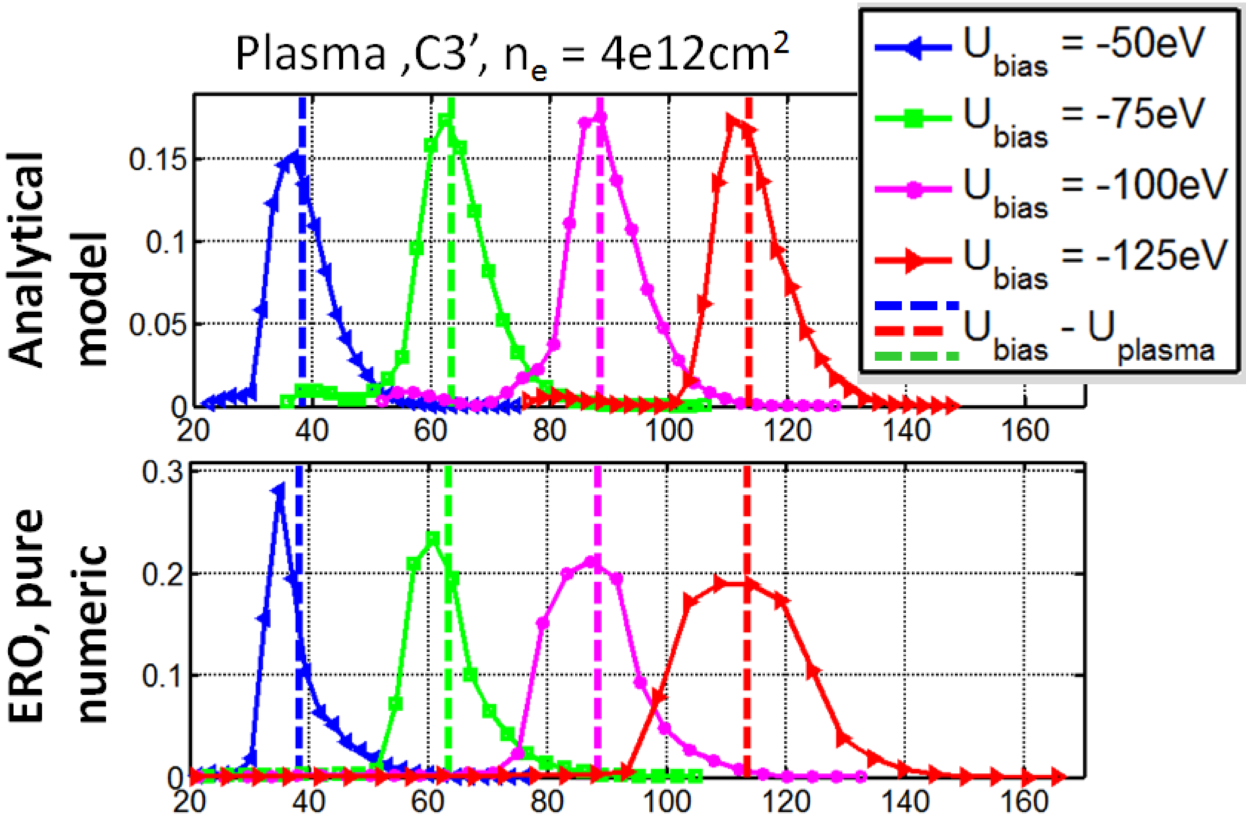


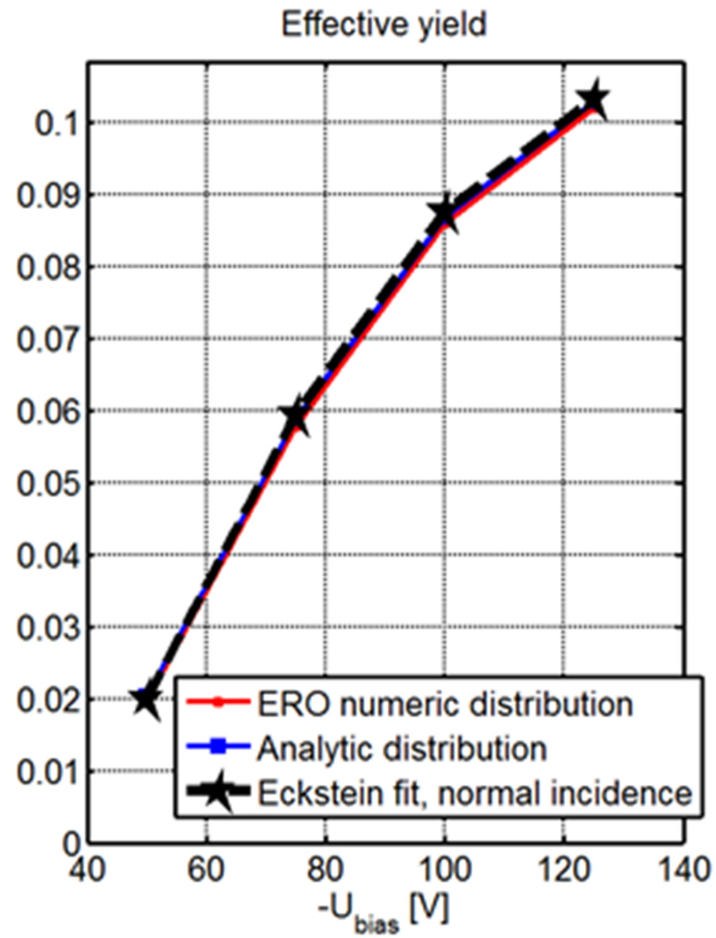


Dedicated experiment for ERO benchmark:

- **3 plasma coditions * 4 target biasings**
- **He plasma (no Be-D release effect)**
- **Target weight loss + witness plate depostion experiments is expected.**

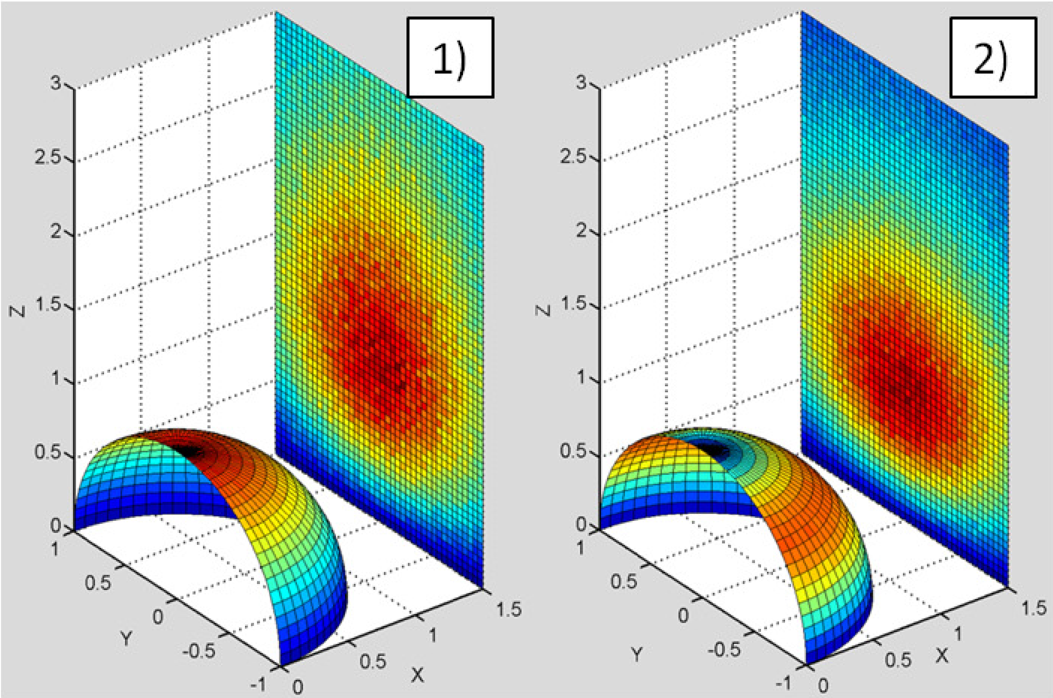
Effect of MS tracking in ERO

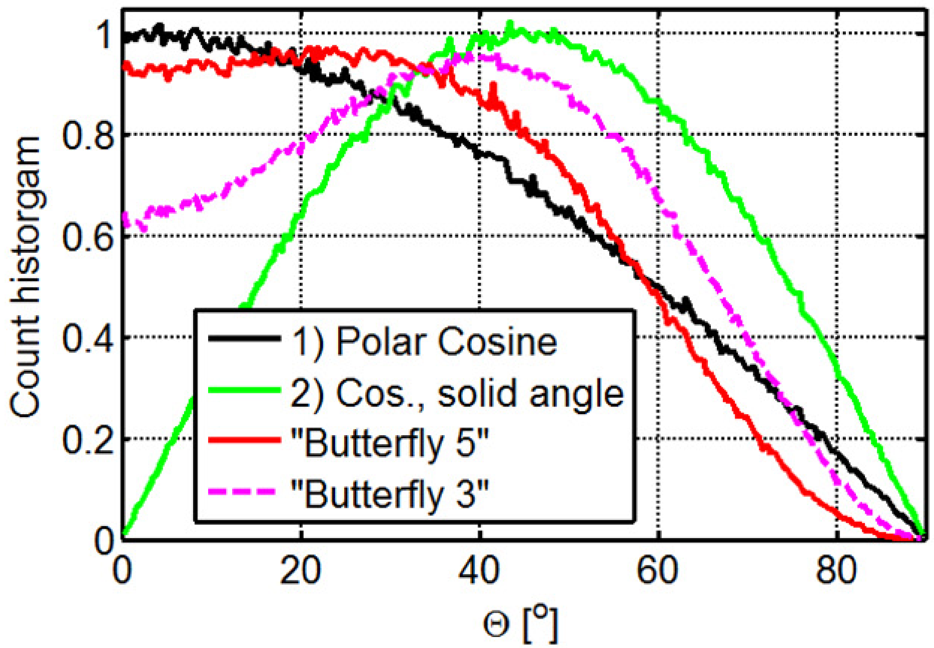




- The angle distribution of sputtering paticles on impact in nearly normal.
- Energy distributions on impact by numeric ERO “pre-simulation” are somewhat different from analytical ones, however both have **negligible effect on the effective sputtering yields**.

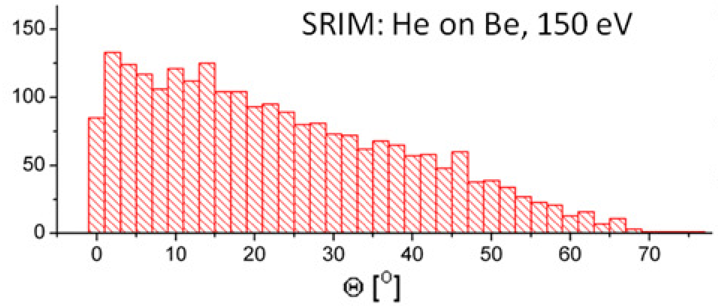
Angle distribution after sputtering

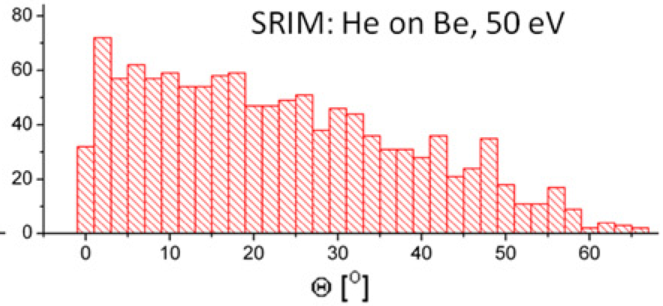




1) $dN_\theta = N_0 \cos\theta \cdot d\theta$

2) $dN_\Omega = \dfrac{N_0}{\pi} \cos\theta \cdot \underbrace{d\Omega}_{d\Omega = \sin\theta \cdot d\theta \cdot d\varphi}$

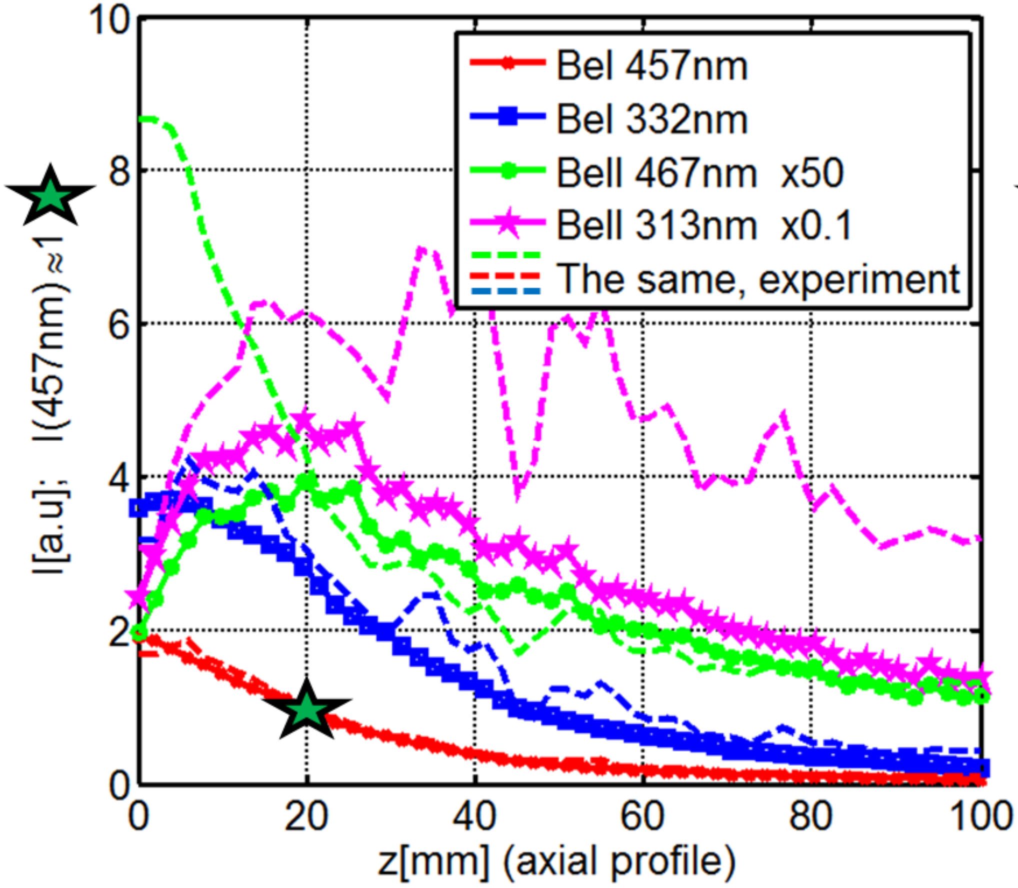


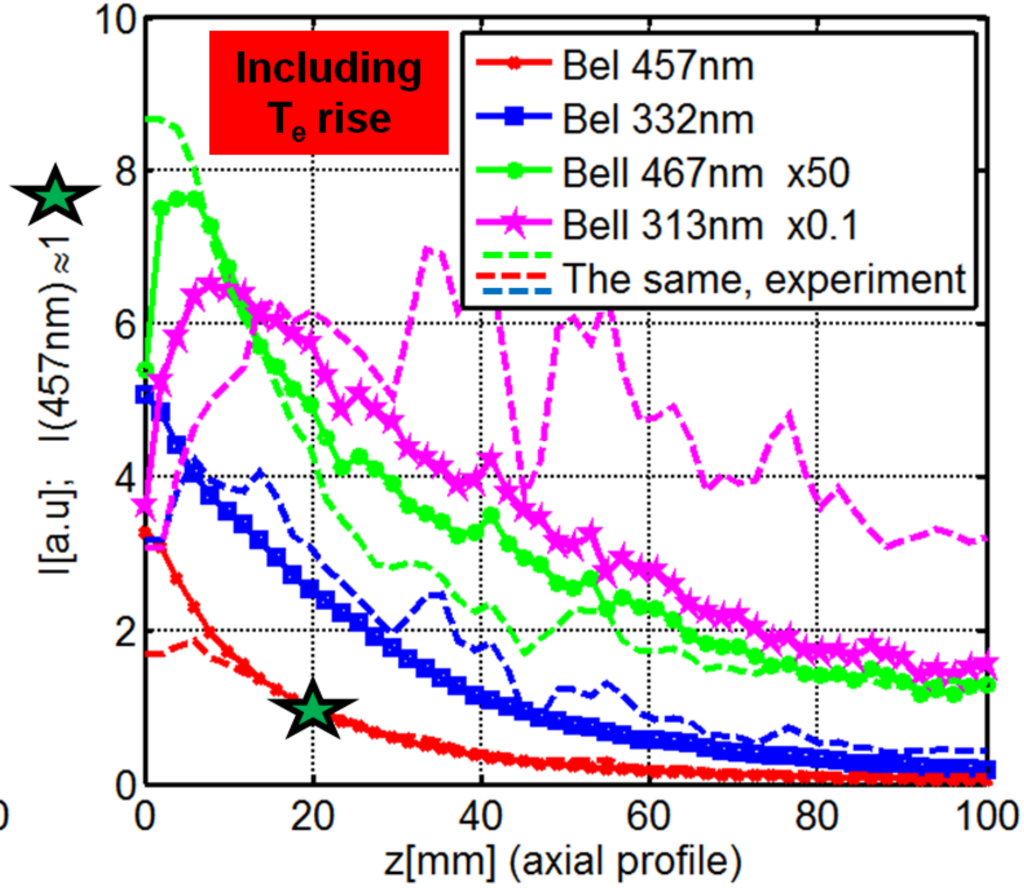


- Despite some confusion in literature, “polar cosine” distribution seems to be the right one for physical sputtering process, it is also necessary to reproduce PISCES-B measurements.
- Moreover, an additional cut-off angle is necessary to get best match for BeII lines.

Simulation of axial profile shapes

ERO&Experiment: plasma 'C2'; optimal release angle cut-off at 30°



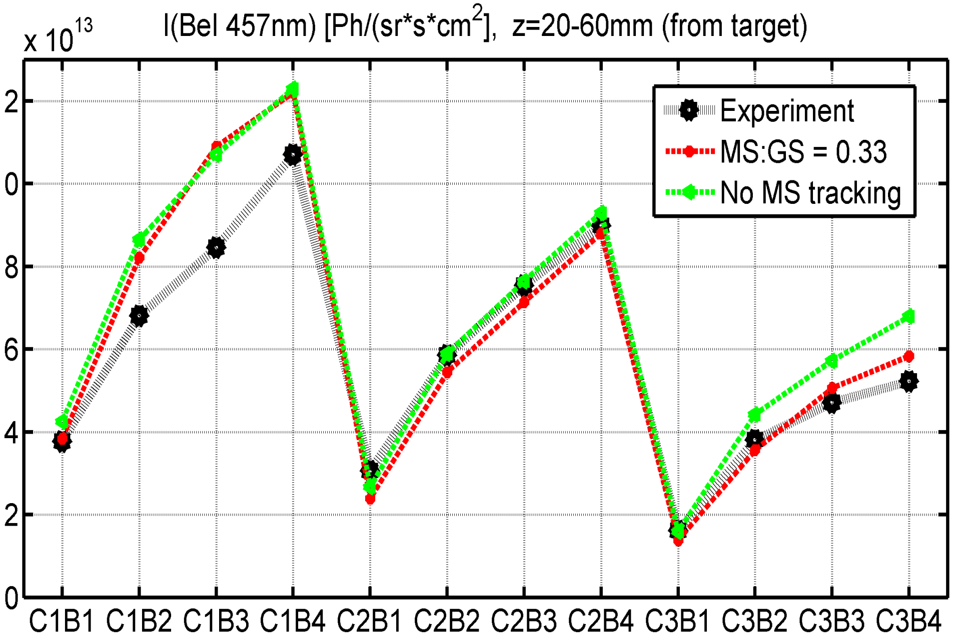


The profile shapes and line ratios are in perfect agreement for BeI and in a good agreement for BeII: used ADAS'96 data and intitial angle distributions are very resonable!

BeI 457nm for z in [20..60mm] are very stable against varios assumptions: perfect for producing of the **integrated values!**

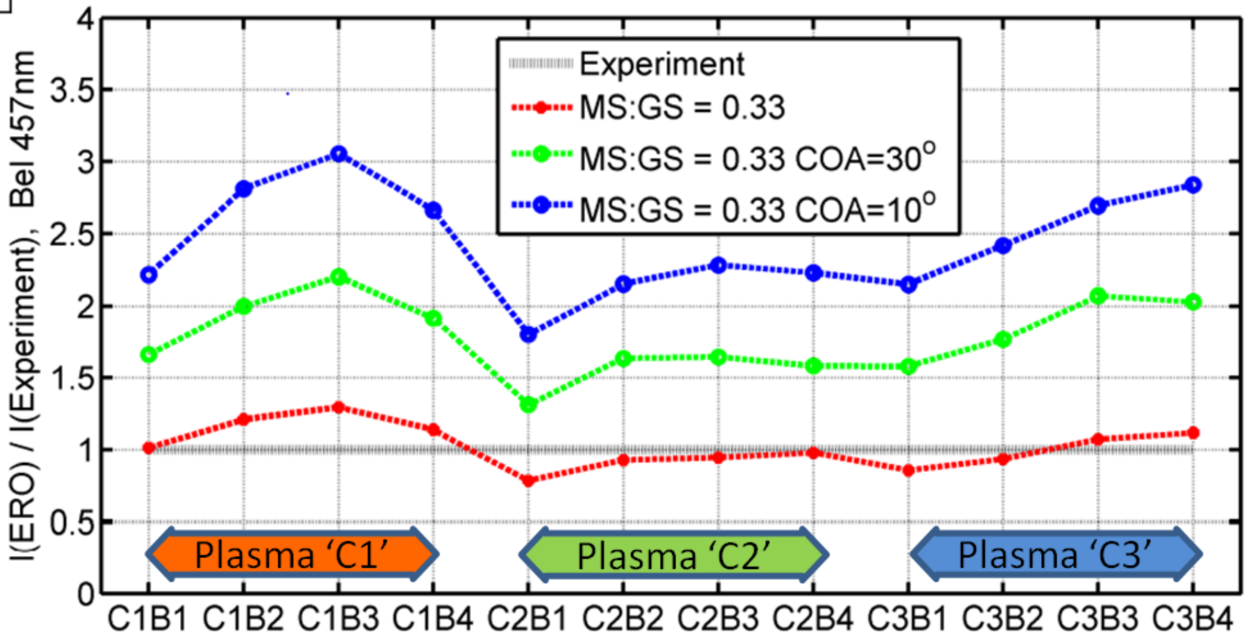
Absolute line intensites charachterising sputtering yields

Plasma	At axis, z=150mm	Biasing	ERO 'name'
'C1'	n_e=12*10^{12}cm^{-3} T_e=4.8eV $P_{neutrals}$=7.3mTorr B=0.0152T	'B1' V=-50V	1) 'C1B1'
		'B2' V=-75V	2) 'C1B2'
		'B3' V=-100V	3) 'C1B3'
		'B4' V=-125V	4) 'C1B4'
'C2'	n_e=6.5*10^{12}cm^{-3} T_e=7.7eV $P_{neutrals}$=3.8mTorr B=0.0152T	'B1' V=-50V	5) 'C2B1'
		'B2' V=-75V	6) 'C2B2'
		'B3' V=-100V	7) 'C2B3'
		'B4' V=-125V	8) 'C2B4'
'C3'	n_e=4.0*10^{12}cm^{-3} T_e=11.5eV $P_{neutrals}$=2.5mTorr B=0.0152T	'B1' V=-50V	9) 'C3B1'
		'B2' V=-75V	10) 'C3B2'
		'B3' V=-100V	11) 'C3B3'
		'B4' V=-125V	12) 'C3B4'



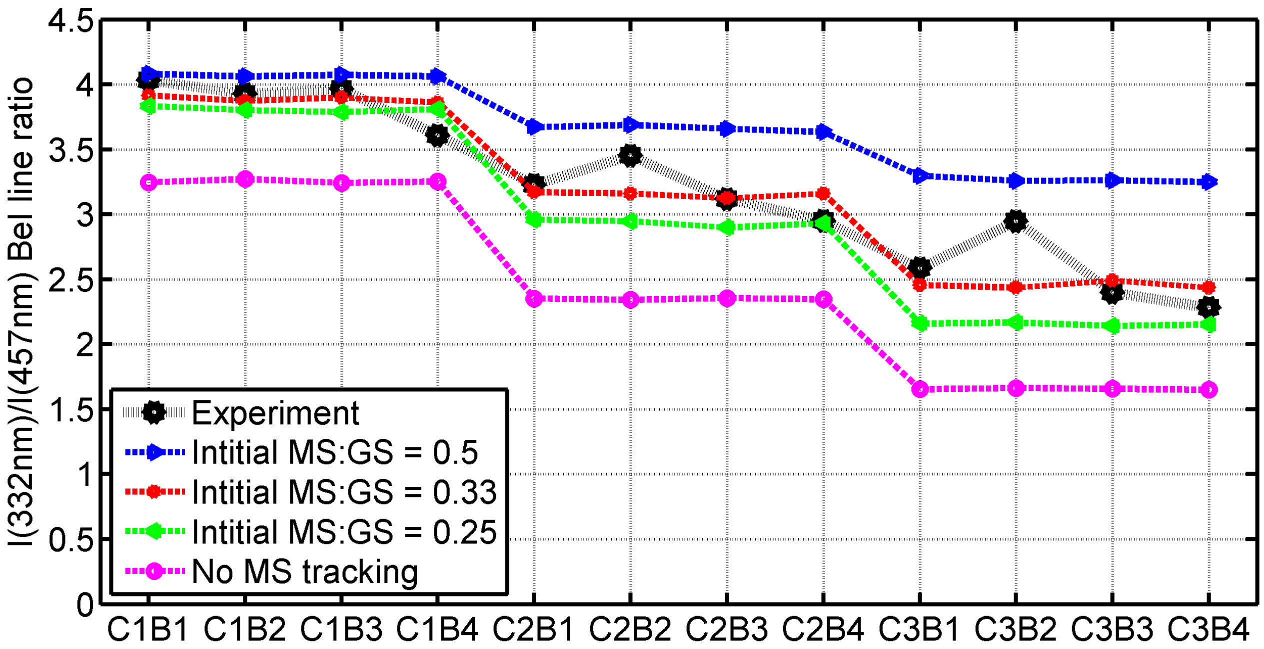
Nearly perfect reproducing of SDTrimSP data (Eckstein 2007 fit by C.Björkas)

