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D. Borodin<sup>1</sup>, S. Brezinsek<sup>1</sup>, J. Miettunen<sup>2</sup>, M. Stamp<sup>3</sup>, A. Kirschner<sup>1</sup>, C. Björkas<sup>4</sup>,  
M. Groth<sup>2</sup>, S. Marsen<sup>5</sup>, S. Lisgo<sup>4</sup>, D. Matveev<sup>1</sup>, M. Airila<sup>4</sup>, V. Philipps<sup>1</sup>  
and JET EFDA contributors\*

*JET-EFDA, Culham Science Centre, OX14 3DB, Abingdon, UK*

<sup>1</sup>*Institute of Energy and Climate Research - Plasma Physics, Forschungszentrum Jülich GmbH, Association EURATOM-FZJ, Partner in the Trilateral Euregio Cluster, Jülich, Germany*

<sup>2</sup>*Department of Applied Physics, Aalto University, P.O. Box 14100, 00076 AALTO, Finland*

<sup>3</sup>*EURATOM-CCFE Fusion Association, Culham Science Centre, OX14 3DB, Abingdon, OXON, UK*

<sup>4</sup>*EURATOM-Tekes, Department of Physics, P.O. Box 43, FI-00014 University of Helsinki, Finland*

<sup>5</sup>*Max-Planck-Institute for Plasma Physics, EURATOM Association, Greifswald, Germany*

<sup>6</sup>*ITER Organization, Route de Vinon sur Verdon – 13115 St Paul Lez Durance – France*

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## **ABSTRACT**

Estimations of the ITER first wall (FW) life time, previously made by the 3D Monte-Carlo ERO code [1], depend strongly on the assumptions of the physical sputtering yield for beryllium (Be). It is of importance to validate the respective model and data at existing devices including the JET ITER-Like Wall (ILW) as most ITER- relevant experiment. Applying the same sputtering input data in ERO as before in the ITER-predictions, the ERO simulations for the Be light intensity (up-to-date atomic data is used) near the solid Be limiter in the JET-ILW case reveal a factor 2 overestimation of the assumed yield even if the low estimate assuming 50% D surface content is used. This result indicates the preference of this assumption for plasma-wetted areas. It points to a possible (after eliminating of uncertainties) necessity to correct (reduce) the respective estimates for the Be sputtering yield and accordingly, re-visit the ITER FW life time predictions.

## **INTRODUCTION**

The ITER duty cycle is determined by the lifetime of the first wall (FW) plasma-facing components (PFC) and retention of tritium (T), which must not exceed the safety limit (1kg). Both factors were analysed first by 2D LIM code [2] and later confirmed by more detailed 3D ERO code simulations [1]. In [2] it was shown that the retention issue in the main chamber is less critical than the life time and retention mostly determined by T co-deposition (also in divertor [10]), thus also largely governed by Be erosion in the first place. Therefore, ERO studies focus on the erosion issues. The estimated life time of the most critical beryllium blanket module is about 1500 ITER discharges for both codes using sputtering data [3]. The codes predict the same maximal erosion point, but at some other locations more general 3D ERO simulations lead to different results. ERO considers also 1) various assumptions (discussed below) concerning physical sputtering which lead to different high and low estimates for the life time (1100-4200 ITER discharges) and 2) self-sputtering by Be plasma impurity which can be very significant.

It is important to reduce the uncertainties of beryllium sputtering yields by applying the same ERO code to the most ITER-relevant device (by the 3D wall and plasma configuration) which is JET with the recently installed ITER-Like Wall [4] with massive Be limiters and a full W divertor. We apply the benchmark to dedicated discharges in limiter configuration in order to have best controlled conditions for the Be sputtering. The Be light emission was measured during a plasma density scan which reflects a variation of the impact energies of impinging deuterium to characterize the physical sputtering from the solid Be shaped limiter [9]. Initial ERO JET-ILW modelling results were published in [5]. Note that the same ERO code is also applied to various other experiments including Be erosion at the linear plasma device PISCES-B [11].