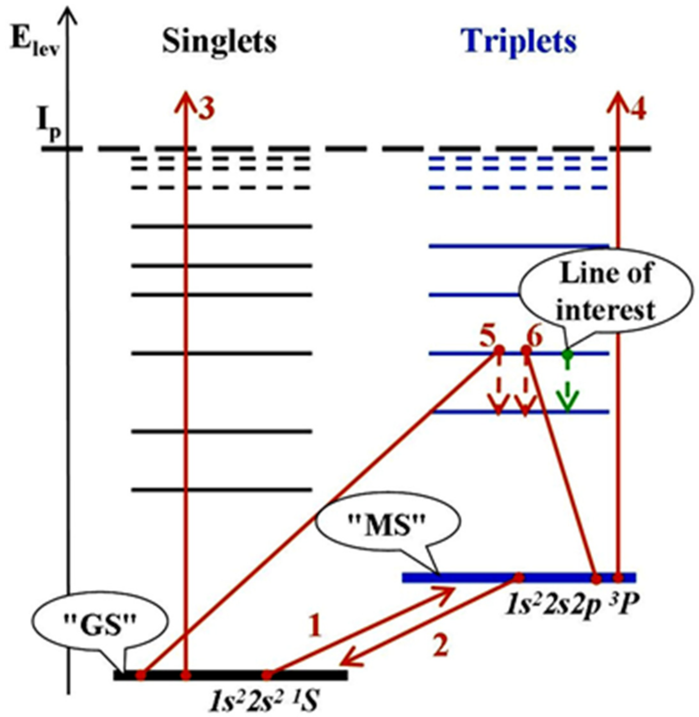
….with a coefficient depending on “cut-off” angle



Effect of MS tracking in ERO

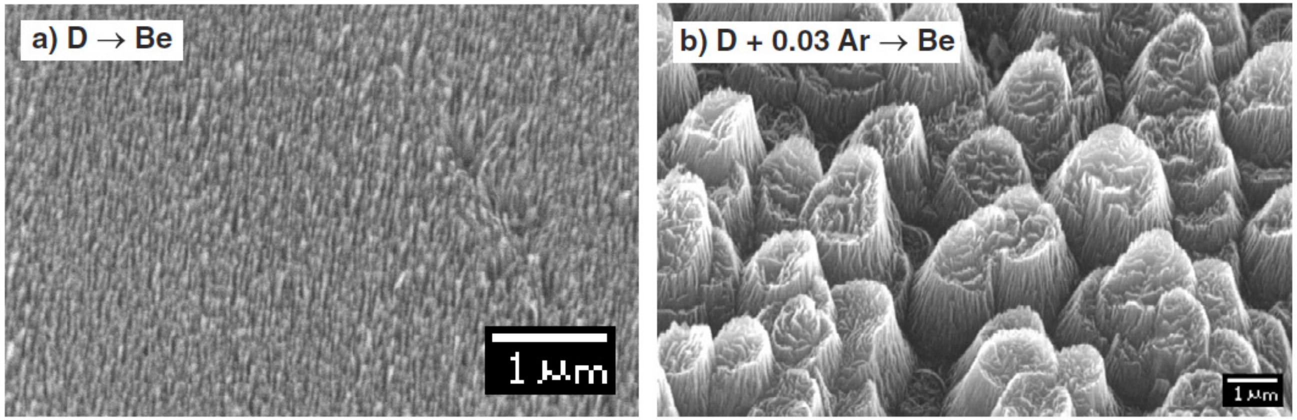
Triplet to singlet line ratio:





- The initial populations in Be after sputterig seems to be always close to MS:GS=0.33.
- This is independent on target biasing and plasma conditions.
- For D plasma situation is similar (ongoing simulations).

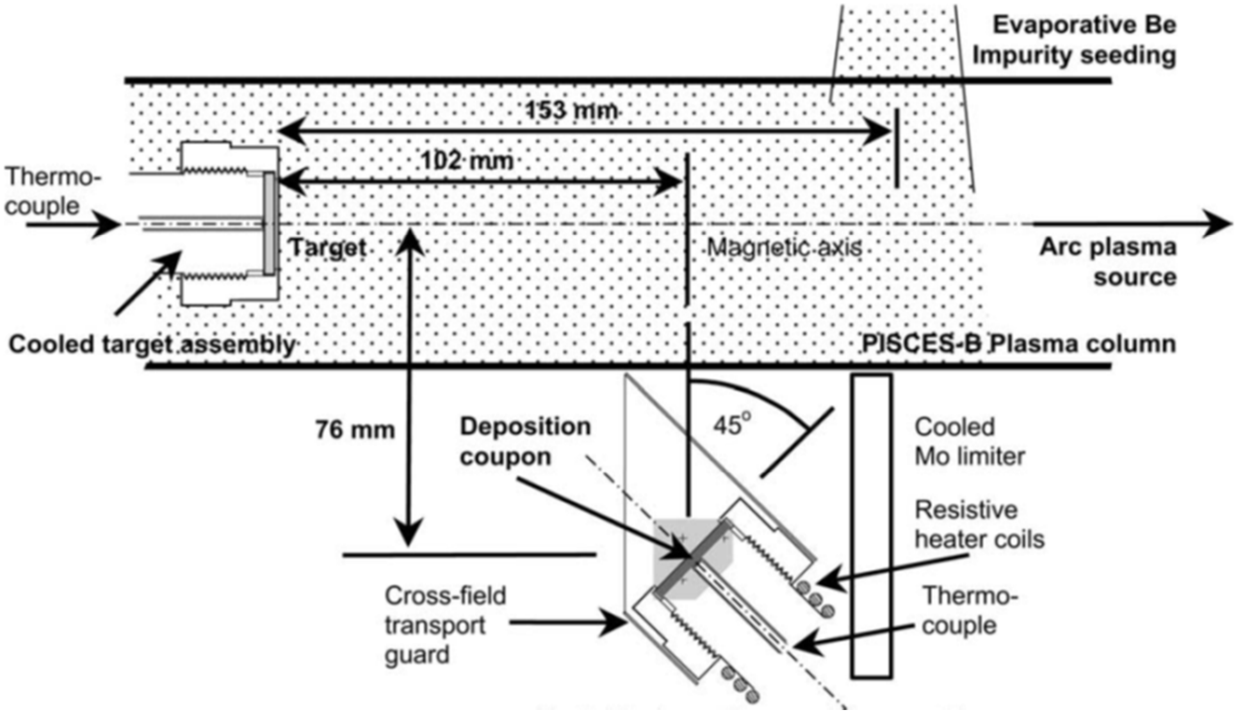
Yields absolute value discussion



A.Kreter et al., Phys. Scr. **T159** (2014) 014039

The growing with fluence „cone-like structures“ are known to intrease the decay length of axial profiles of Be in PISCES-B.

Can it be an explanation for the „cut-off angle“?



Weight loss / wittness plate available only for D plasma (just 1 measurement)

D plasma case simulations though more difficult

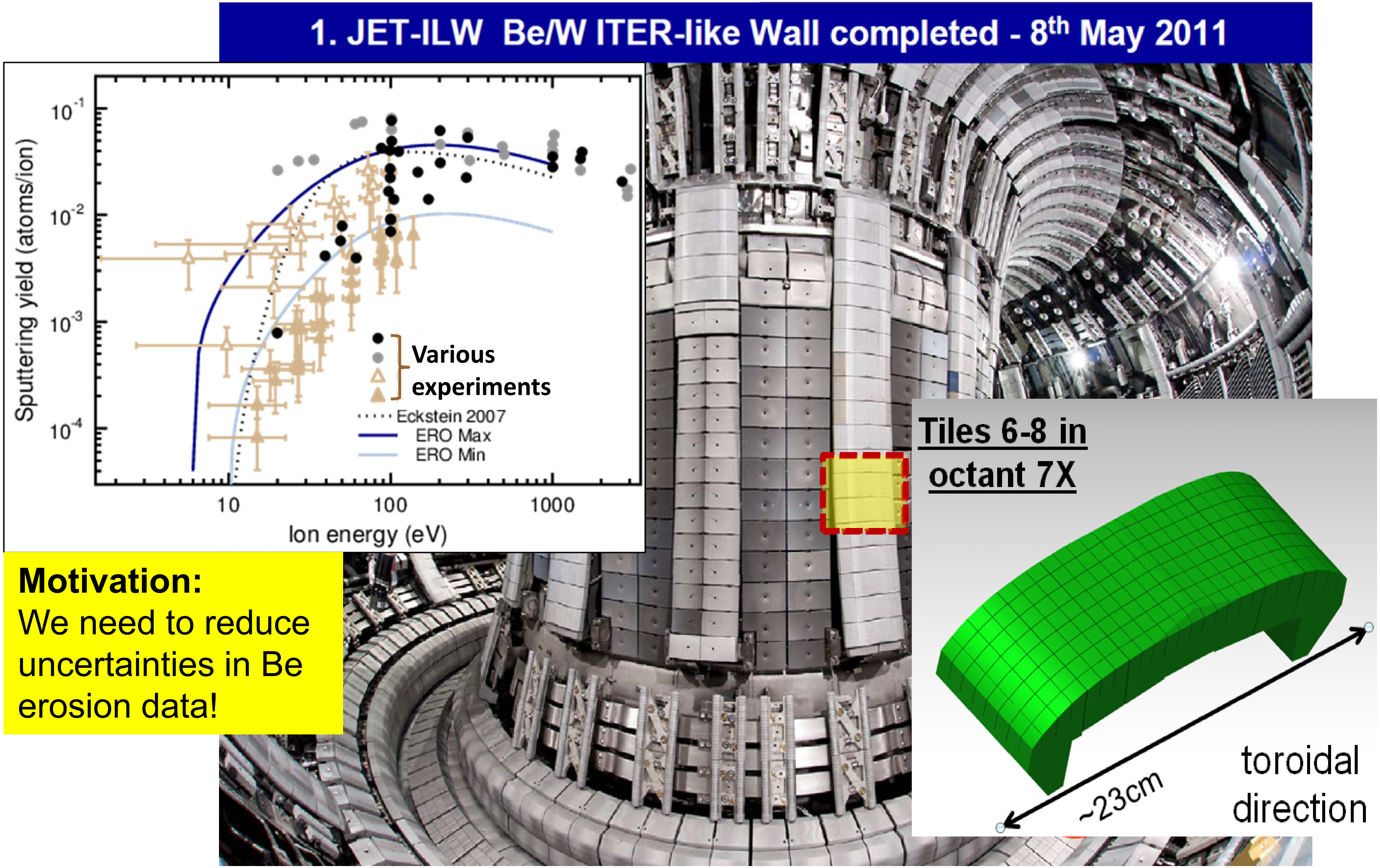
- ***BeD_x and D^{2+}, D^{3+} ions***

can help to clarify many issues!

Indispensible to implement the BeDx reaction data (M.Probst)!

Benchmark at JET ITER-like wall, IW Be limiter

Spectroscopy at inner-wall Be limiter



Motivation:
We need to reduce uncertainties in Be erosion data!

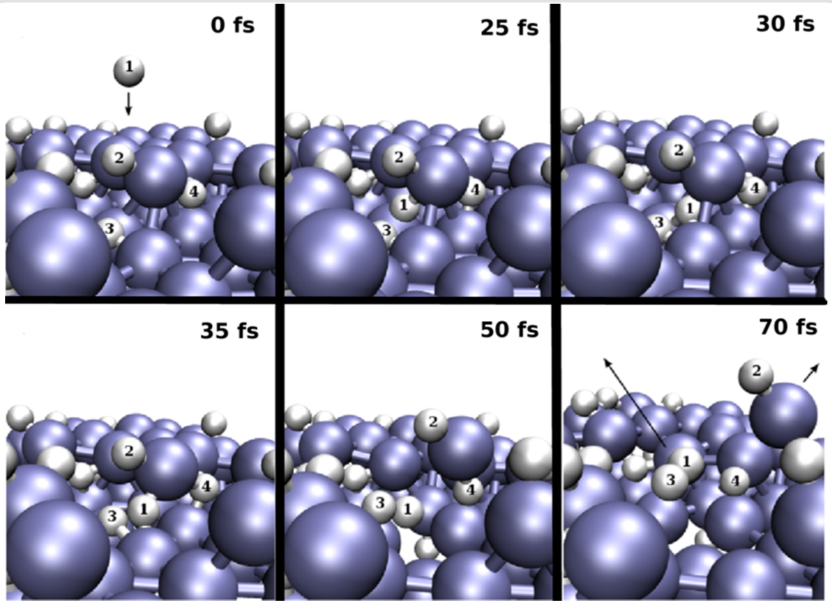
Be erosion mechanisms

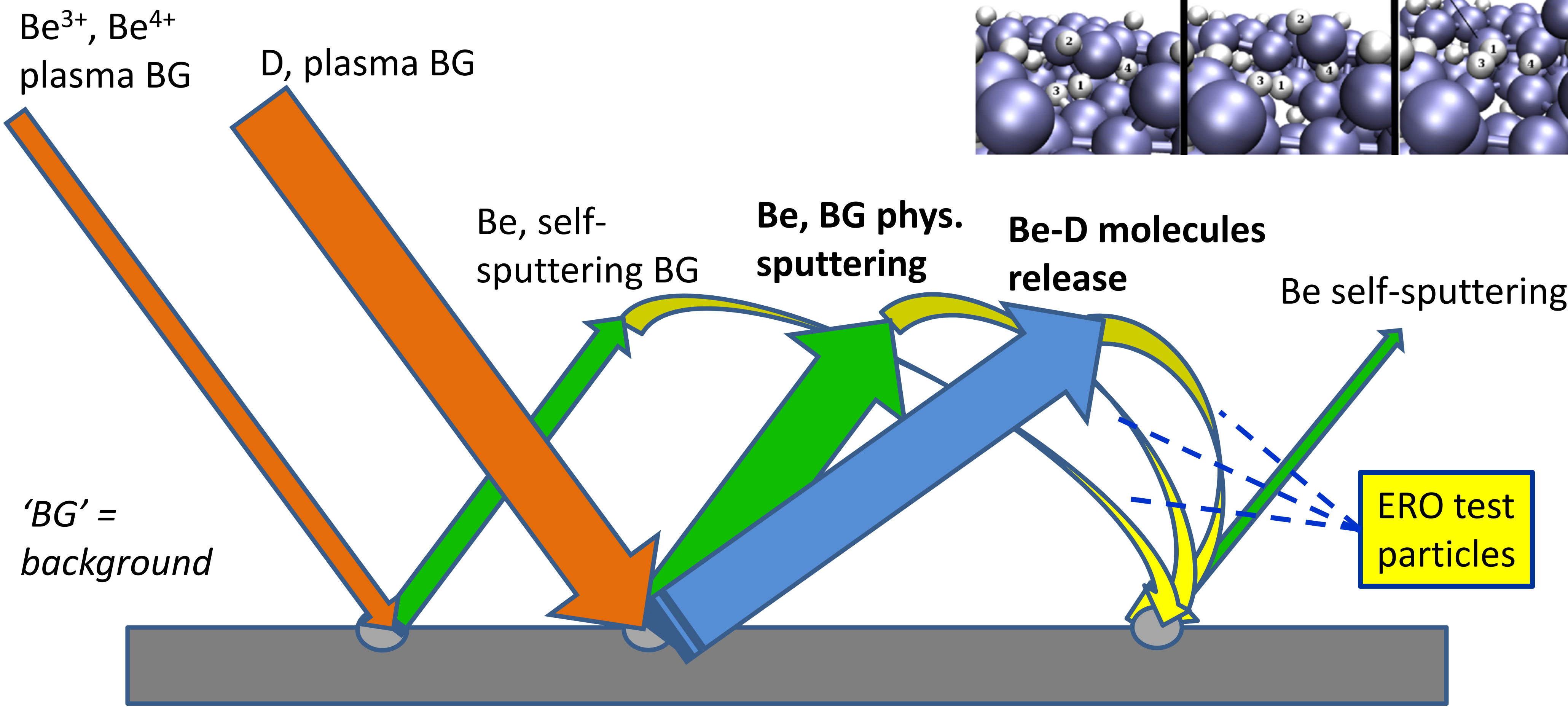
Energetic ions are needed for all the processes!

MD simulations demonstrate «swift chemical sputtering»:

C. Björkas et. al, PPCF (2013)

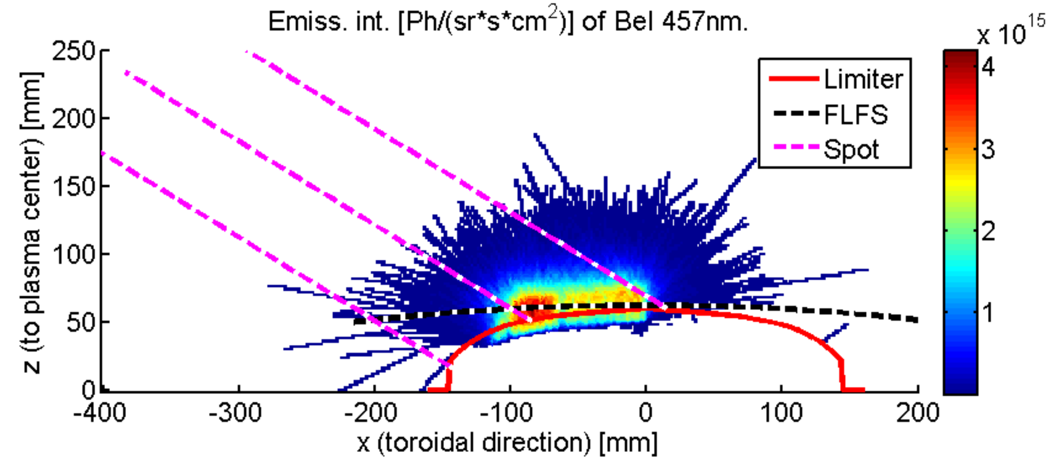
„Chemically assisted (CA) erosion“



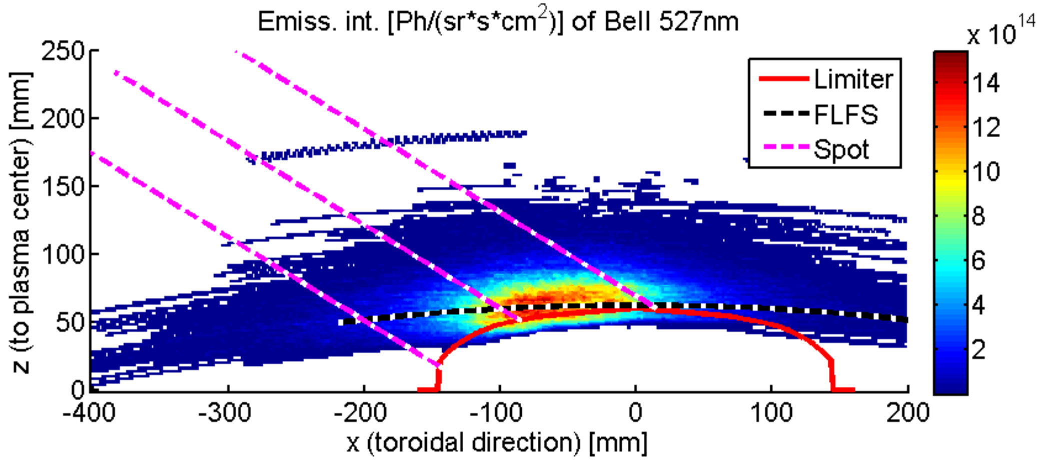


Local Be transport (3D) and light emission

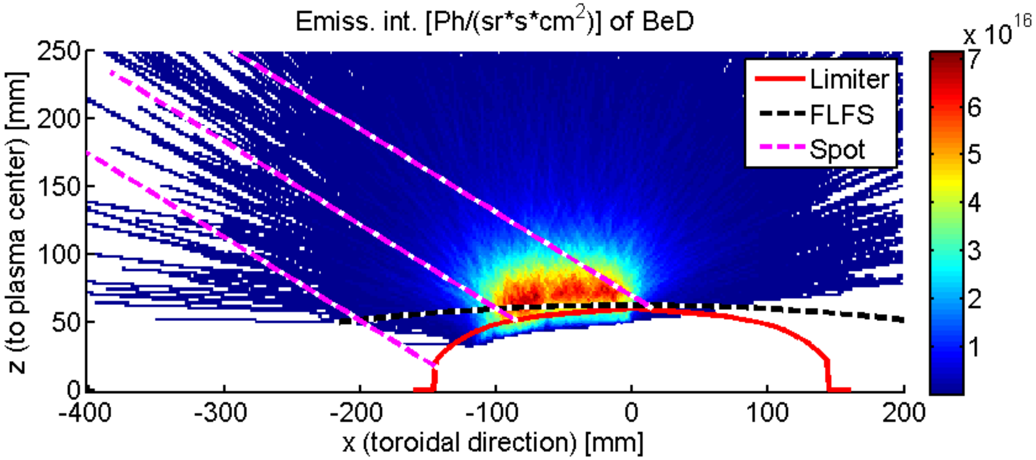
BeI, physically eroded Be



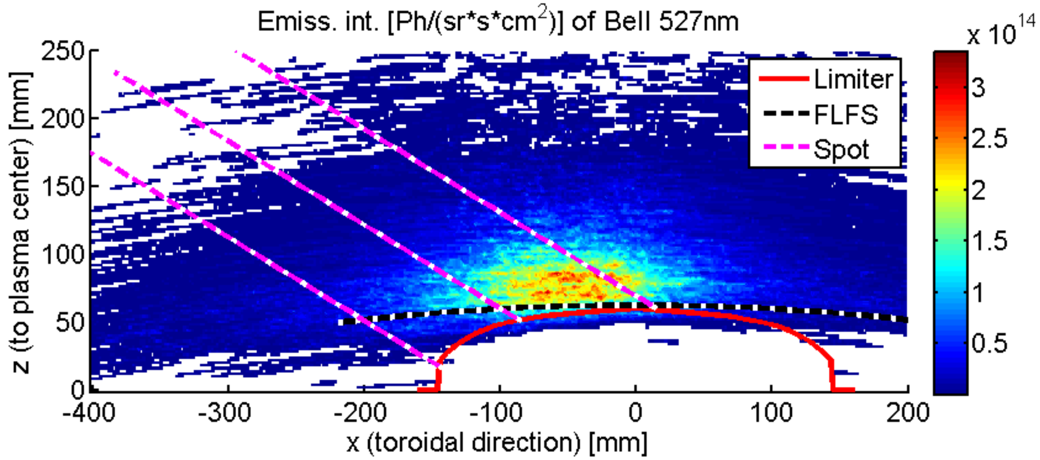
BeII, physically eroded Be



BeD band, CA eroded Be (BeD)

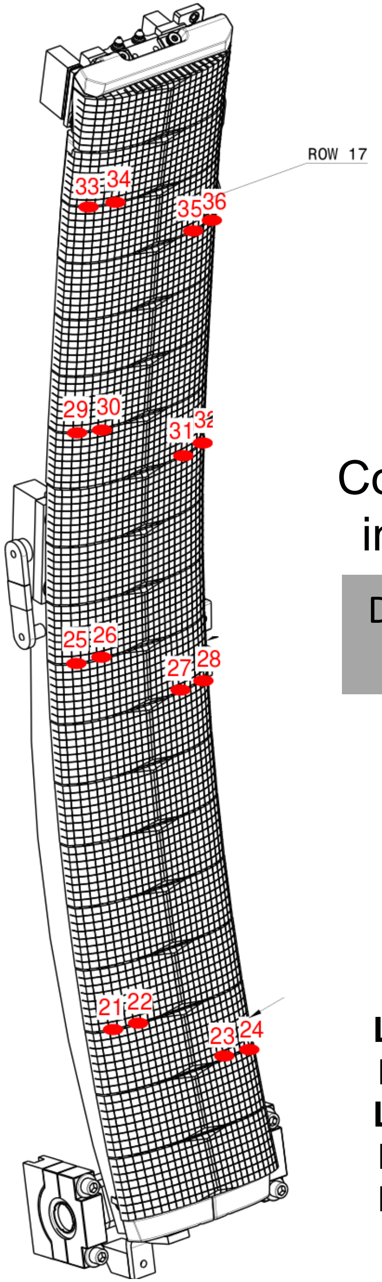


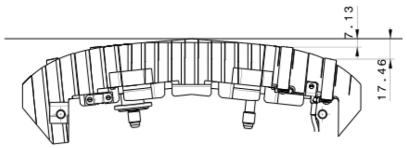
BeII, CA eroded Be (BeD)



BeII intensity and fraction coming to the observation chord depends on the erosion mechanism

Embeded probe measurements



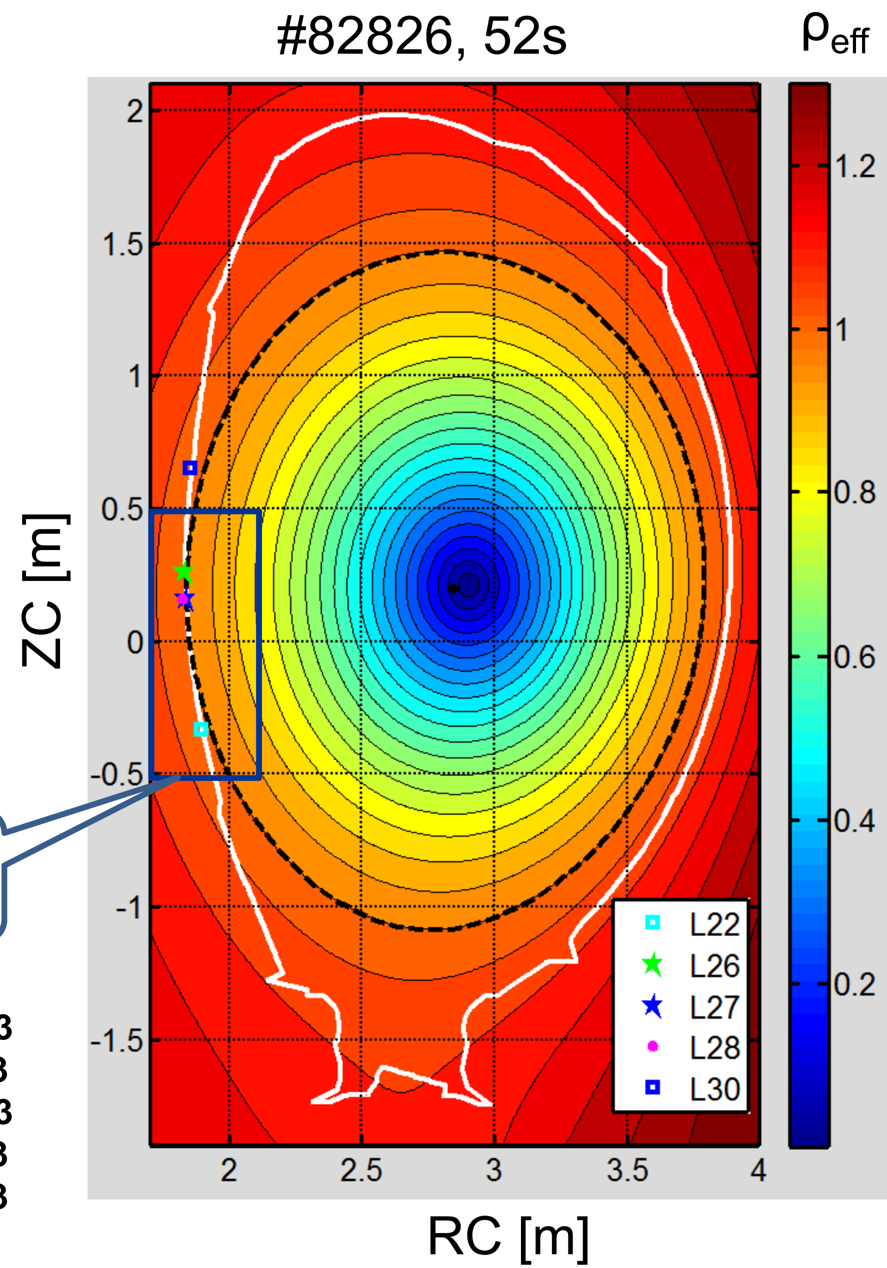


T_e (separatrix) ~ 15eV

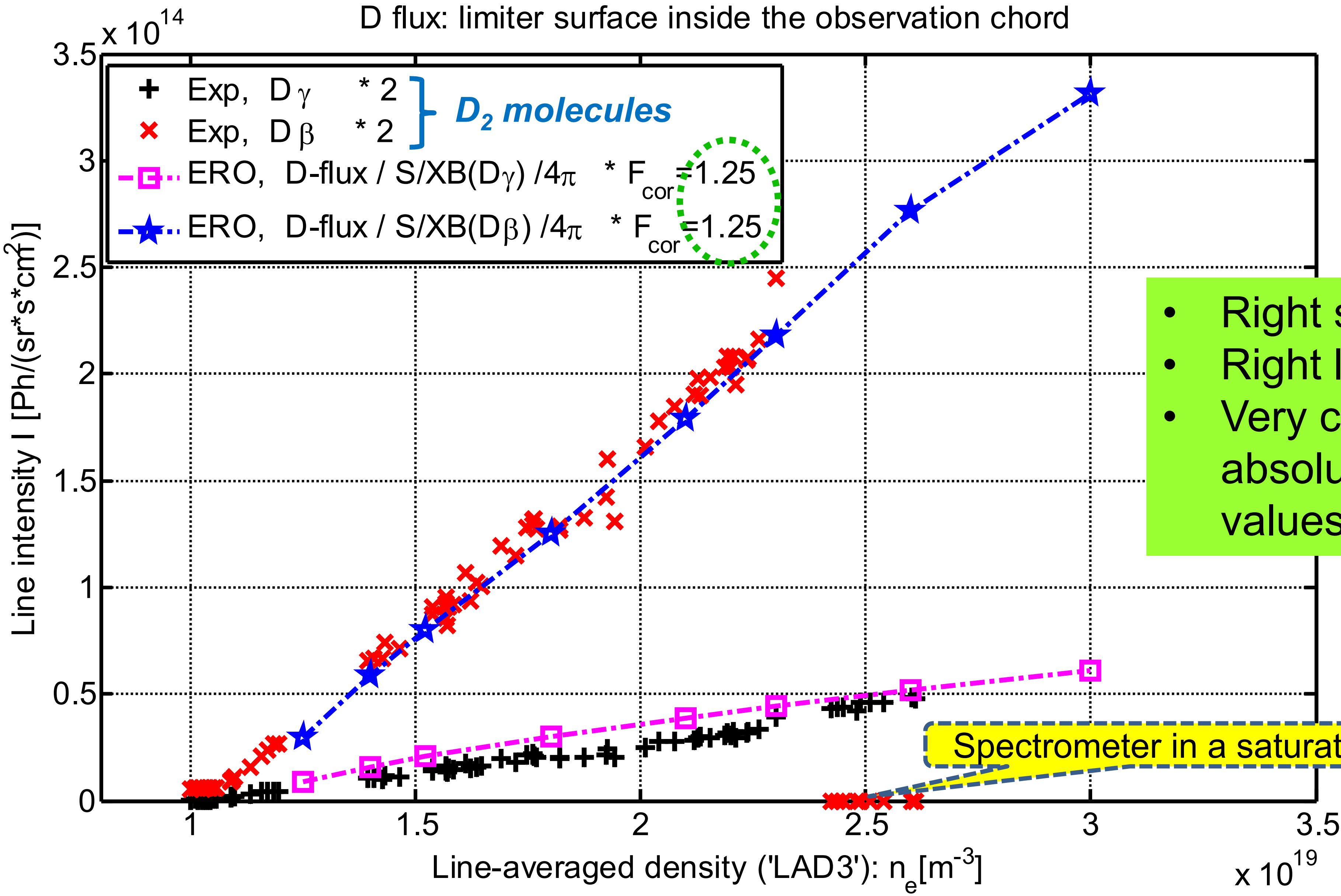
Corrected plasma parameters lead to improvement for the earlier results:

D.Borodin et. al, PFMC-2013, Phys. Scr. (2014) 014057

L22:	**rho=1.013**	**Te=16.82eV**	**Ne=7.30e+018m^-3**
L26:	**rho=1.004**	**Te= 4.57eV**	**Ne=1.66e+018m^-3**
L27:	**rho=1.003**	**Te=14.05eV**	**Ne=5.51e+018m^-3**
L28:	**rho=1.007**	**Te= 4.06eV**	**Ne=1.41e+018m^-3**
L30:	**rho=1.021**	**Te= 3.14eV**	**Ne=1.75e+017m^-3**



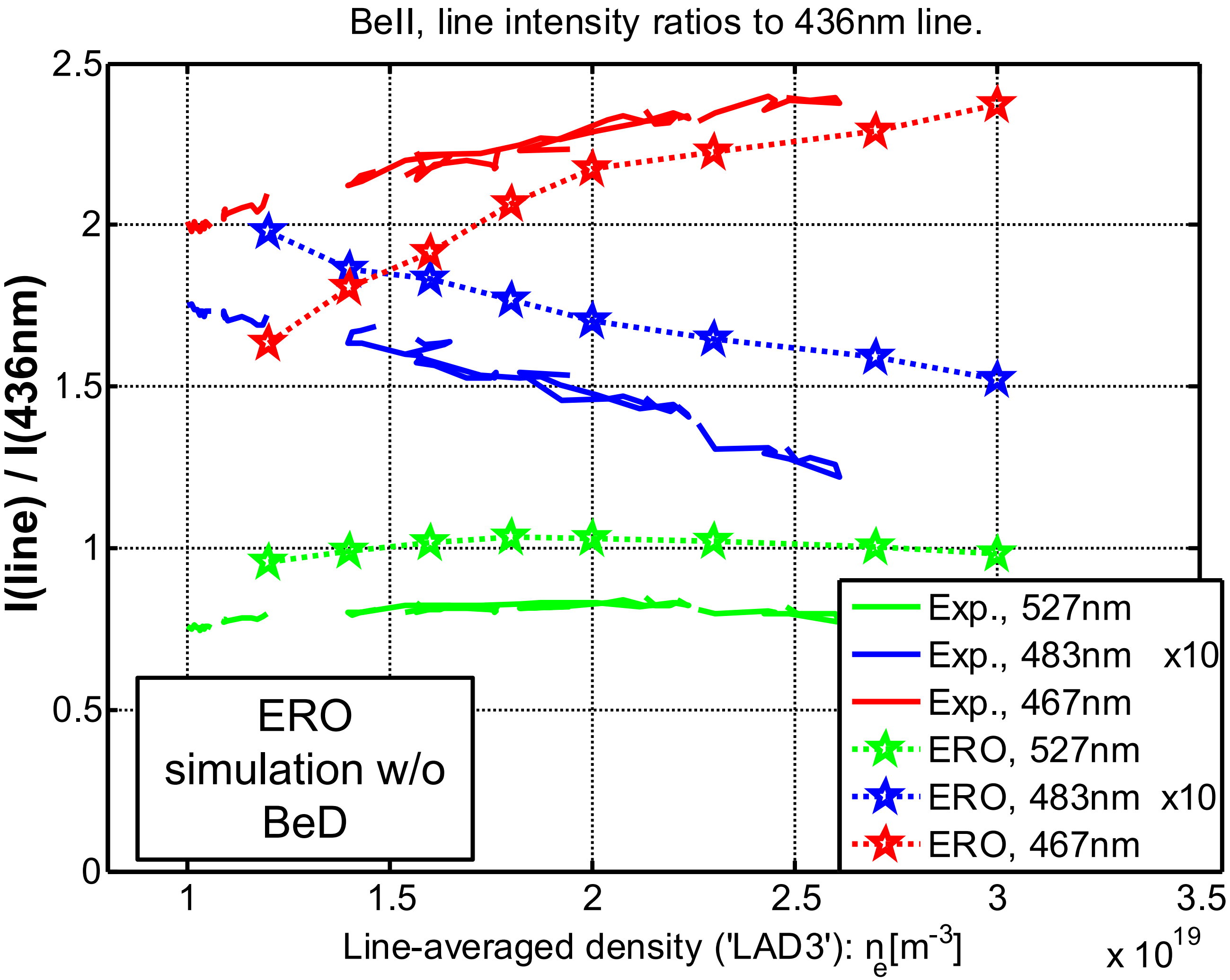
D spectroscopy and recycling flux



- Right shape!
- Right line ratio!
- Very close absolute values!

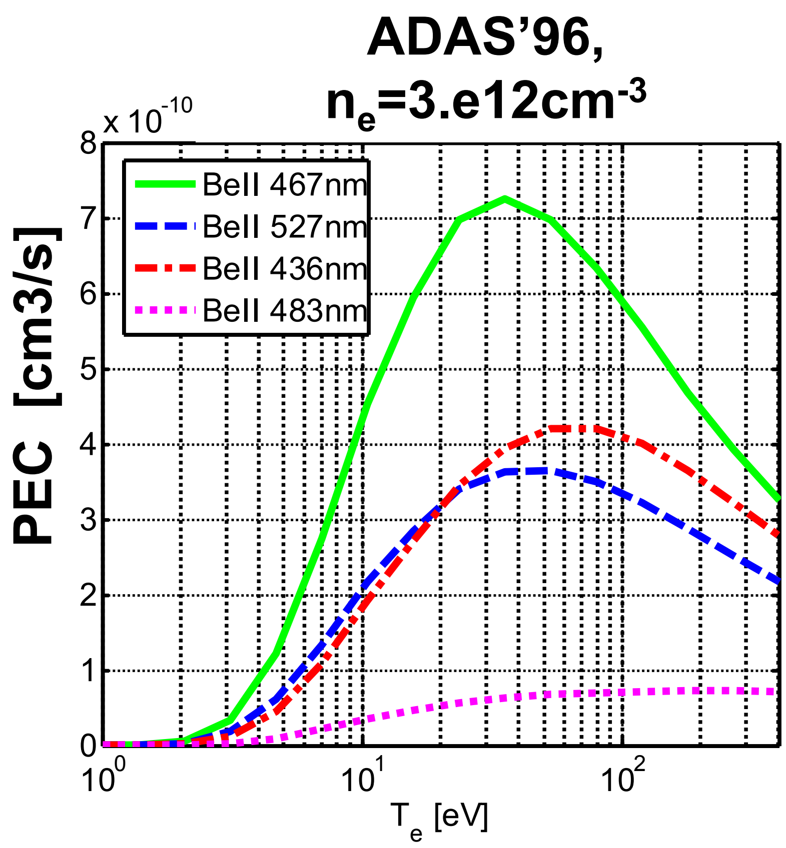
T_e ← Density scan in limiter plasmas → n_e

Line ratios in BeII



T_e ← Density scan in limiter plasmas → n_e

ERO reproduces (all 3!) ratios within 25%.

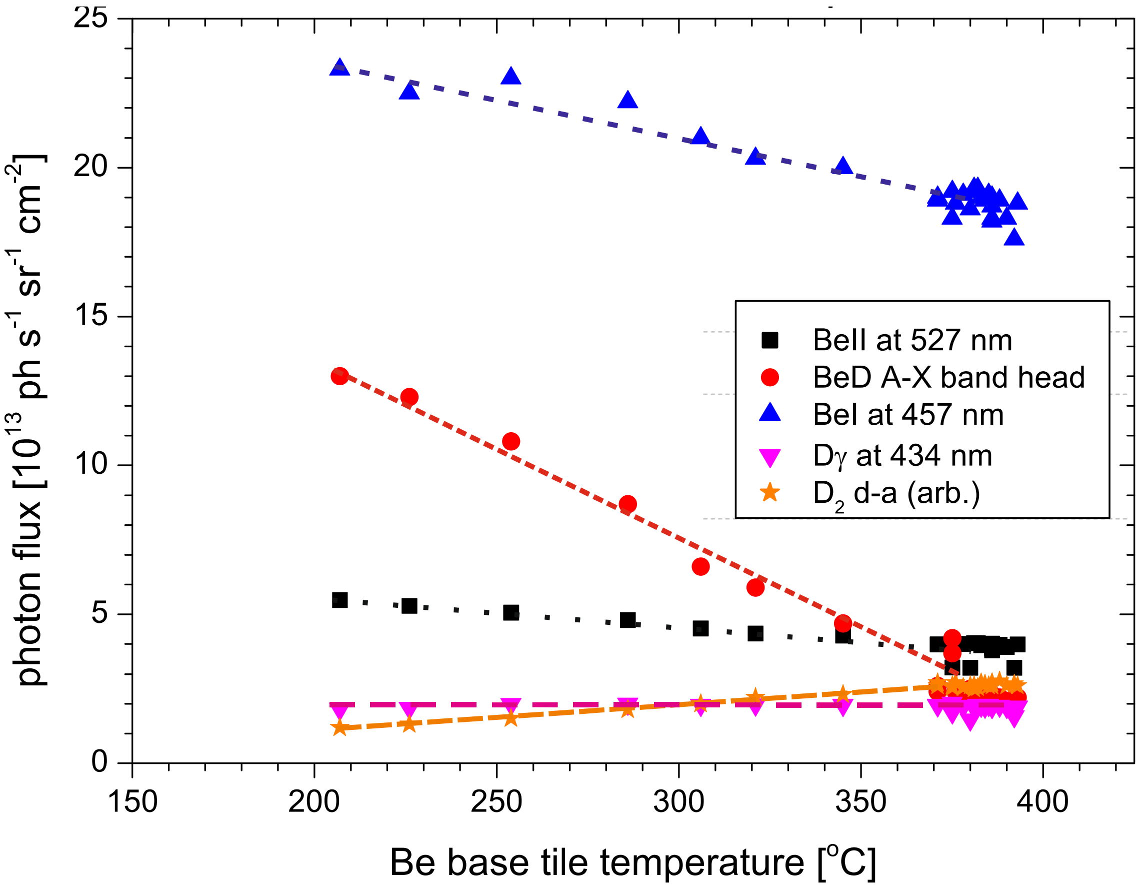


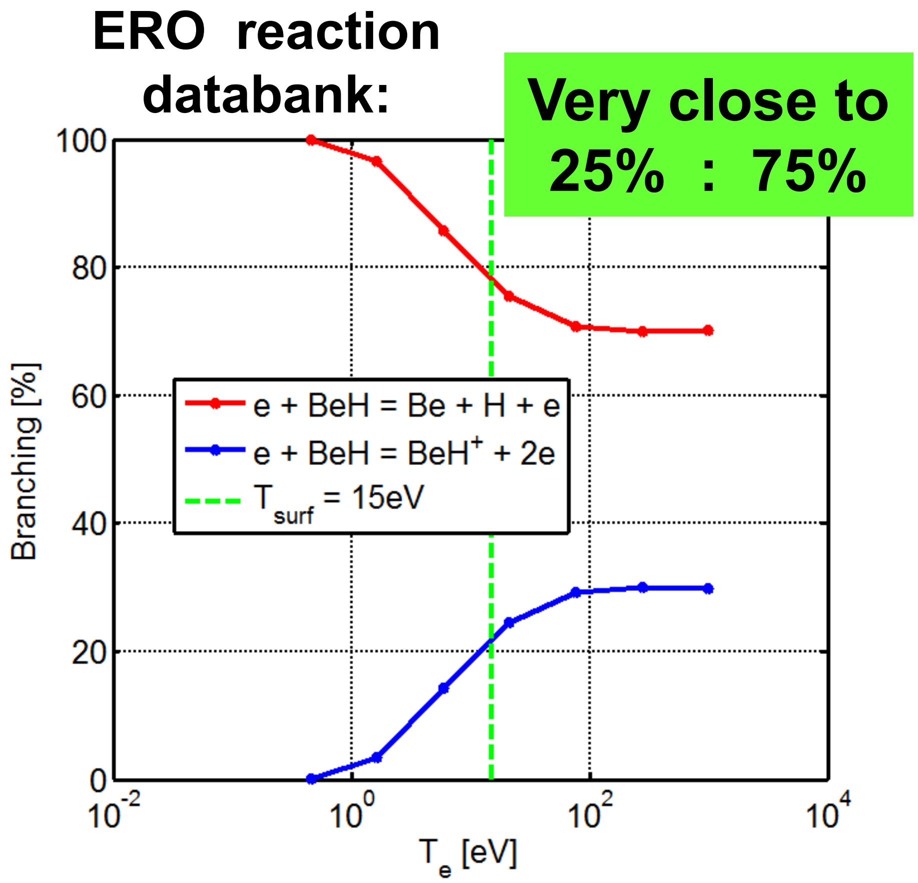
- *Measurement error(s)?..*
- *ADAS PEC uncertainties?..*
- *Be released as BeD penetrates deeper into the plasma . . .*

T_{surf} scan: spectroscopic observations

Spectroscopic observation under otherwise constant plasma conditions:

- Reduction of BeI, BeII and BeD photon flux with increase of surface temperature



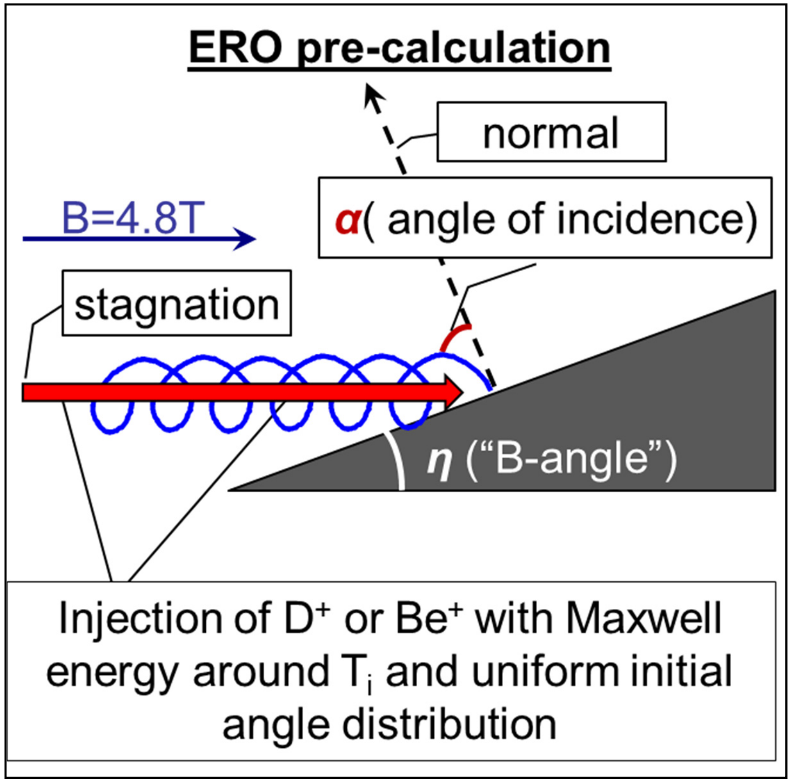


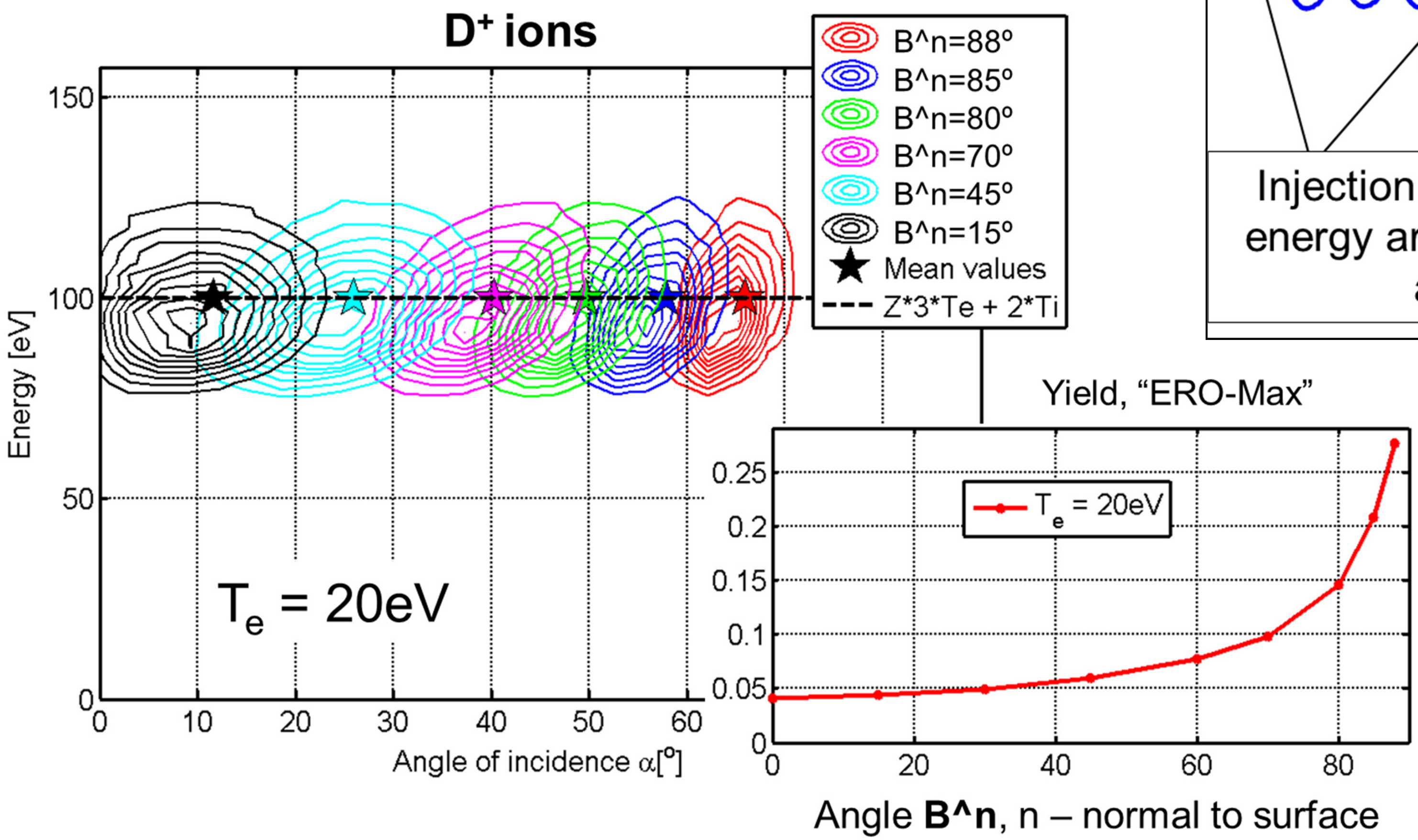
- Comparison of BeD A-X band, BeI and BeII provides information on dissociation path
  - Dominant path BeD + e ->Be + D + e (75%) over BeD + e-> BeD^+ + 2e (25%)