ERO is a 3D Monte-Carlo plasma-surface interaction and impurity transport code allowing tracking the eroded species including gyration in the electromagnetic field. ERO simulates in addition the light emission of impurities (using atomic data from ADAS [3]) and provide a synthetic diagnostic output which can be compared with experimental data obtained e.g. in the observation chord of the JET-ILW spectroscopic system [9]. In the present work the ERO modelling [5] was

significantly refined by applying improved plasma parameters as well as the integration procedure for the effective Be sputtering yields allowing the comparison of modelled and measured absolute emission intensities in the same observation volume. The high “ERO-max” and low “ERO-min” estimates for physical sputtering yields of Be derived in [1, 5] were applied. Moreover, in the present work the angular and energy dependencies of the sputtering yields was taken into account on the basis of pre-calculated distributions of the impact angles and energies.

## 1. SPUTTERING YIELDS INTEGRATION IN ERO

The sputtering yield as a function of the angle  $\alpha_{in}$  and energy  $E_{in}$  of the impinging particle can be factorized [7] as

$$Y(E_{in}, \alpha_{in}) = Y(E_{in}, 0) * A(E_{in}, \alpha_{in}), \quad (1)$$

where  $E_{in}$  is the energy and  $\alpha_{in}$  is the angle of incidence;  $Y(E_{in}, 0)$  is the yield at normal incidence ( $\alpha_{in} = 0$ ) and  $A(E_{in}, \alpha_{in})$  the angular factor.  $Y(E_{in}, 0)$  is determined by four fitting parameters; the values for high and low estimates ‘ERO-min’ and ‘ERO-max’ based on fitting of various simulated data (in binary collision approximation [7] or by molecular dynamics approach [18]) are given in [5]. ‘ERO-min’ is largely determined by simulation points produced in assumption of 50% concentration of D in the surface interaction layer. To calculate  $A(E_{in}, \alpha_{in})$  the dataset of three additional fit parameters, each depending on  $E_{in}$  are necessary. In ERO optimal datasets corresponding to respective  $Y(E_{in}, 0)$  fit are used. Dataset from [7] leads to similar results for ‘ERO-max’  $A(E_{in}, \alpha_{in})$ .

In case of the B-field perpendicular to the plasma-facing surface the assumption of normal incidence for impinging ions is justified, because the angular part of equation (1) has values close to 1 for incident angles in the range of 0°–20°. However, at shallow magnetic field angles relevant for the JET-ILW limiters or ITER blanket modules most plasma particles hit the surface at angles between 50°–60° according to ERO simulations described below and also according to analytical solution [8]. This leads to an increase of the sputtering yield by a factor of about 10 compared to normal incidence.

As ERO is primarily an impurity tracing code for locally eroded particles (for which formula (1) is applied directly), plasma particles are normally not tracked and thus their impact angle and energy is not calculated within the simulations. Therefore, a dedicated yield integration procedure is introduced in ERO for the primary plasma impact including the self-sputtering by intrinsic Be plasma impurities. The sputtering by D and Be ions is treated separately respective to their concentration (steady state assumed) in the plasma flux at the given surface point. To determine the angle and energy distributions of impinging plasma ions a series of preliminary ERO simulations is performed. In each of those runs D or Be ions from the plasma start away from a flat surface (at a distance about the connection length), which is inclined by various angles with respect to the magnetic field. The ions start with Maxwell-distributed velocities. The movement of the ions is determined by the friction force with the plasma flow, and the Lorentz force in the electric and magnetic field. Acceleration in the pre-sheath and sheath electric fields is considered automatically.

The electron and ion temperatures are assumed to be equal and constant in the simulation volume, whereas the electron density along the magnetic field lines drops by a factor of two at the sheath entrance compared to its value at the stagnation point. Figure 1 shows histograms of simulated distributions of impact angle and energy for various plasma temperatures (Fig.1a) and surface inclination angles (Fig.1b). Applying formula (1) and using the simulated distributions one gets the respective effective Be sputtering yield (Fig.1c).

The effective yields  $Y_{\text{eff}}(T_e, \alpha_B)$  have been calculated for pairs of plasma temperature  $T_e$  and magnetic field angle  $\alpha_B$  (between B and normal to surface) considering ‘ERO-min’ and ‘ERO-max’ estimates for  $D^+$  and  $Be^{3+}$  ions. ERO calculates  $T_e$  and  $\alpha_B$  for each surface cell and uses linear interpolation to get the respective  $Y_{\text{eff}}$ . Multiplying this with the corresponding local ion fluxes ERO provides the gross erosion patterns along the surface.