Treating angular part of a sputtering yield

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

Preliminary ERO runs . . .
"Integration" produces
effective sputter yields:



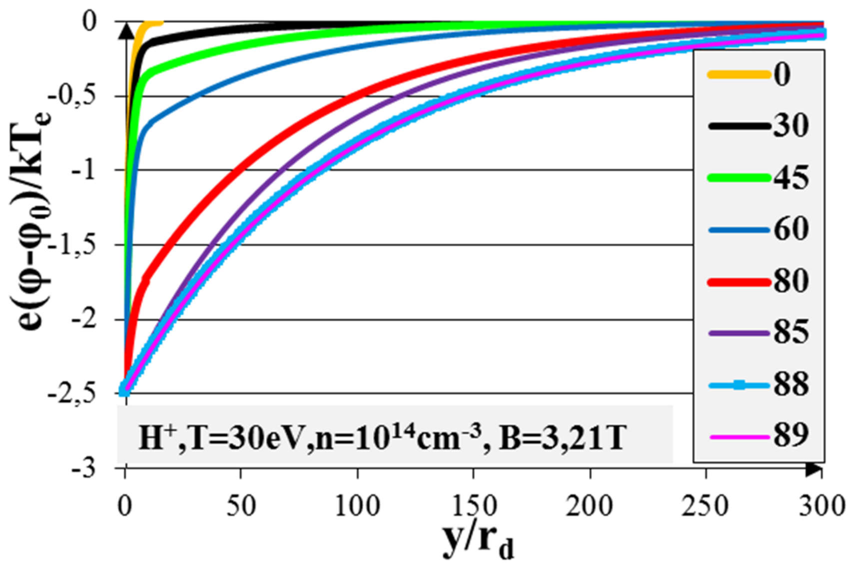


Very recent: analytic solution

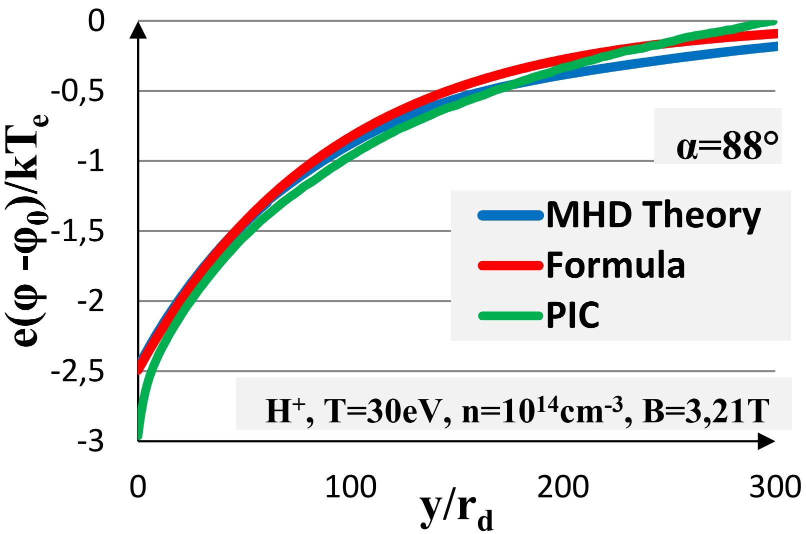
I.Borodkina et al., PET-2015, submitted to CPP

Analytical approach

1) Sheath potential

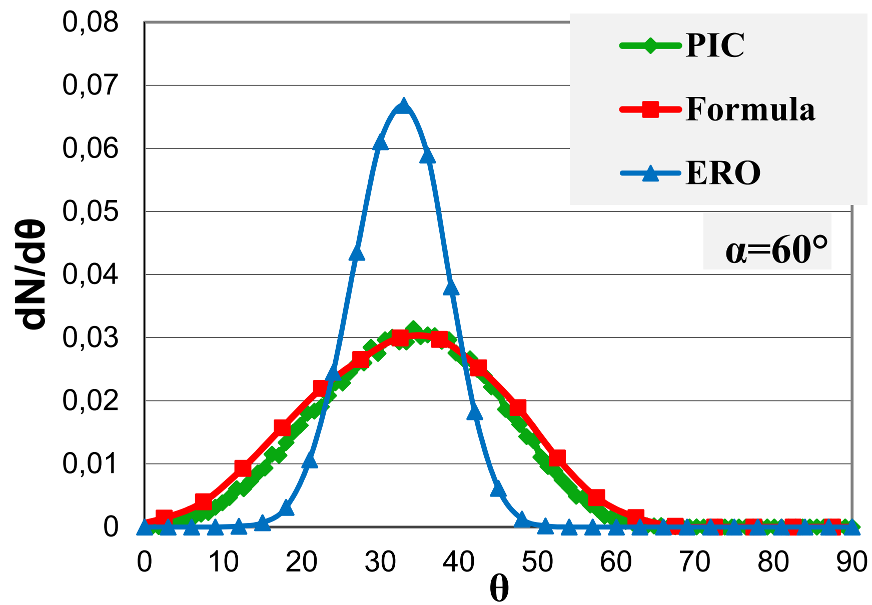


The expression benchmarked with another analytics and



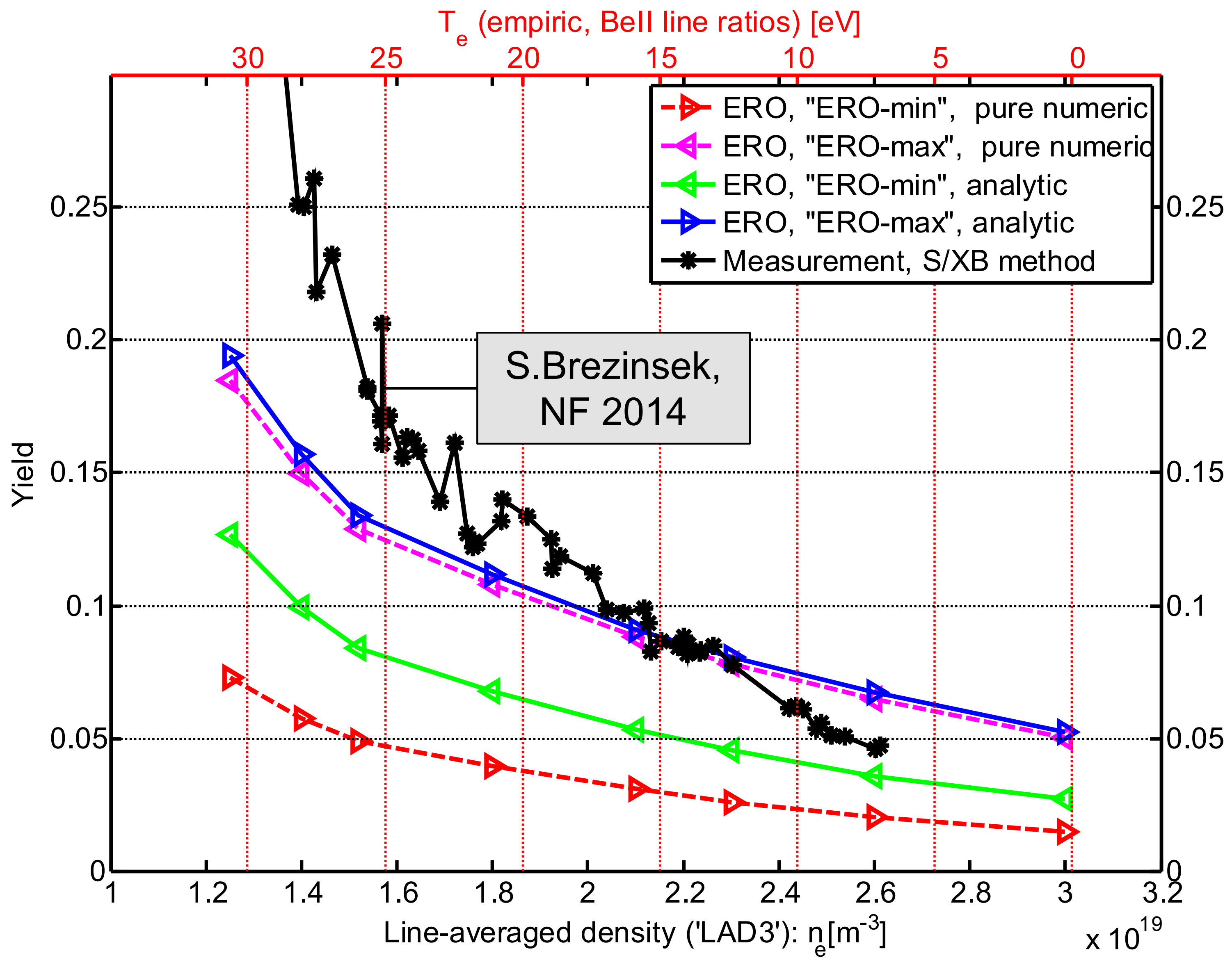
2) Formula for velocity at the part of trajectory just before the impact

- *Energy distribution on impact is somewhat more peaked than ERO one.*
- *Angular distribution in ERO pre-runs seems to be clearly too peaked:*



- ***Analytic result is in a good agreement with various PIC simulations***
- ***On the other hand, ERO can follow ion thermalization with plasma . . .***

S/XB approach – plasma density scan



T_e ← Density scan in limiter plasmas → n_e

Corrections from analytical approach:

+10% for 'ERO-max'

+30% for 'ERO-min'

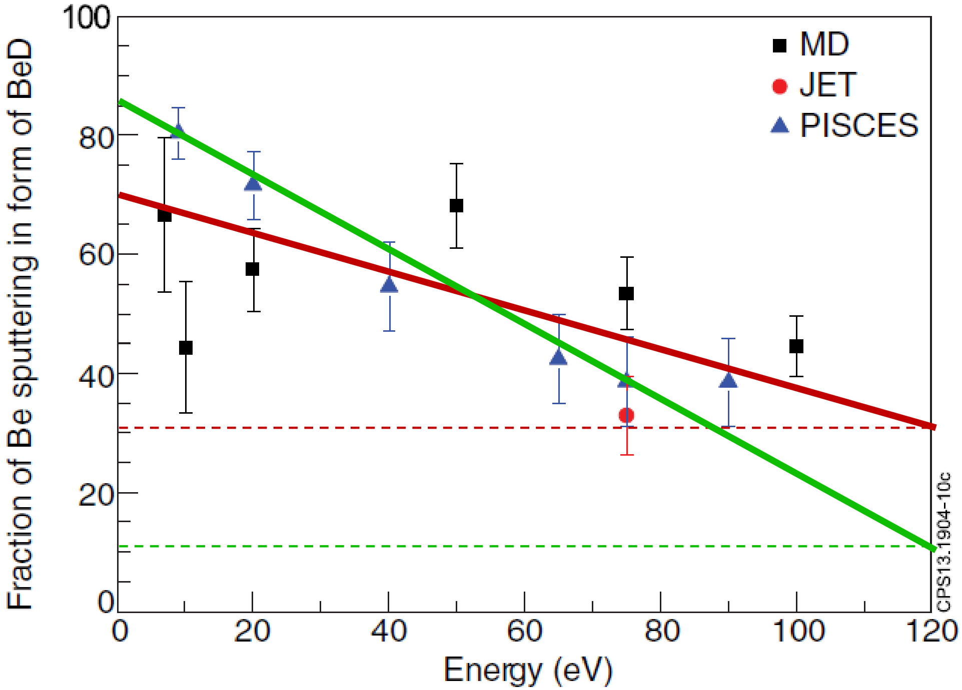
Dedicated experiment for testing erosion:
limiter plasmas shifted towards "our" inner wall guard limiter

→ Enormous Be erosion

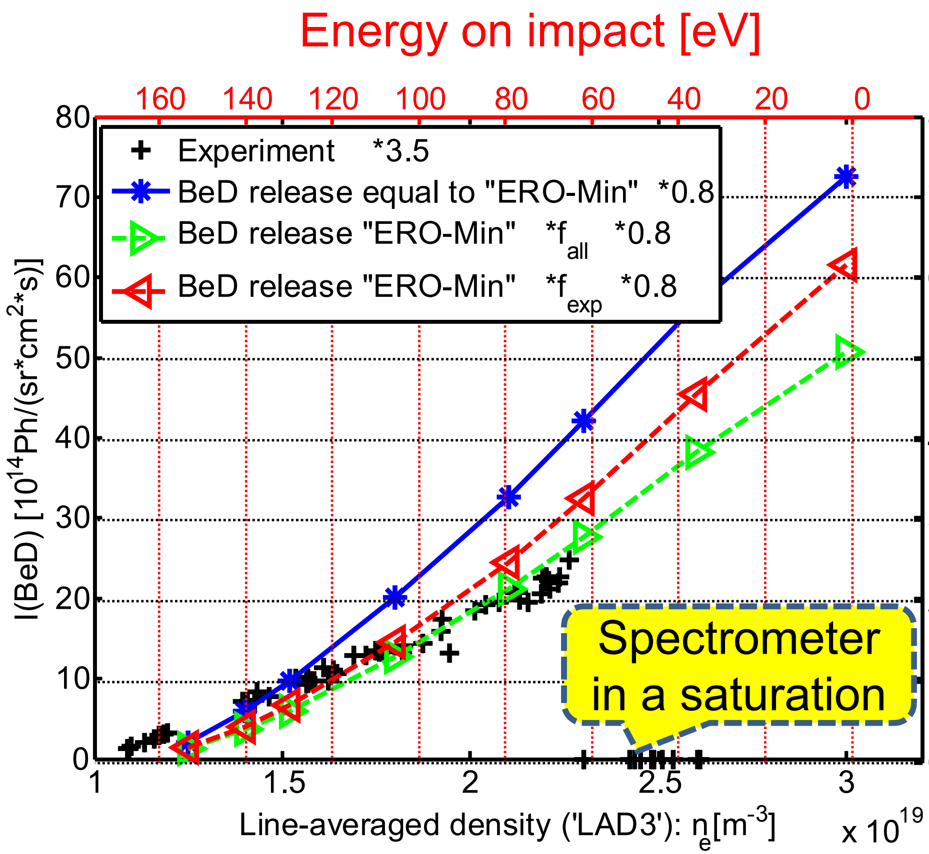
→ Enormous Z-effective

BeD fraction (density scan)

$f_{all}(BeD) = 70 - 40/120 \cdot E_{imp}$ [eV]
$f_{exp}(BeD) = 85 - 75/120 \cdot E_{imp}$ [eV]



S.Brezinsek et.al, Nucl. Fusion 54 (2014) 103001



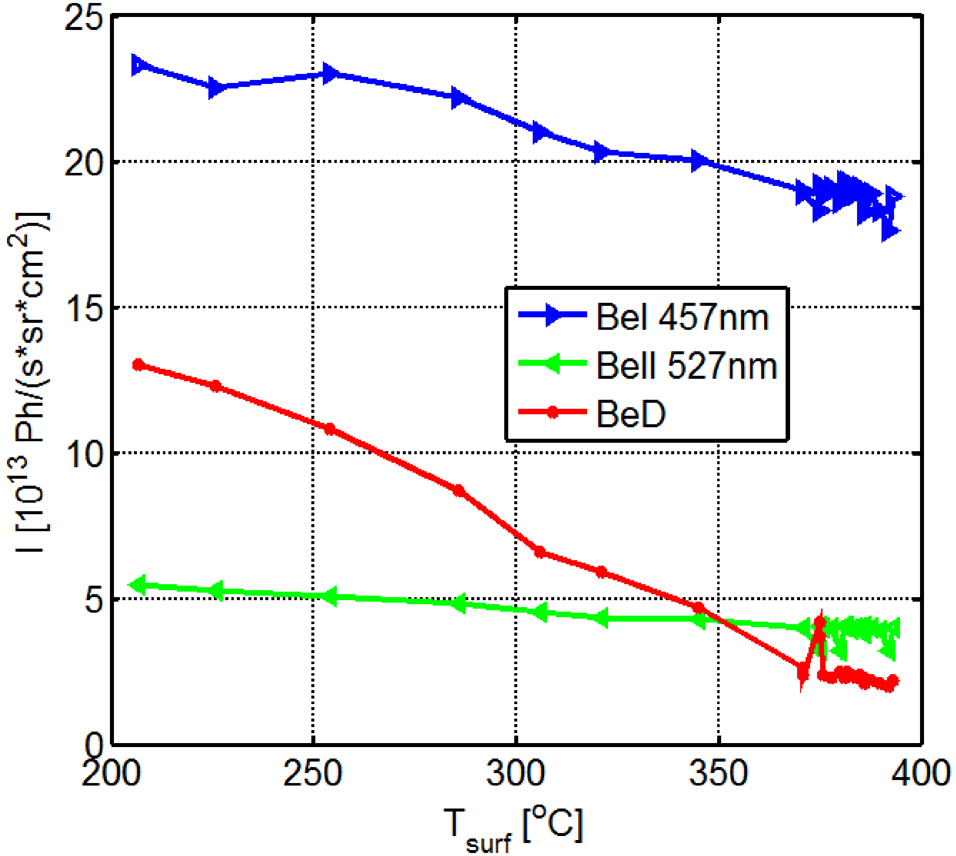
T_e ← Density scan in limiter plasmas → n_e

BeD fraction from experiments at JET, PISCES and earlier MD modelling

- **The shape is nearly reproduced.**
- **The absolute value within 20%**

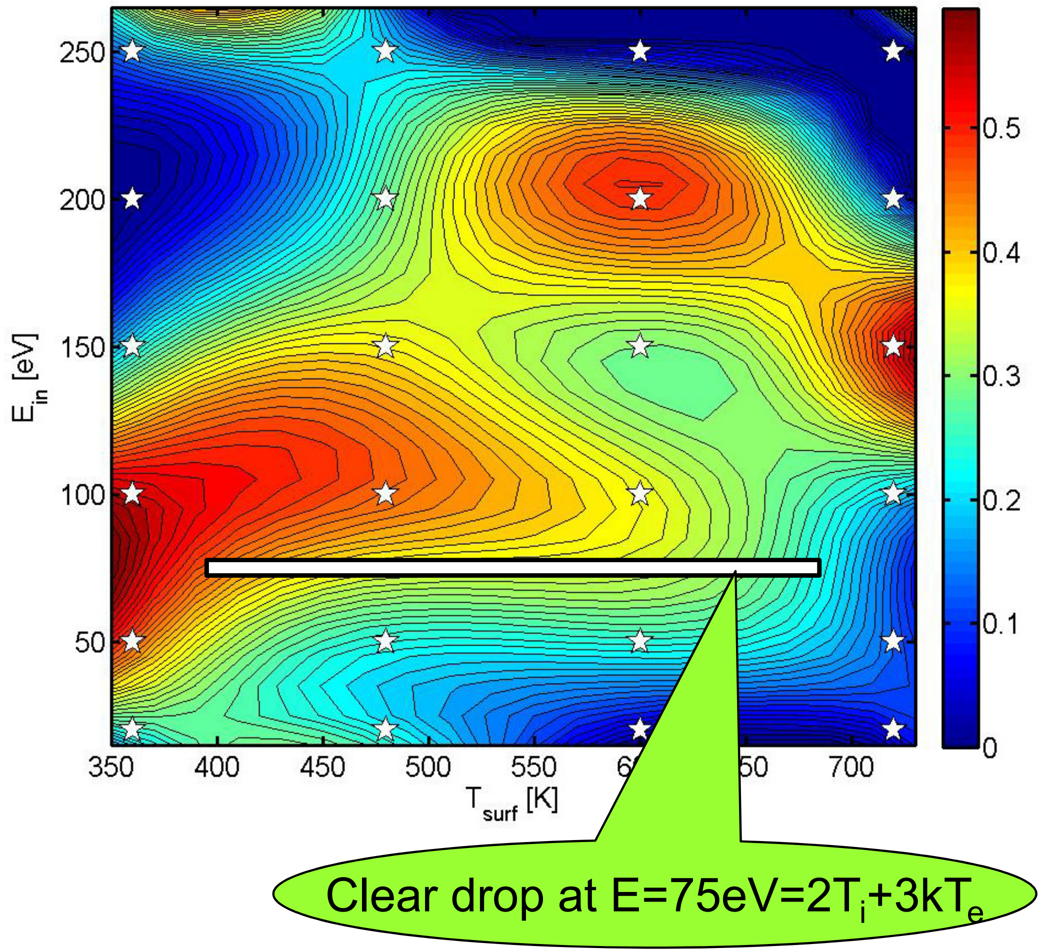
BeD release – T_{surf} scan

JET ILW surface density scan



Surface temperature scan

BeD/Be released (MD)



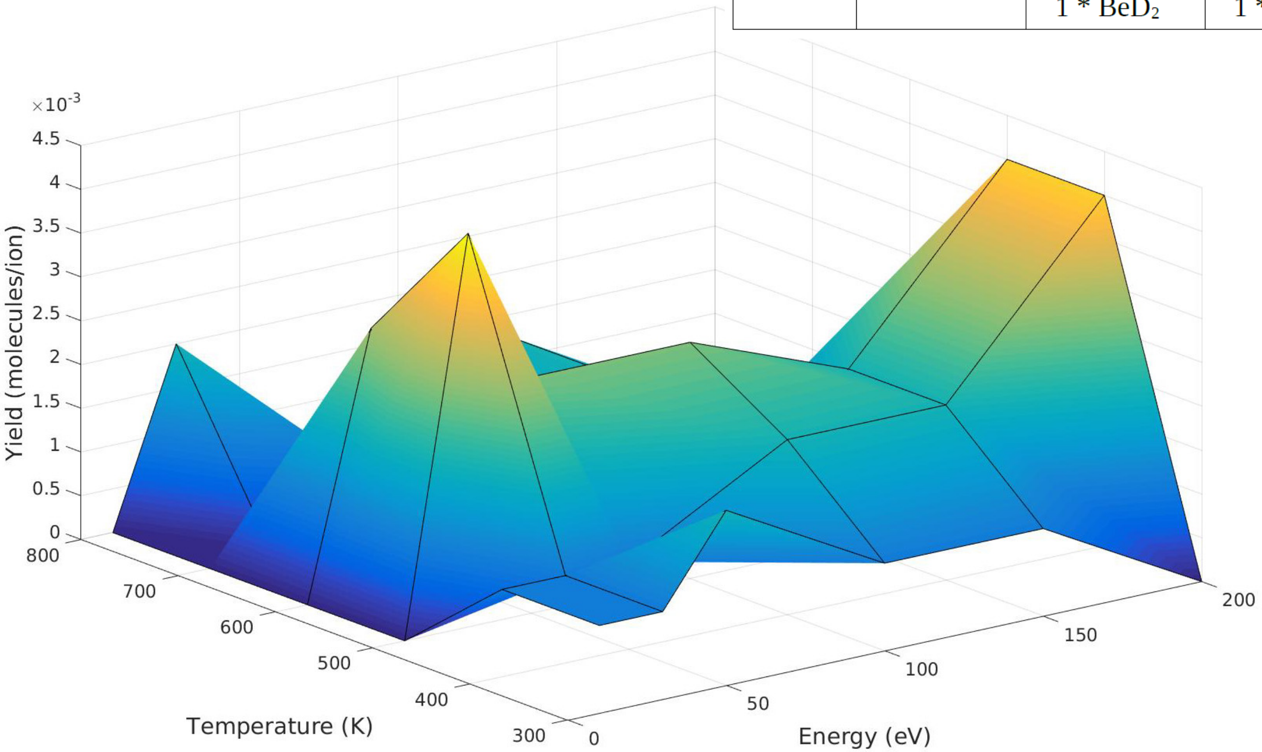
MD simulations for BeDx are really CPU-time consuming. MD strongly overestimates ion flux and hence D diffusion. KMC simulations of D deposition diffusion at realistic fluxes currently underway . . . **For now we can do ERO simulations using empiric data.**

BeD_x release – MD with KMC

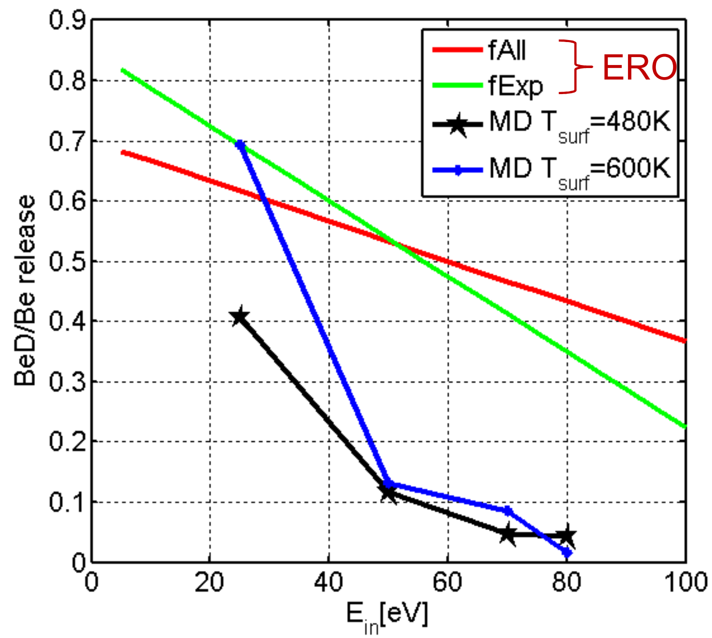
Simulations by E.Safi, MD cumulative + KMC, status 22.04.2016

MD simulations will demand more time . . .

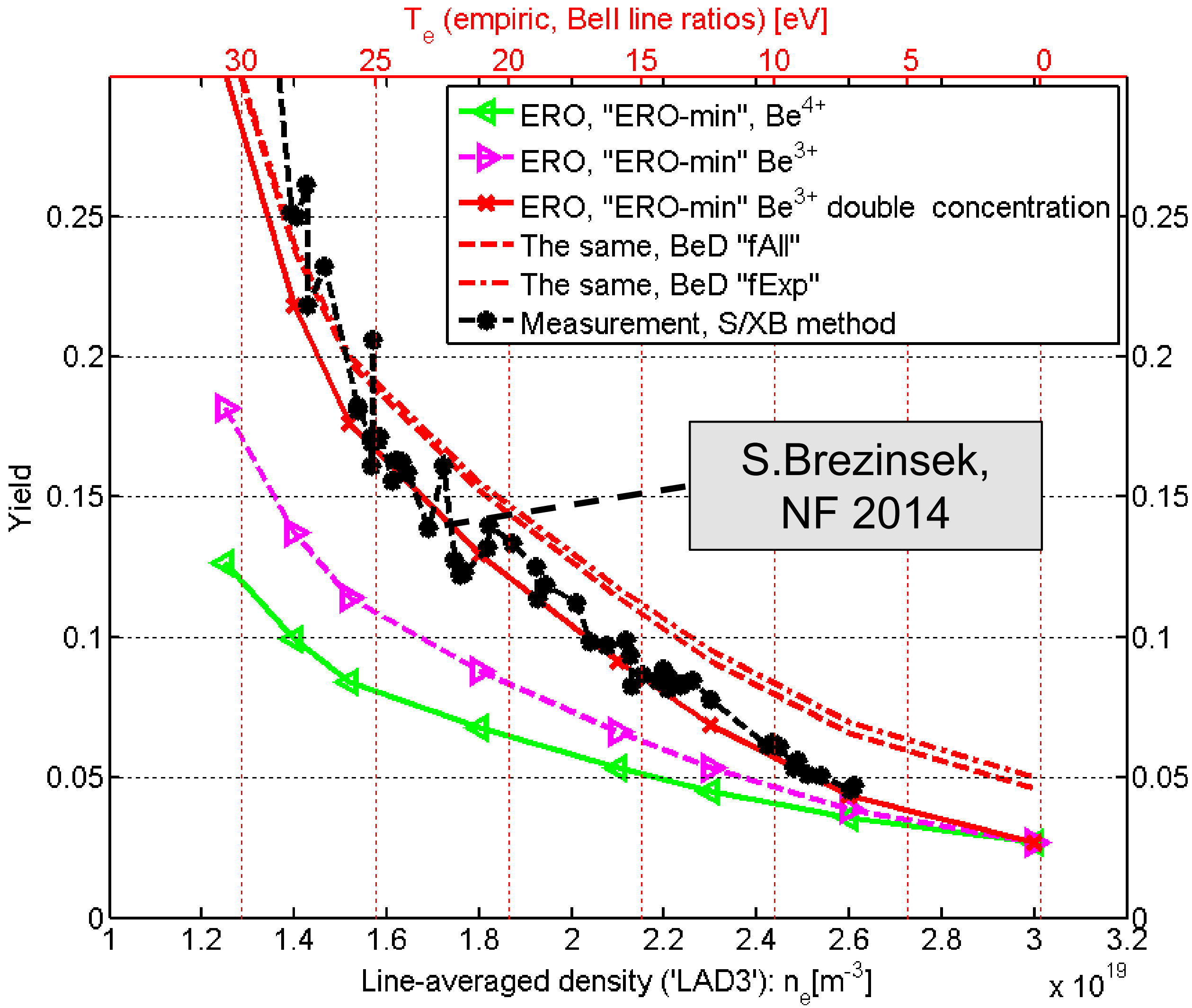
	300K	400K	500K	600K	700K	800K
10 eV	1 * BeD_2	1 * BeD_2	-	-	-	-
30 eV	1 * BeD	1 * BeD	5 * BeD	3 * BeD	-	2 * BeD
50 eV	2 * BeD	1 * BeD	3 * BeD	1 * BeD	1 * BeD	-
100 eV	1 * BeD	2 * BeD	3 * BeD	2 * BeD	2 * BeD	-
150 eV	1 * BeD	2 * BeD_2	2 * BeD	1 * BeD	-	-
200 eV	-	4 * BeD 1 * BeD_2	4 * BeD 1 * BeD_2	-	-	-



Alternative MD simulations by I.Sukuba (non-cumulative)



S/XB approach – Be plasma impurity



T_e ← Density scan in limiter plasmas → n_e

$$Y_{total} = Y_{Be \leftarrow D} * (1 - f_{Be}) + Y_{Be \leftarrow Be} * (f_{Be})$$

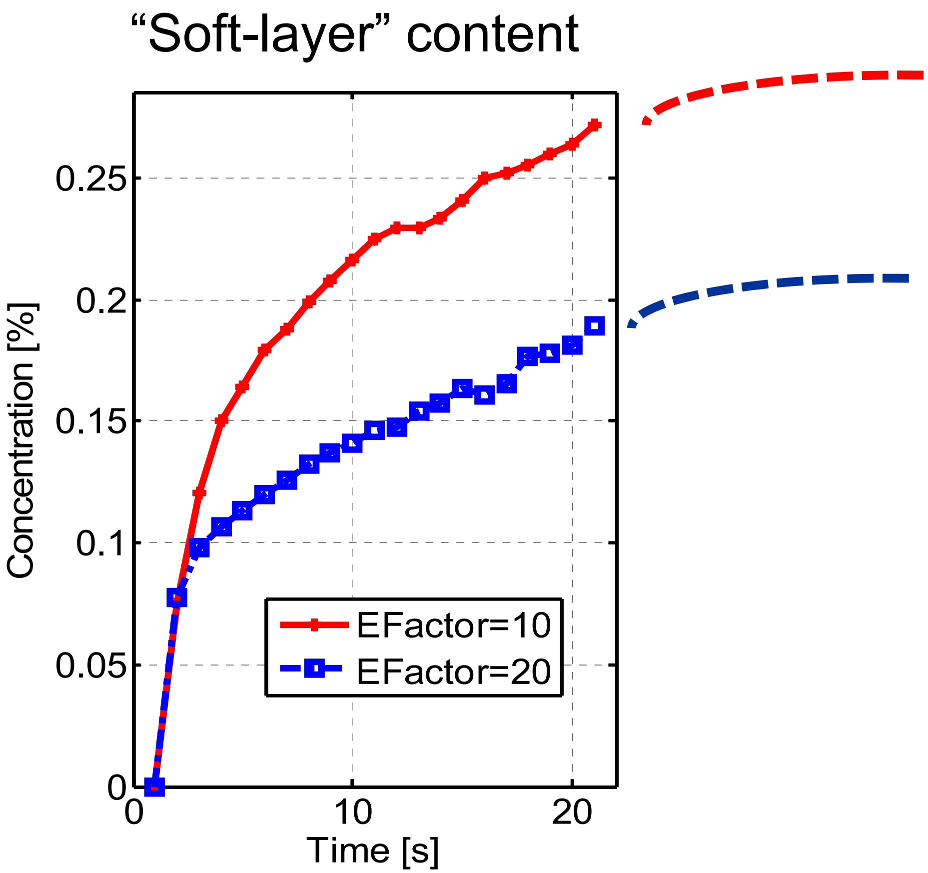
Intrinsic Be concentrations f_{Be} determined from Z_{eff}

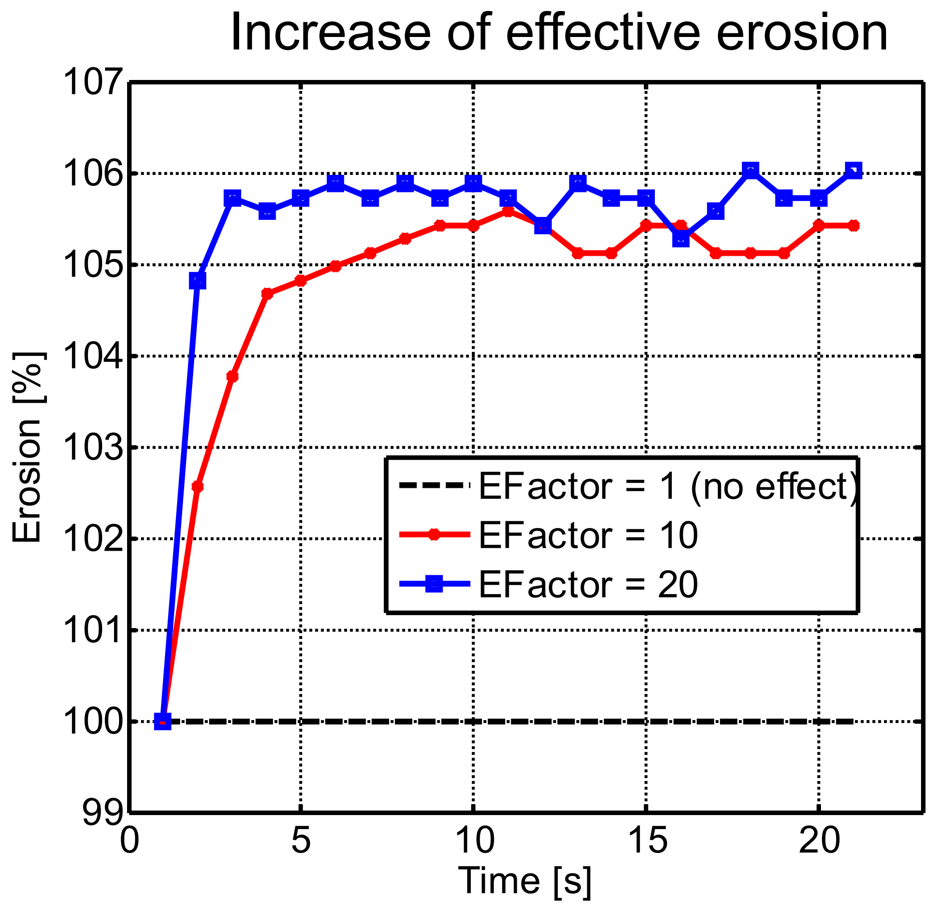
T_e in the active light emmission zone is detemined from the Bell line ratios

BeD effect is within errorbars

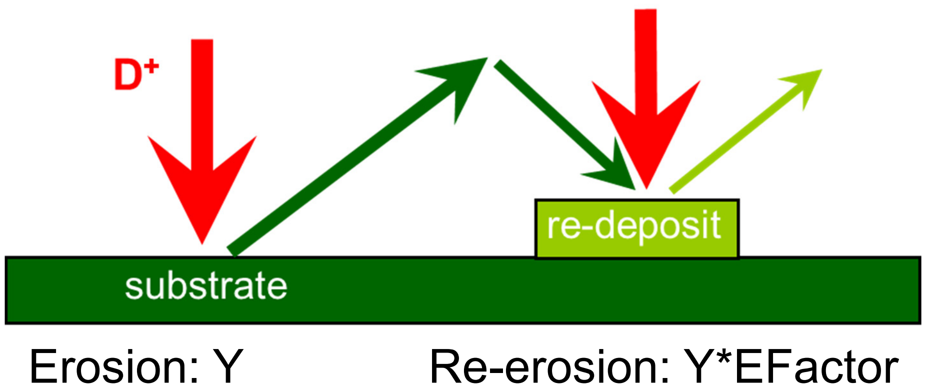
'ERO-min' for Be←D sputtering agrees with experiment!

Enhanced re-erosion



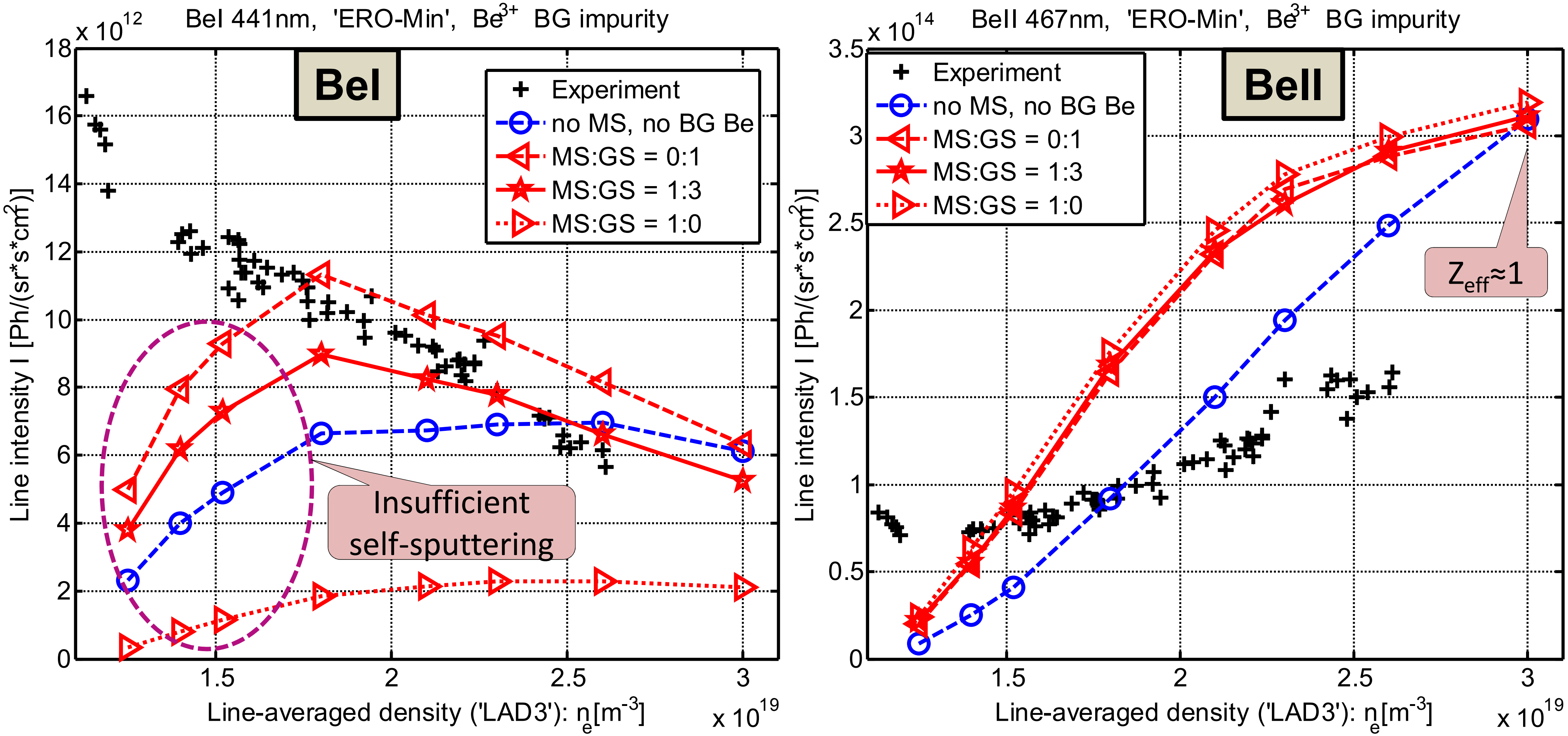


Why so small effect?
Erosion zone + low re-deposion efficiency.



EFactor independent <10% increase of erosion
This is fully within our uncertainties . . .

ERO synthetic emission in the chord



T_e ← Density scan in limiter plasmas → n_e

1. **Self-sputtering assumptions in ERO at low densities are insufficient**
2. **Initial MS population after sputtering is of importance for BeI, but has no effect for BeII**
3. **Absolute values are within a factor of 2, however BeI to BeII ratio is wrong.**

In these ERO simulations Be-D was not included . . .

Main points (IW JET limiter)

1. **The modeling of Be erosion at JET ILW (IW tile, limiter plasmas) was revisited.**
   - ✓ *The new **analytical solution for angles and energies on impact** lead to increasing of effective yield by 10-30%.*
   - ✓ ***Corrected plasma parameters** (T_e based on embedded probes data) lead to a better agreement for line ratios in BeII, branching in BeD decay reactions etc.*
   - ✓ *Even 20 times **enhanced re-erosion** leads to a **negligible** effect below 10%.*
   - ✓ *Initial **MS population** is of importance for BeI, but there are no means to determine it.*
   - ✓ ***BeD light intensity trend** by density scan **reproduced**. Absolute value within 20%.*

2. **JET ILW: "ERO-min" physical sputtering assumption (Eckstein's 2007 fit) is confirmed (BeII passive spectroscopy) to suit well for the plasma-wetted areas with high D content in the interaction layer. Treatment of angle and energy distributions on impact is provided.**

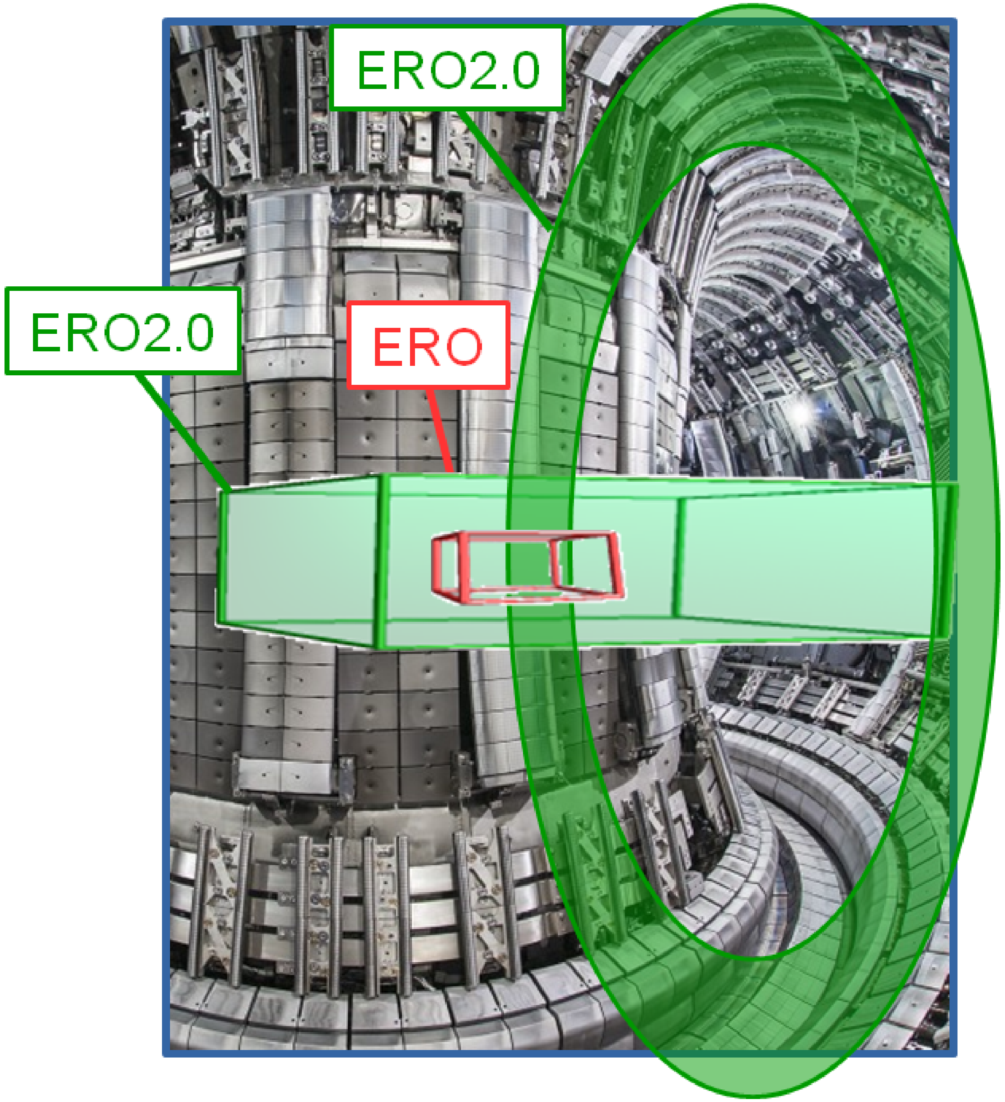
3. **ERO predictions for ITER with "ERO-min" (4200 discharges critical BM life time) can be used as a basis. One should: 1) improve treatment of Be self-sputtering and shadowing (PFCFlux); 2) consider the influence of the Be-D release and updated BM shaping.**

4. **New experiments and further ERO benchmark are necessary (scheduled to 25.07).**

5. **Plasma parameter from SOLEDGE2D-EIRENE ongoing (H.Bufferand).**

From ERO1.0 to ERO2.0: volume

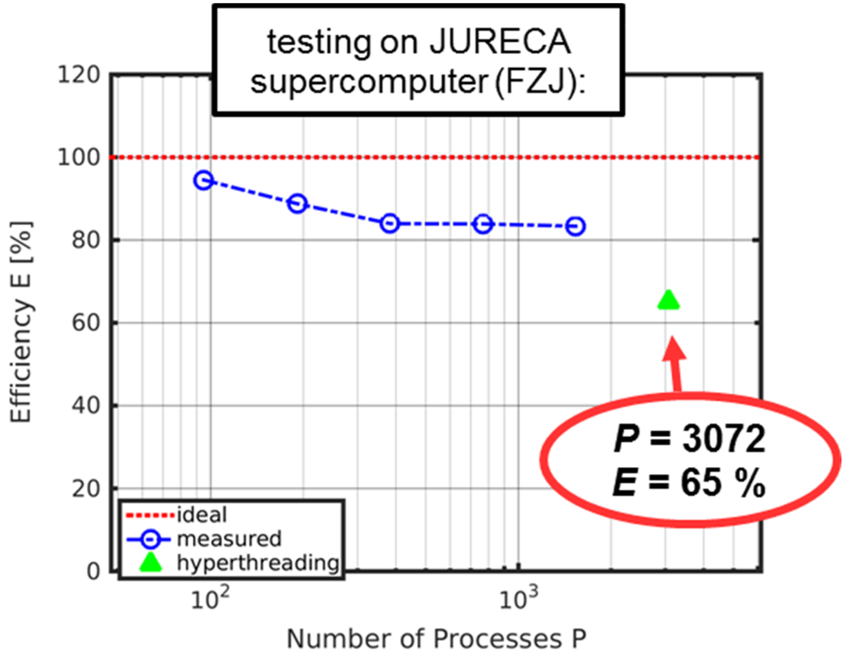
JET's Iter-like Wall



J.Romazanov et al., DPG-2016

The limits of ERO1.0

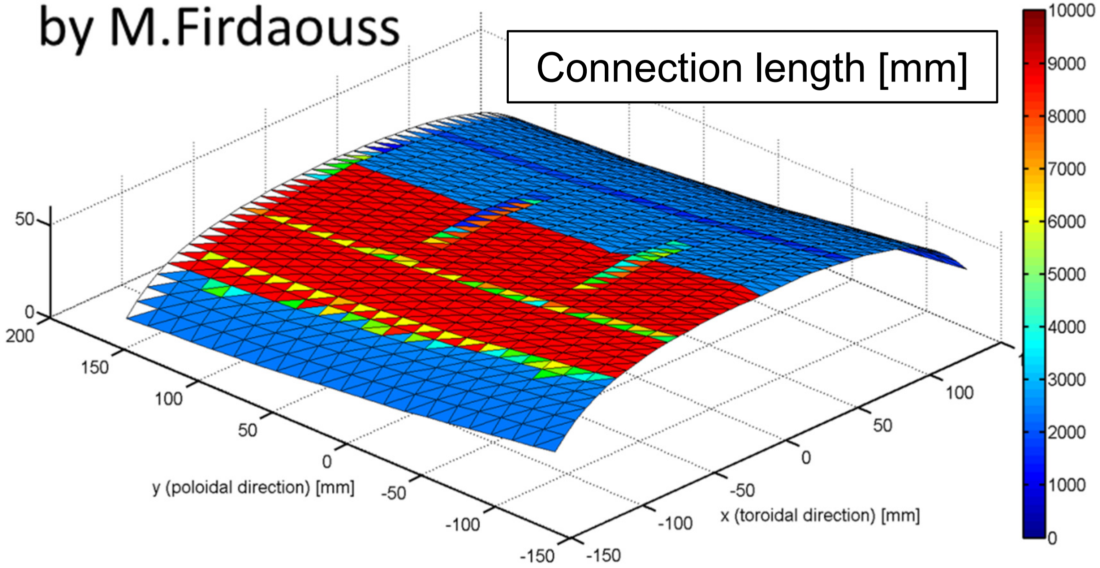
- small simulation volumes of ~(10 cm)³
- typically covering a single PFC part

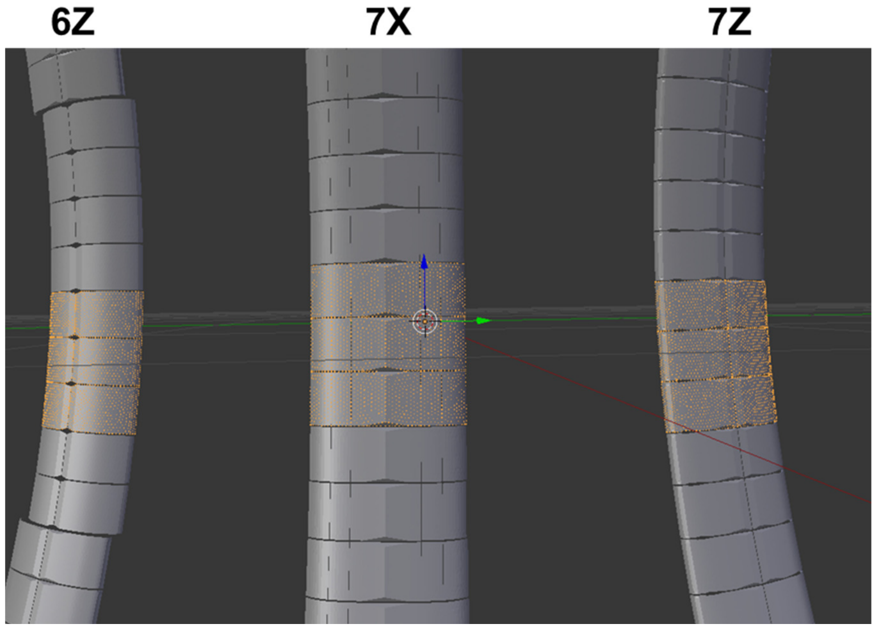


on **3072** processes we can simulate 3072 x 0.65 ≈ **2000** more particles without increase of wall clock time

From ERO1.0 to ERO2.0: shadowing

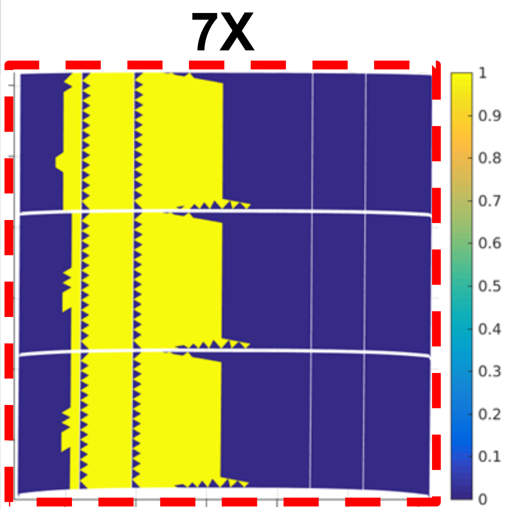
PFCFLUX simulations
by M.Firdaouss

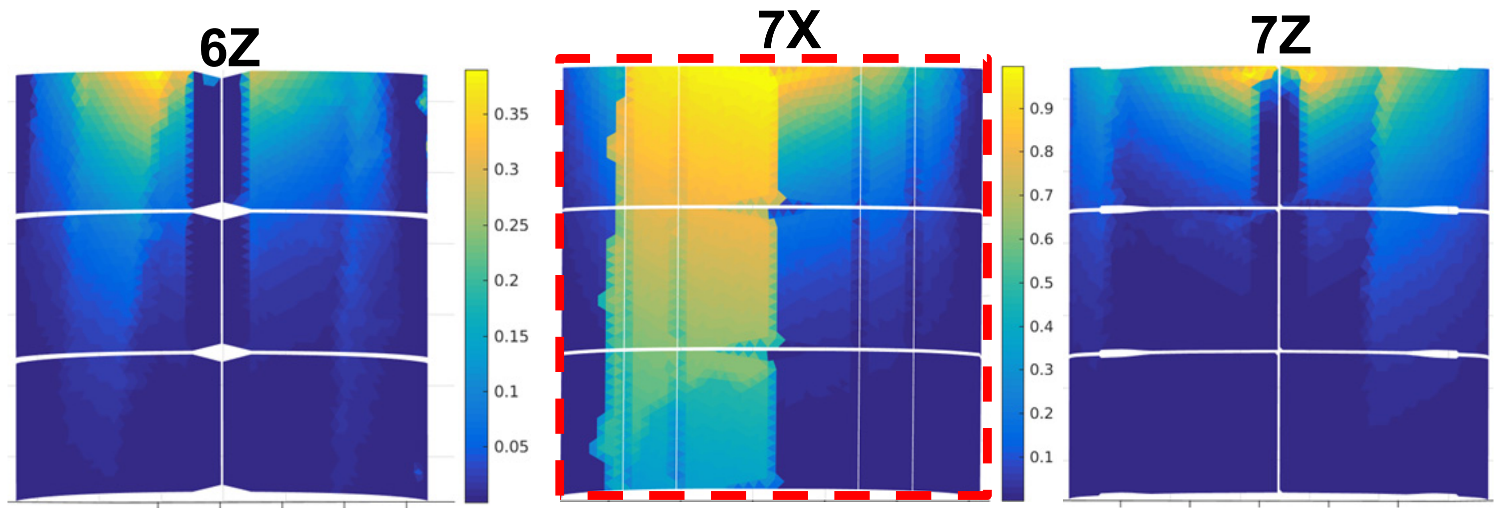




ERO1.0 | **ERO2.0**

J.Romazanov et al., EPS-2016

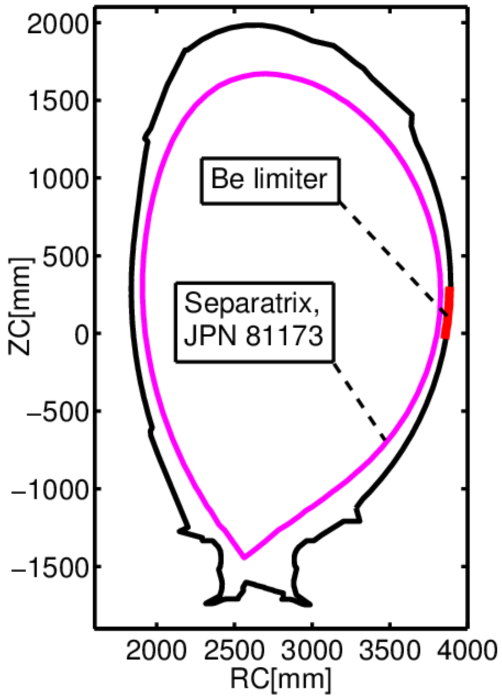


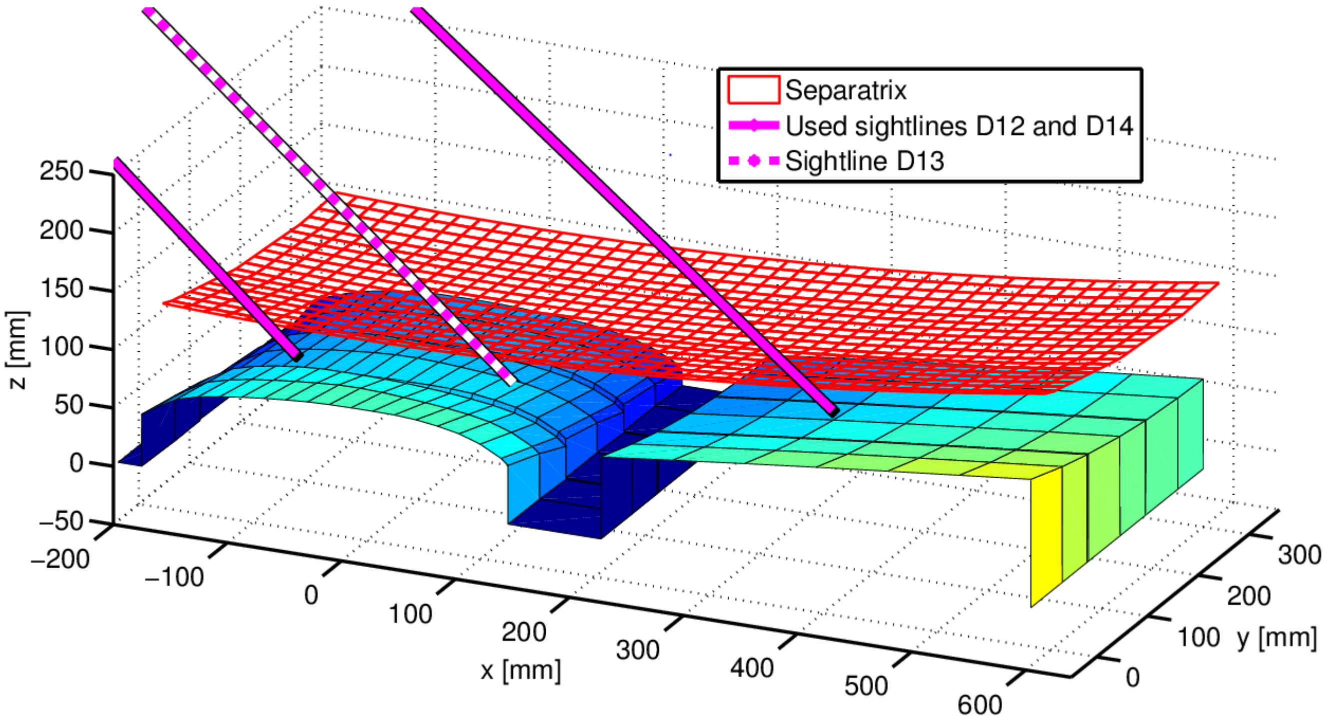


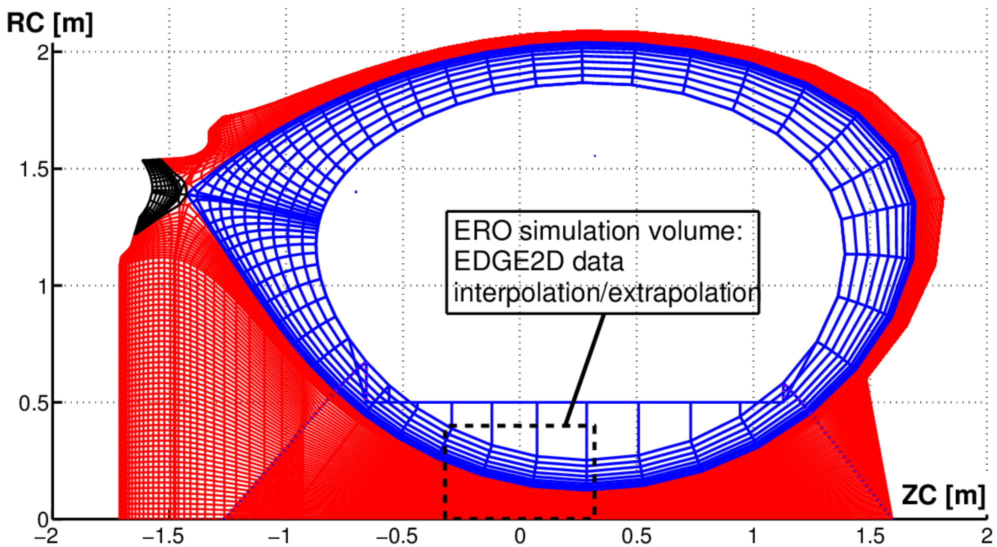
Benchmark at JET ITER-like wall, OW Be limiter near ICRH antenna

7 papers at PFMC-2015, APS-2015, PSI-2016 by
Ch.Klepper, I.Borodikina, A.Lasa, V.Bobkov, D. Borodin.

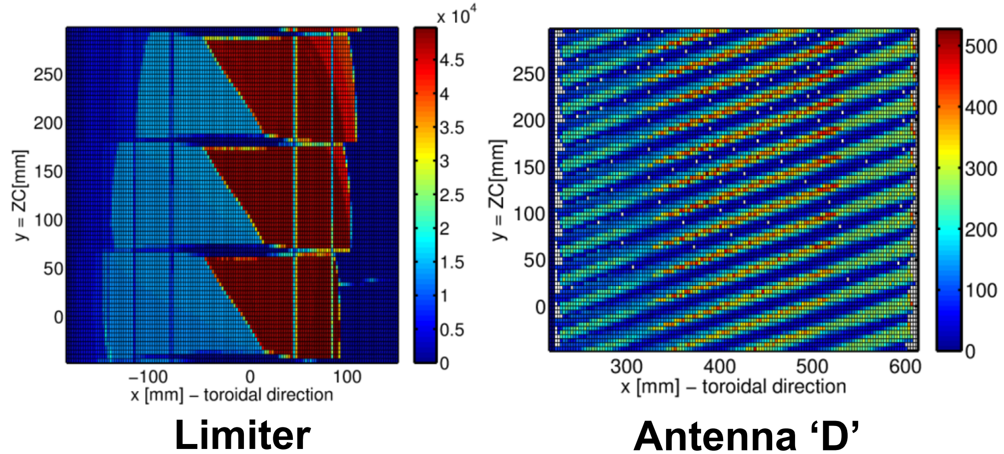
Be erosion near ICRH antena



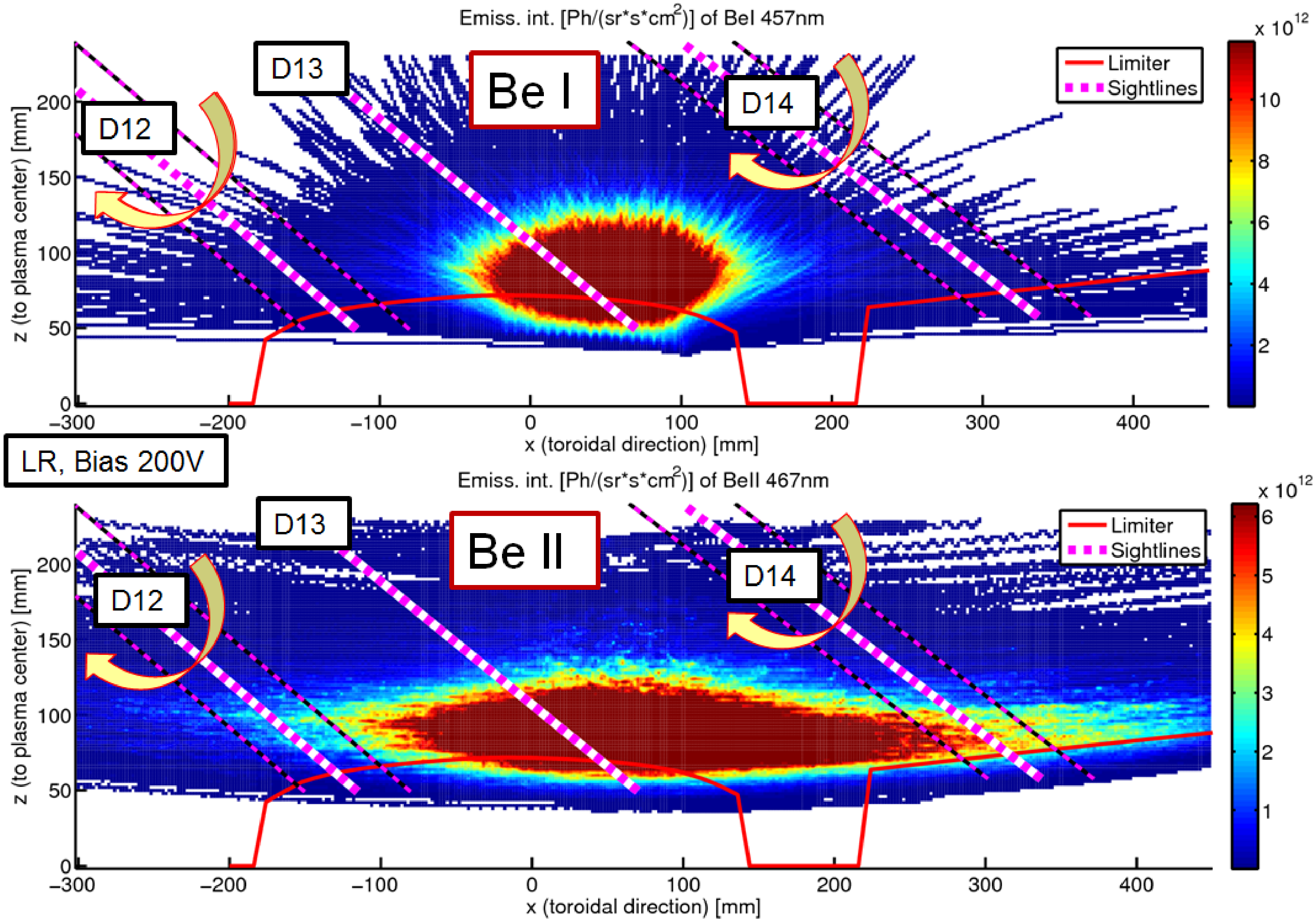




PFCFlux code shadowing:



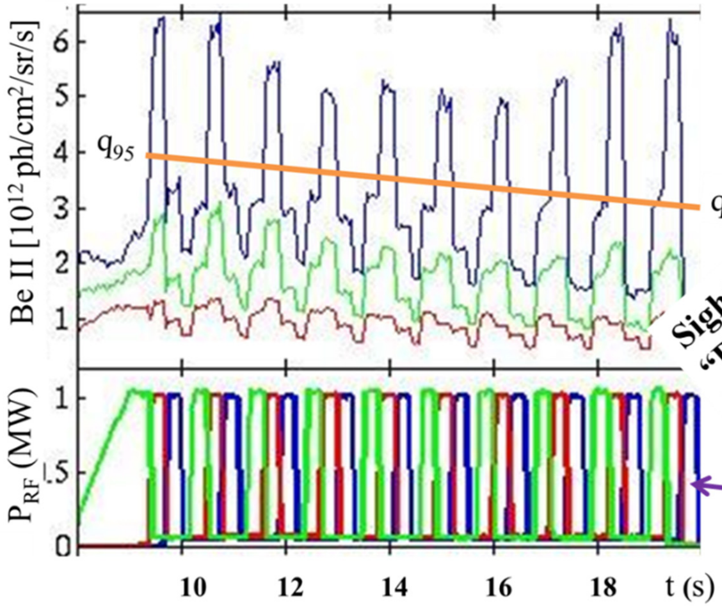
Be erosion near ICRH antena – ERO side view

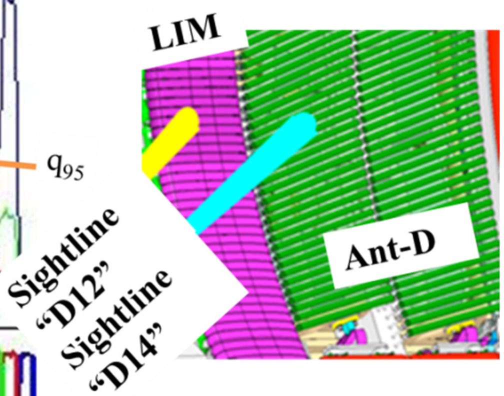


The fractions of BeI and BeII light comming into D13 and D14 sight lines depends on plasma parameters, plasma flow, shadowing pattern and multiple other factors.

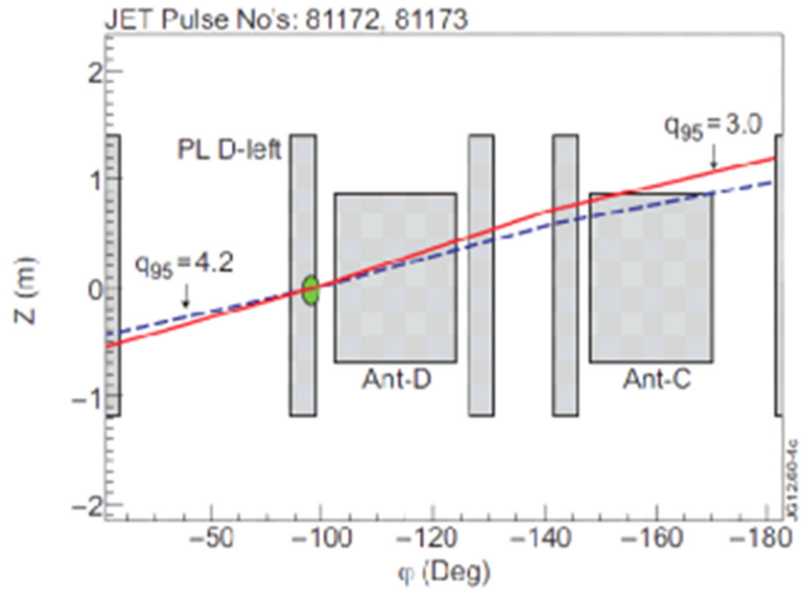
Be erosion near ICRH antena – ERO side view

Antenna sightlines (~ tangential)
"D14" passes by antenna side of limiter
"D12" views side of limiter away from antenna
"Background" (far left of LIM, antenna-free region)





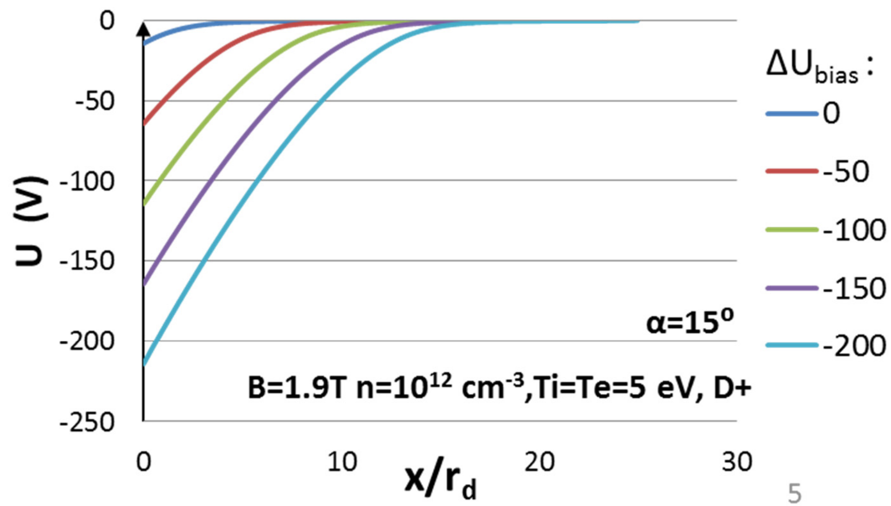
Antenna Toggling
Ant-D ---------
Ant-C ---------
Ant-A&B -----------



*P. Jacquet et al., Physics of Plasmas (1994-present) 21, 061510 (2014); doi: 10.1063/1.4884354

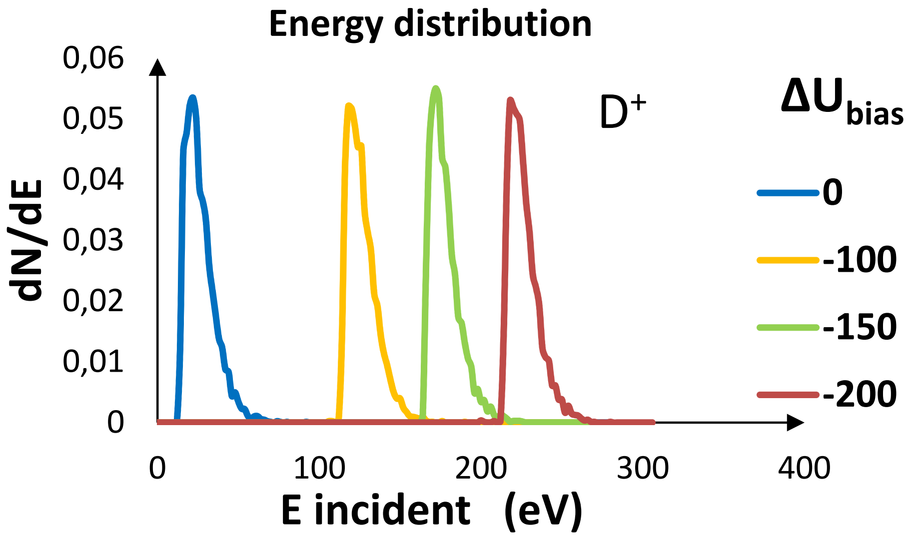
Enhanced erosion of Be limiter correlates with Antenna C toggling. Emission increases by **factor of 2-3.**

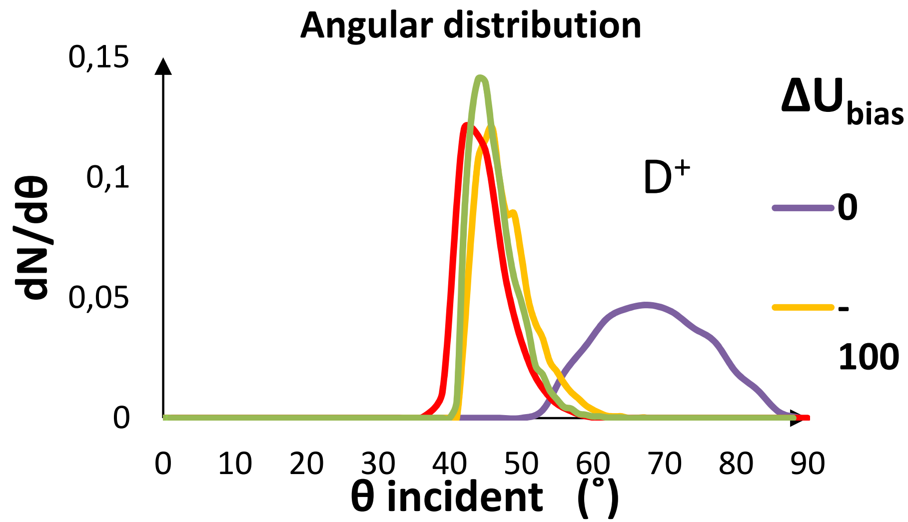
- The effect can be reproduced through addiitional surface biasing of ~200V.
- The analytical model of I.Borodkina for the sheath E-field and imapct angle and energy distributions is refined to include biasing

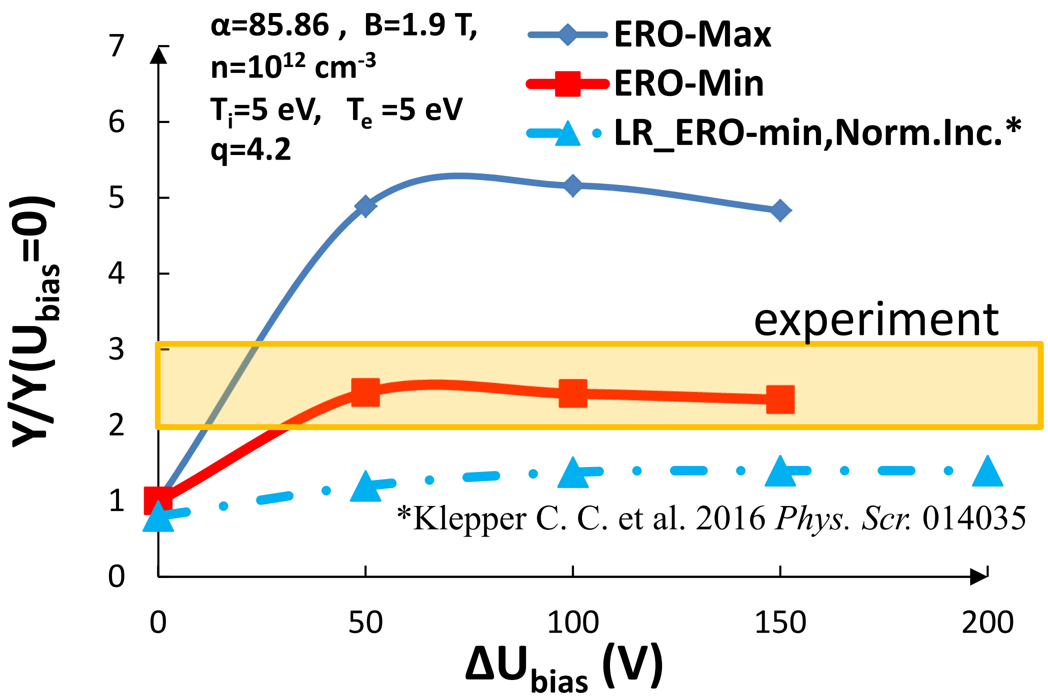


5

Effective yields from analytical model: biasing (RF) effect





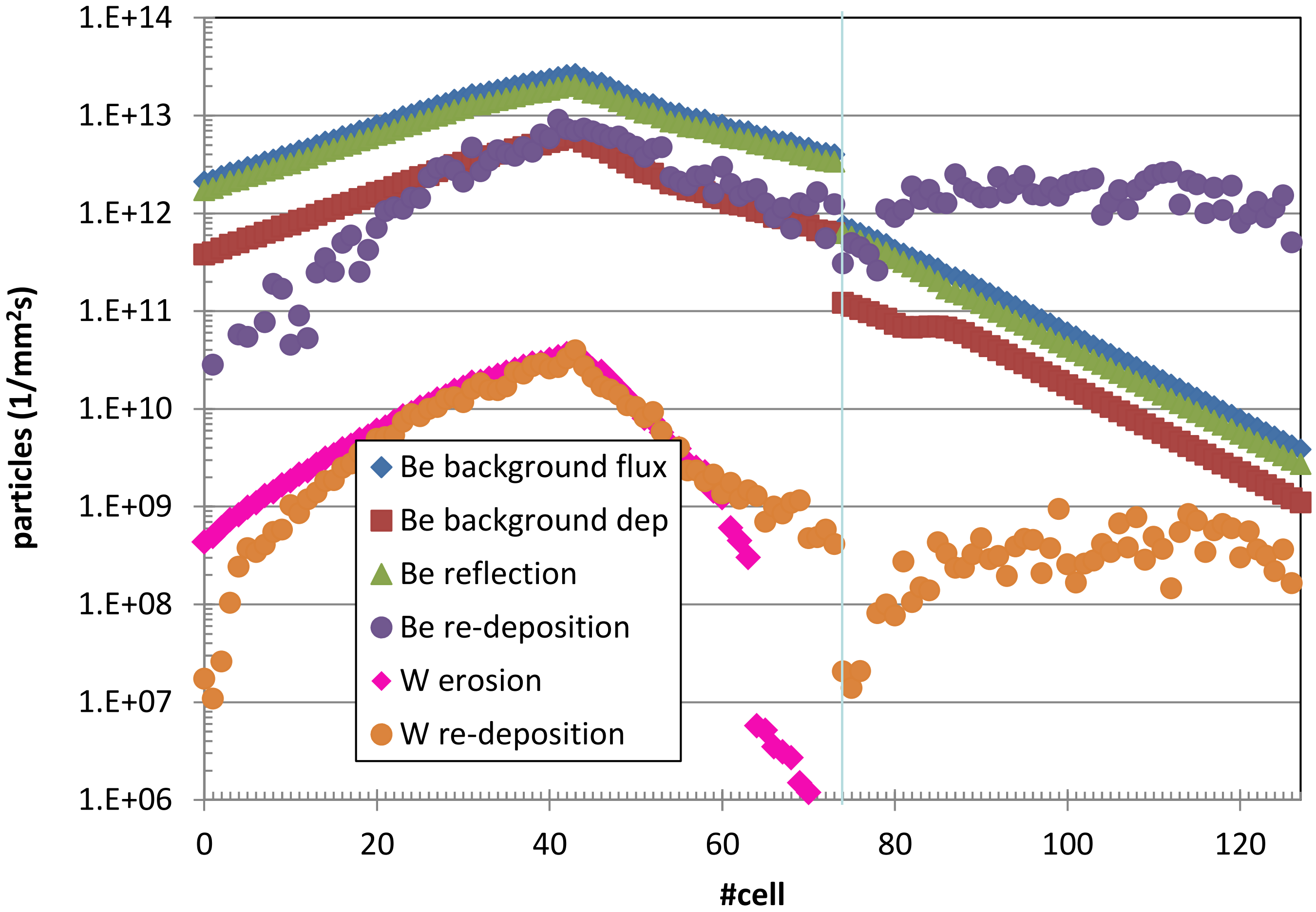


The updated model leads to an increased biasing effect, that matches the experiment (factor 3 increase of 'ERO-min' Be erosion due to RF power), due to the properly treated angular factor in the sputtering yield.

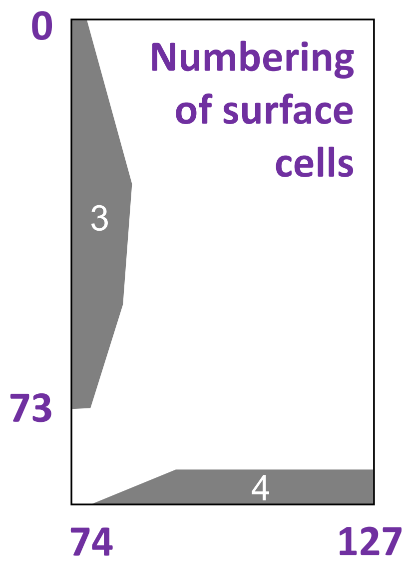
ERO simulations for JET/ITER divertors

A.Kirschner et. al, ITPA DivSol-2015, PET-2015

L-Mode, strike point on tile 3 – erosion/deposition profiles

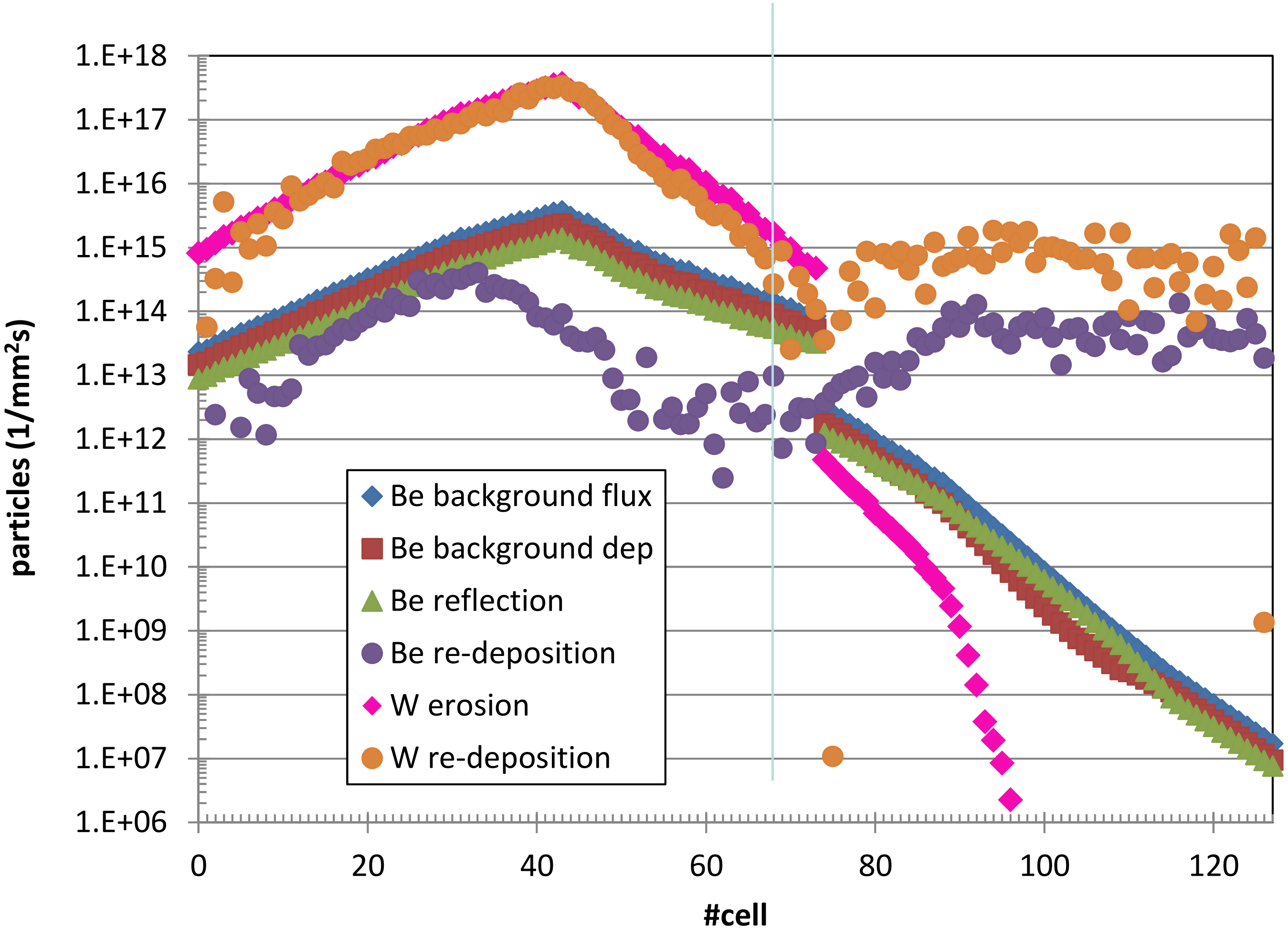


- ~80% of incoming Be is reflected
- ~41% of reflected Be is re-deposited on tiles
- no Be layer formation on tile 3
- No significant W erosion

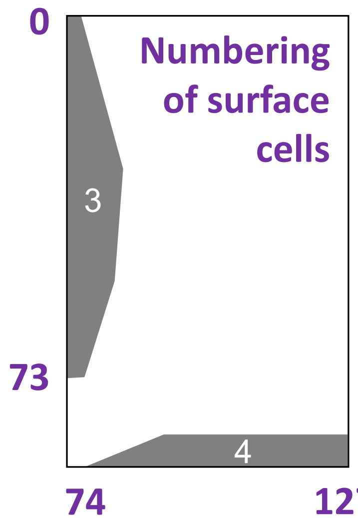


Rotating collector data reproduced, incoming **beryllium flux** into inner divertor is **small** (about 0.1% relative to D^+ flux, i.e. about 10 times smaller than C influx in JET-C)

ELM, strike point on tile 3 – erosion/deposition profiles



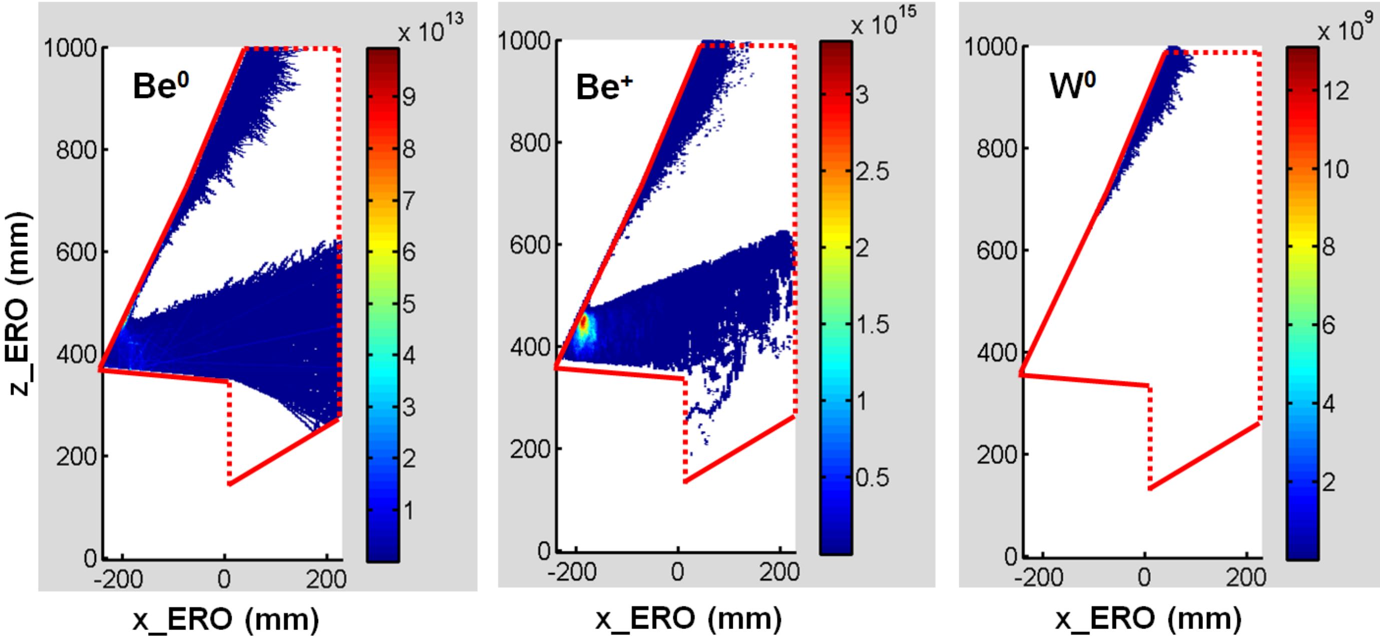
- ~40% of incoming Be is reflected
- ~32% of reflected Be is re-deposited on tiles
- Large W erosion: W flux at strike point ~100 times larger than Be influx !
- ~92% W re-deposition on tile 3 and 4

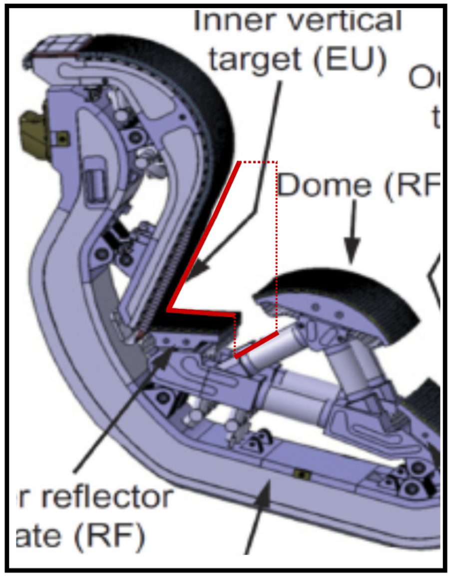


W erosion of divertor is dominated by ELMs!

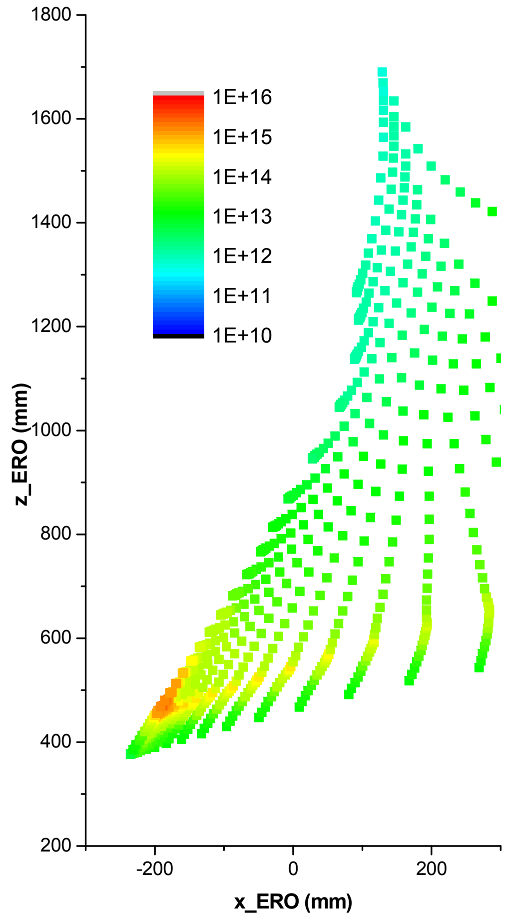
ERO: Be migration into ITER divertor

Simulated impurity densities (particles/cm²)





- ~99% of reflected Be is re-deposited (large electron density)
- Very small W erosion – but: significant W erosion expected during ELMs
- Mixing of Be/W, net layer formation: has to be studied …



- B2-Eirene as input (A. Kukushkin),
- 0.1% Be^{2+} influx to inner divertor

Thermodesorption: kinetic modelling "CRDS"

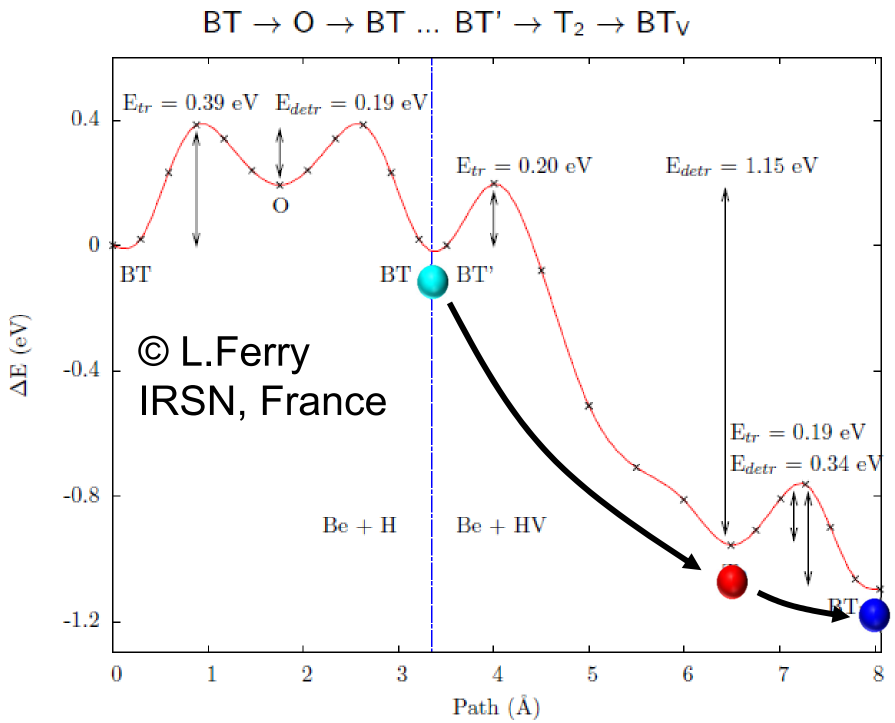
D.Matveev, Mirko Wensing et al., PSI-2016 (Hydrogen WS)

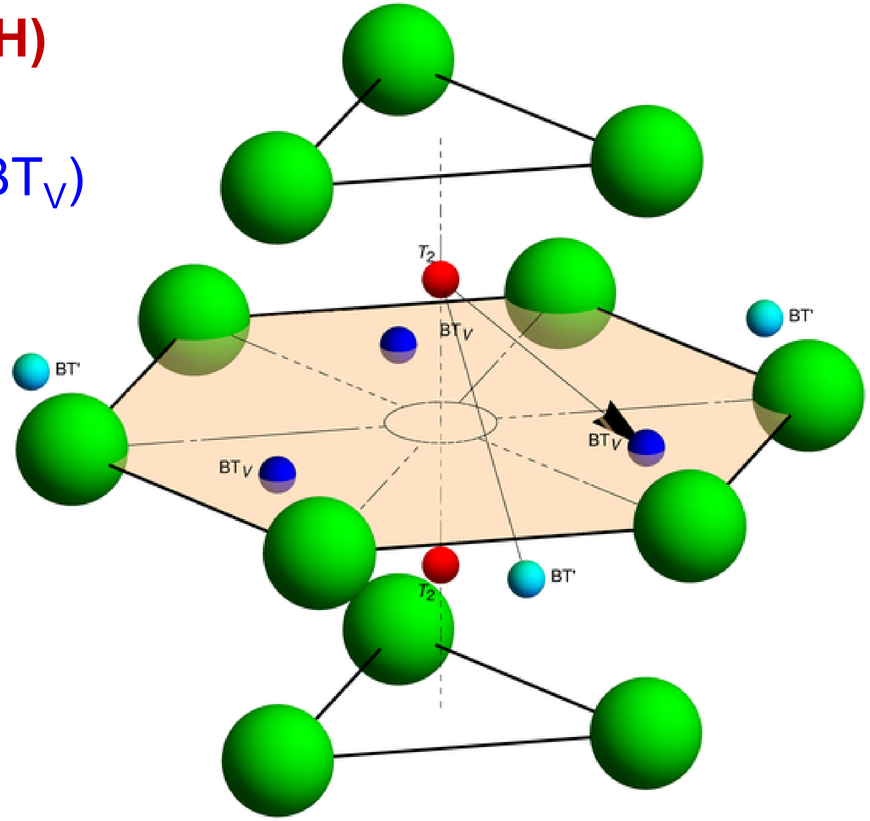
Trapping of H in vacancies (DFT: up to 5H)

	[eV]
H1V	1.30
H2V	1.25
H3V	1.20
H4V	0.98
H5V	0.86

basal-tetrahedral positions (BT_V)

tetrahedral positions (T_2)



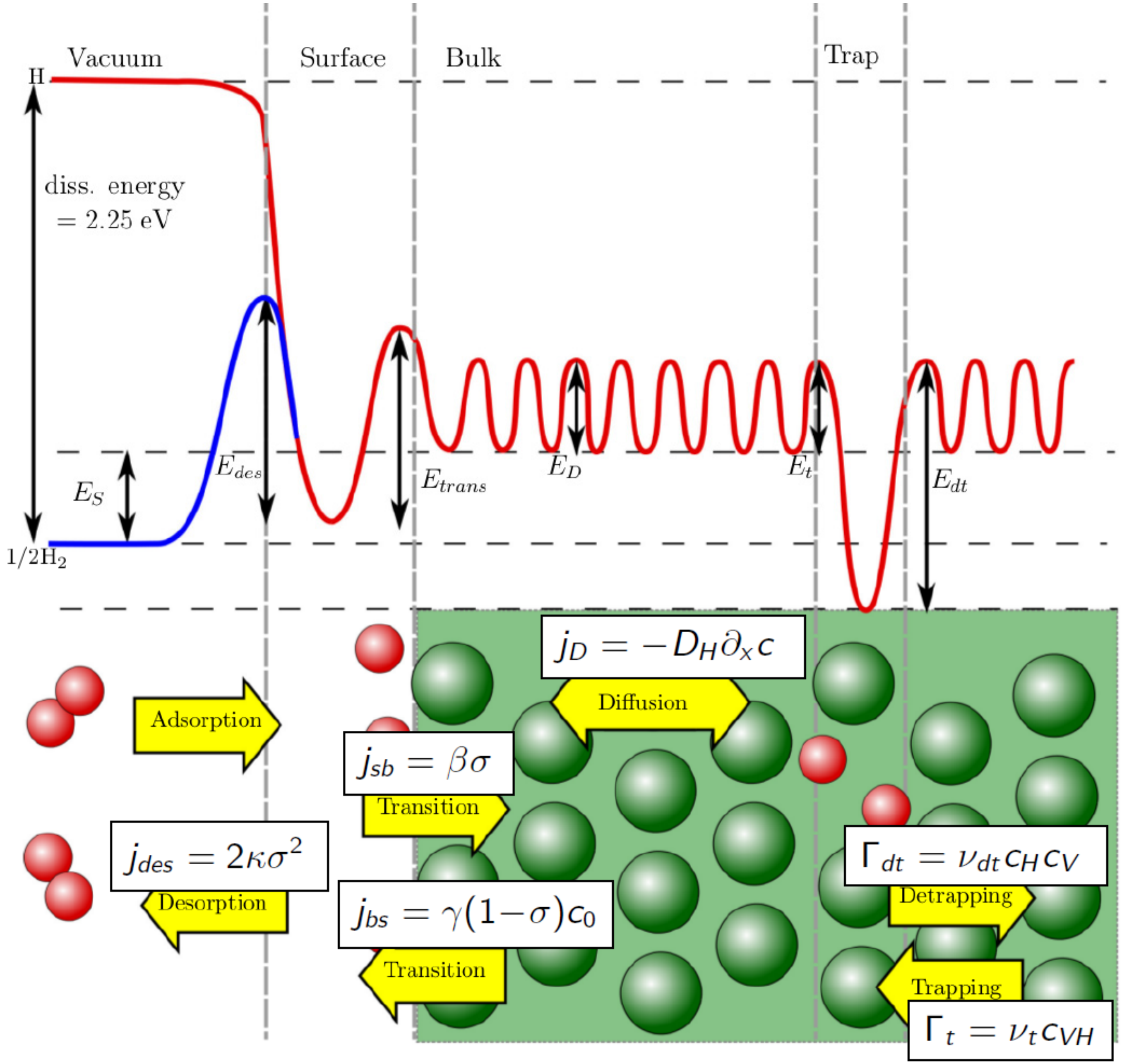


Complex energy landscape

Favorable (de-)trapping via T_2 sites

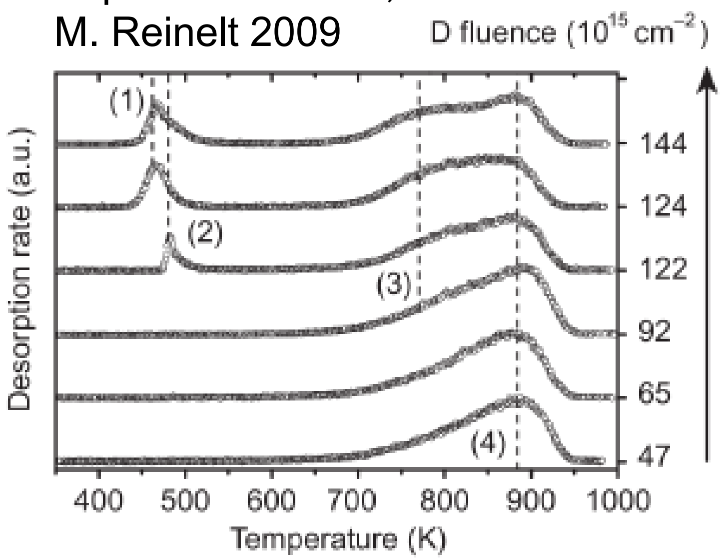
De-trapping frequencies not known

Desorption model overview

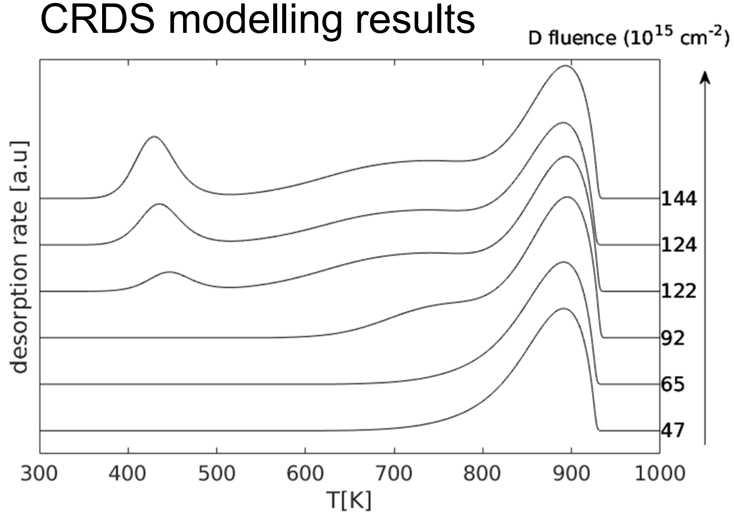


Reaction-diffusion modelling of fluence dependence of hydrogen retention and release in beryllium

Experimental data,
M. Reinelt 2009



CRDS modelling results



Collaboration with IRSN/PIIM, France:

- new DFT data on multiple trapping of hydrogen (H) in vacancies (V), detailed energy landscapes, H and V diffusion, stability of di-vacancies

Coupled Reaction Diffusion Systems (CRDS):

- rate equations approach with multiple trapping and surface limited desorption implemented

Important conclusions:

- determinative role of ratio of total H to total V
- with increasing fluence V become populated up to 5 H, then H occupies the surface
- good qualitative agreement with experiments: low-T and high-T peaks evolution reproduced

Open questions and problems:

- available surface sites (pores, open bubbles)
- role of surface hydrides (surface morphology)
- large scatter of experimental data

Summary - ERO

- The ERO code is a useful bridge allowing benchmarking various Be data with plasma experiments, most of which are difficult to interpret
  - *Benchmarks at JET ILW and other devices (both tokamaks and linear devices)*
  - *Implementation of physical effects (sheath E-field, shadowing, BeD release, etc.)*
  - *Testing of atomic, molecular and surface data*

- In the focus of current studies:
  - *Erosion data including BeD release*
  - *Interpretation of spectroscopy*
  - *Influence of 3D geometry of plasma-facing components, fields and plasma parameters configuration*

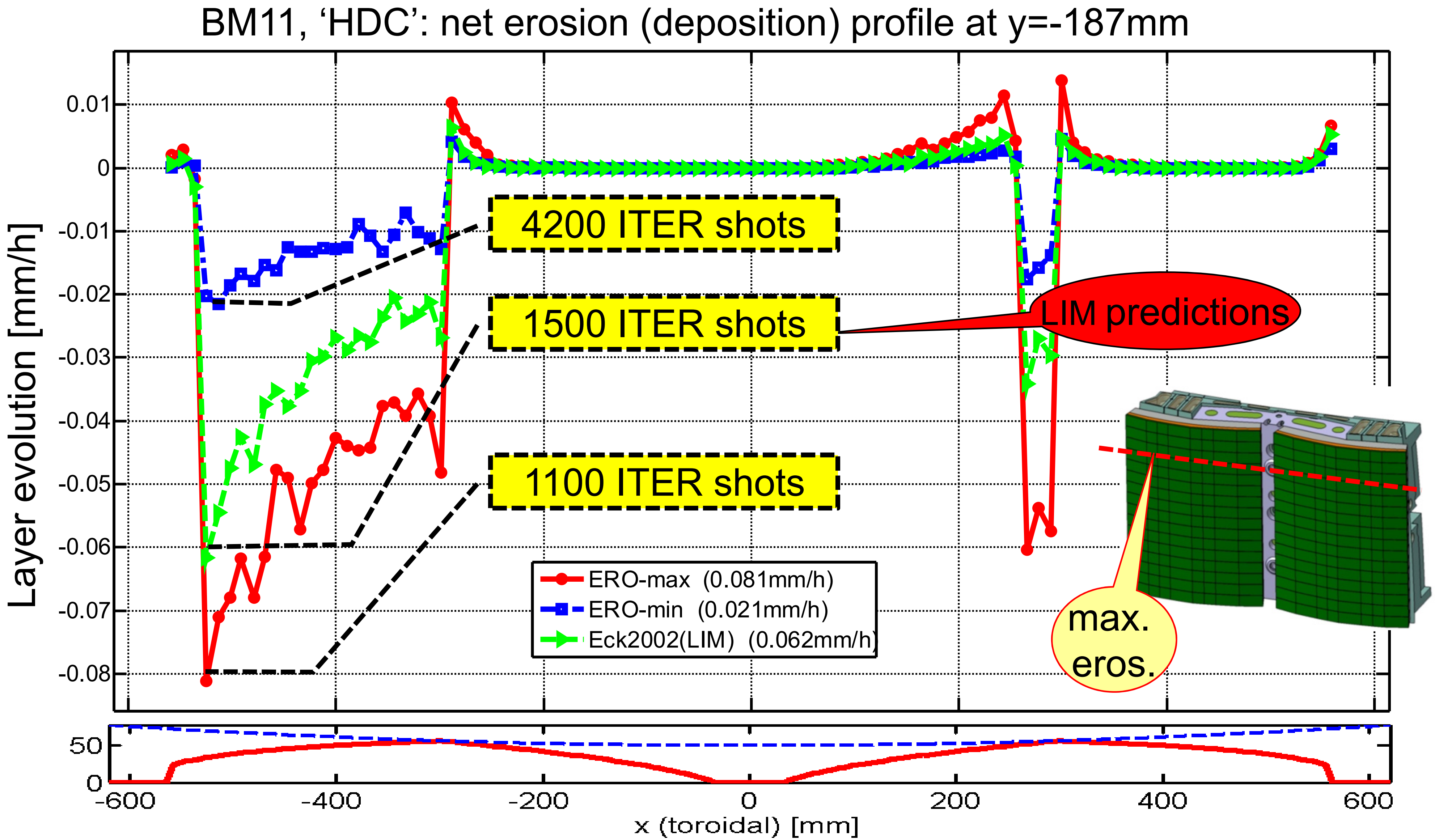
Summary - applications

- JET ILW: Density scan in limiter plasmas confirms 'ERO-min' erosion fit, and effective yield integration procedure (preferable is the analytic solution (AS) for the angle and energy distributions of sputtering particles on impact).
- JET OW L-mode experiments with ICRH antenna influence indicate the correctness of biasing implementation in AS. 'ERO-min' allows to reproduce the observed factor 3 erosion rise by antenna toggling.
- ERO applications to the divertor areas of JET and ITER can help to get an insight into the Be migration and deposition issues.
- PISCES-B He plasma exposure confirms the Eckstein fit based on SDTrimSP data with uncertainties with "cut-off angle" probably related to the surface morphology.
- The new kinetic model CRDS (Coupled Reaction Diffusion Systems) based on DFT data is capable to reproduce some untrivial qualitative features observed in the TDS experiments.

Shortcommings, which are realistic to improve Before the final CRP report

- PISCES-B: simulations for D-plasma exposure.
- Implementation of BeD_x reaction data from M.Probst.
- New experiment is scheduled to measure BeD_x release at 10eV impact energy (close to detached limiter plasmas).
- It would be great to have
  a) weight loss/ witness plate data for PISCES-B with He plasma.
  b) updated data for the D plasma exposure case
- The update of the ITER predictive modelling is expected before IAEA conference this year.

Sputter yields assumptions and net erosion

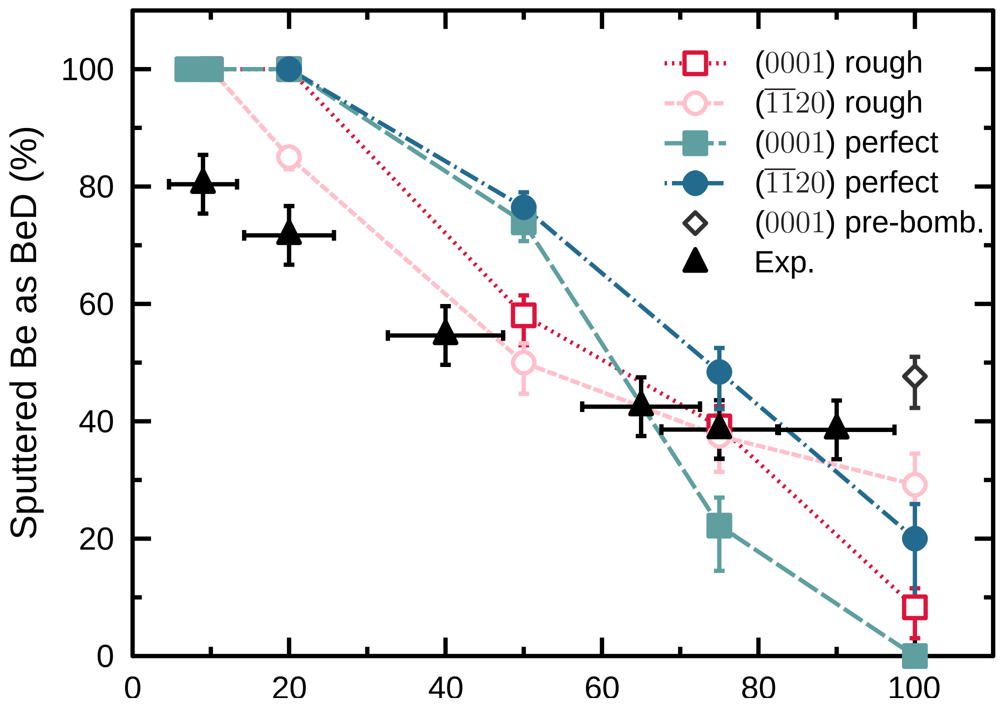


Sputtering data determined the outcome!

PFMC-2011

The End

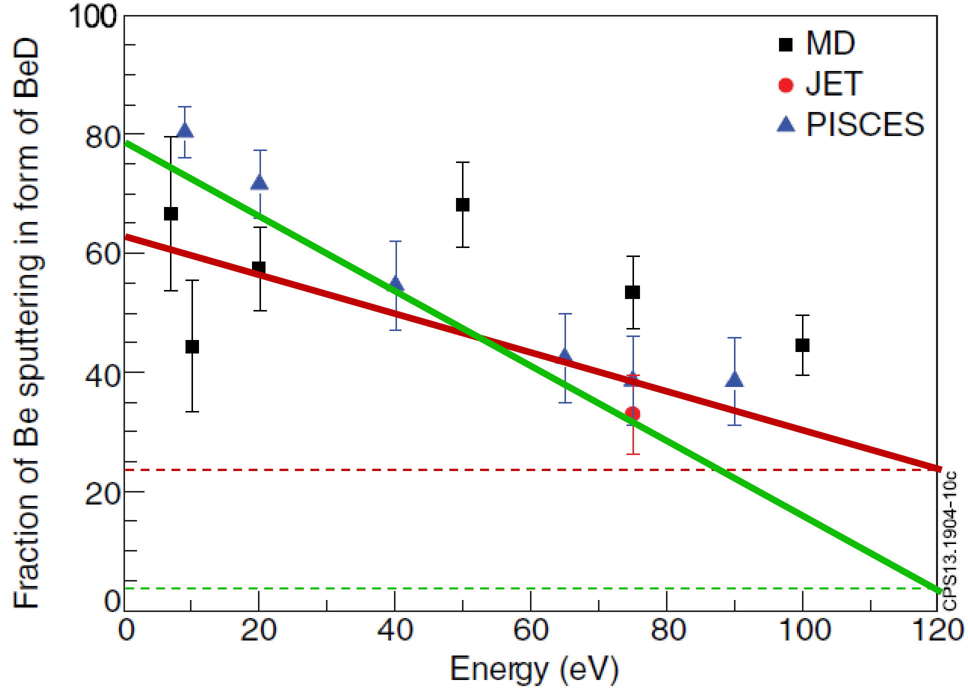
Be sputtering yields – BeD fraction



C.Bjorkas et.al, PSI-2010

f_{all}(BeD) = 70- 40/120·E_{imp} [eV]

f_{exp}(BeD) = 85- 75/120·E_{imp} [eV]



BeD fraction from experiments at JET, PISCES and MD modelling

S.Brezinsek et.al, Nucl. Fusion 54 (2014) 103001

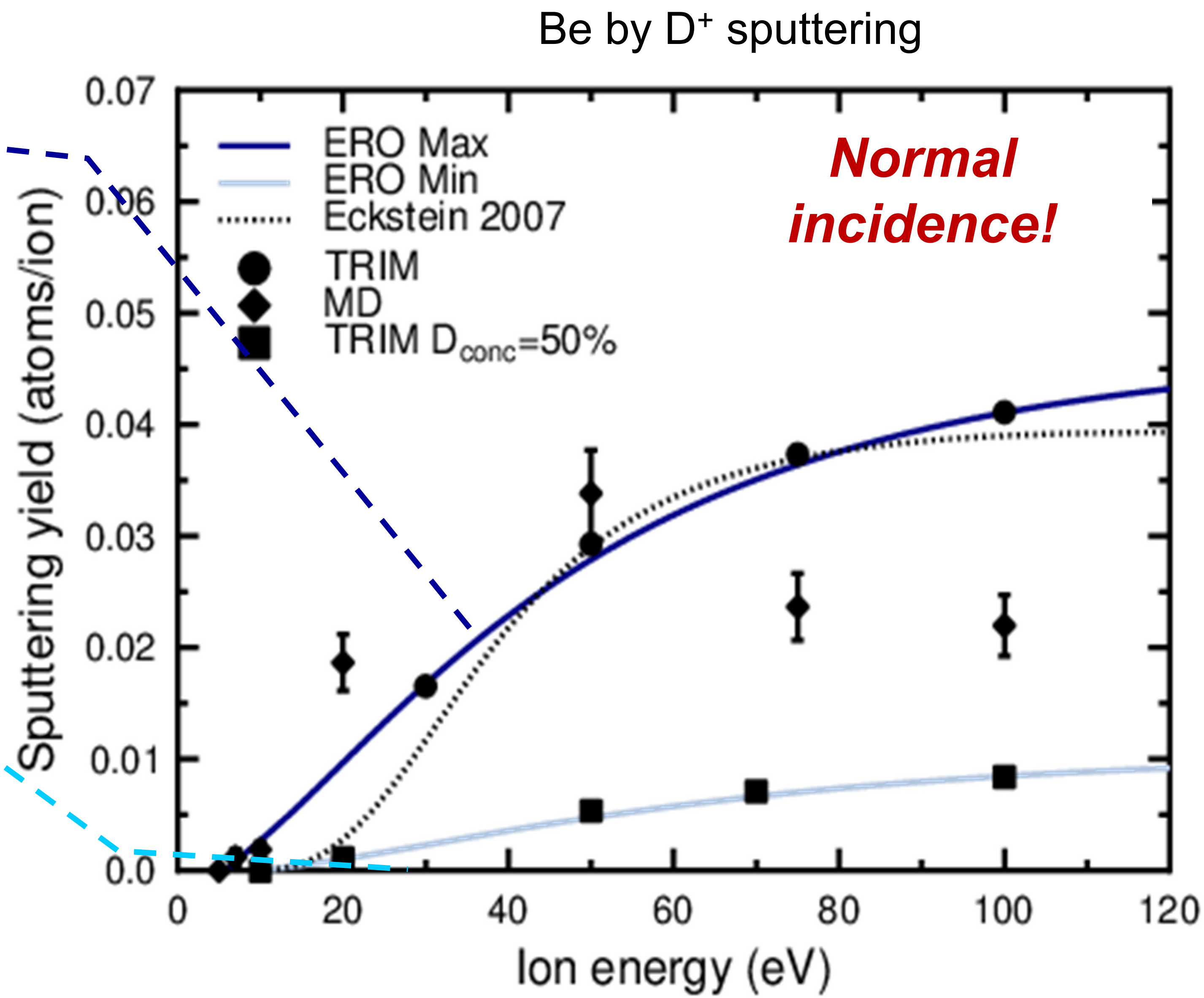
Dependence on surface temperature:
clear drop of BeD fraction with the increasing T_{surf} . . .

Sputtering data – high and low estimates

„ERO-max“
MD + SDTRIMSP
pure Be

Eckstein 2007 fit:
$Y = Y(E_{in}, 0^o) * A(E_{in}, \alpha_{in})$

„ERO-min“
SDTrimSP
50%Be + 50%D



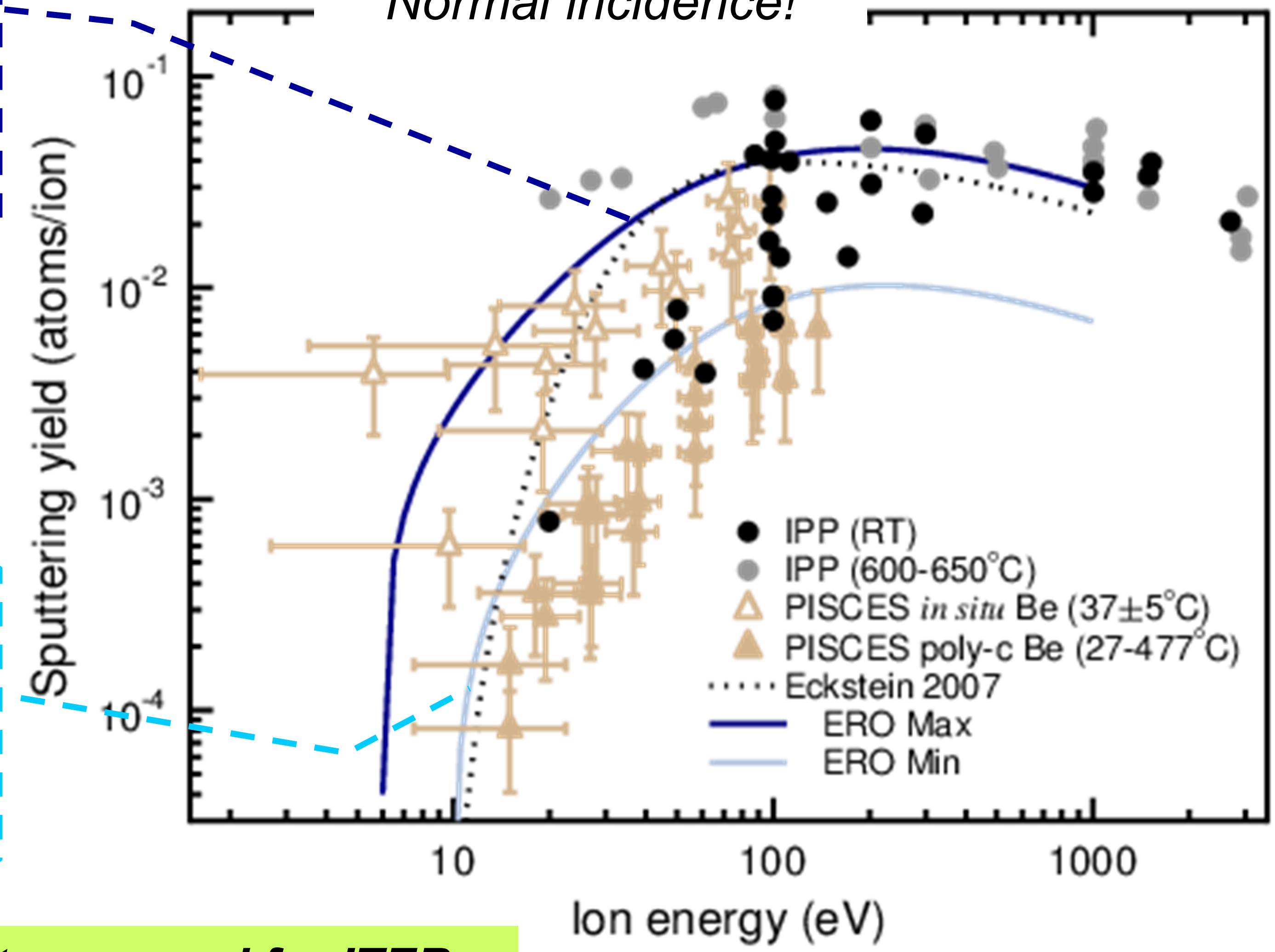
D. Borodin et al., J. Nucl. Mater. (2013), PSI-2012

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.