## 2. BERYLLIUM EROSION EXPERIMENTS AT JET

The erosion experiments by plasma density scan were carried out during special limiter JET discharges, which are more suitable for erosion studies since in the diverted plasmas only low Be spectroscopic emission is observed. The plasma was shifted towards the inner wall with a contact point very close to the solid Be limiter tile (7 in octant 7X) at the spot of the observation system. The geometric details can be found in [5].

The measured plasma parameters  $n_e$ ,  $T_e$  in the scrape-off layer, obtained from a reciprocating magnetic probe (RCP) [12], and in the confined plasma region, measured by Thomson scattering (TS) are used as input for ERO. As no full simulations of the background limiter plasmas under consideration are currently available, the RCP and TS data were combined to restore the resulting  $n_e$  profile for an effective poloidal radius  $\rho$ . In a similar way TS data was used for the  $T_e$  profile, however the  $T_e$  values at  $\rho = 1.02$  obtained from BeII line ratios in the line-of sight [14] near to the limiter surface were used as the RCP data for  $T_e$  at plasma boundary was too scattered. A shift of TS profile by 1cm was required for the best match.

Finally, the measured data of four discrete plasma experiments was mapped into the 2D poloidal cross-section from the linear profiles by the method described in [13], which provides also other parameters required for ERO simulations, like the plasma flow velocity or the E-field parallel to the B-field.

To parameterise the density scan in the limiter experiment, the line-averaged density measured by an interferometer chord in the centre of the JET (‘LAD3’) is used [19]. Correspondingly, the 2D-mapping was carried out for four values of the line averaged density. Linear interpolation is used for the ERO simulated points laying in between those four integrated density values separately for every poloidal location. Figure 3 shows the poloidal ‘maps’ (a) for the electron density  $n_e$  as an example. The density near the target (b) increases with the line-averaged density, at the same time the electron temperature  $T_e$  decreases (c).

The Be concentration in the plasma was estimated using the effective charge  $Z_{\text{eff}}$  measurements assuming Be to be the only impurity (Fig.4). In the modelling it is assumed that all Be hits the limiter

surface as  $\text{Be}^{3+}$  ions. This assumption is done to estimate the maximal possible Be concentration and, thus maximal self-sputtering effect (Fig.5). This of course is a simple approach as for instance the  $Z_{\text{eff}}$  measurements are integrated across the poloidal cross-section.

### 3. BENCHMARK WITH EXPERIMENT AND DISCUSSION

The most straightforward way to determine the Be sputtering yields is to take the ratio of the Be and D particles fluxes estimated with the S/XB method assuming slow varying plasma parameters in the region of emission and ionisation [15] by means of dividing the photon flux of respective spectroscopic lines by the “ionization- per-photon”  $S/XB(T_e, n_e)$  values [9] provided by atomic calculations (ADAS [3]). Figure 4 shows the integrated effective sputtering yields in comparison with the measured yields based on the S/XB approach [14]. The ERO-integrated yields for D ions and self-sputtering by Be ions are combined together according to the impurity concentration (Fig. 3). Measured data lay mostly between the high and low simulated estimates, except for the low density (high temperature) and high erosion region, where uncertainties including Be concentration in plasma are the largest. The S/XB method provides integrated values and plasma parameter gradients are neglected in the first place. To minimize the impact of transport only low ionization stages representative for the source are considered (BeI and BeII). In order to obtain a more detailed insight on the local effects a comparison with modelling is required.

Here, the 3D ERO code is applied for interpretation, which can simulate of the local Be erosion, transport and light emission. The code integrates the light inside the observation chord) as it was reported in [5], where also the observation system is described in detail. One result of such a comparison is given in figure 5 showing experimental and modelled emission of one BeI and one BeII line. ERO reproduces the ratios of these lines to other lines measured in the experiment better than within a factor 2. However, the absolute line intensities, even the ones simulated in the “ERO-min” assumption, are still about a factor 1.5 too high, indicating an overestimation of the Be erosion source in the modelling

The D and D emission registered by the same observation system can be used for independent characterisation of the impinging D ion flux to the surface (Fig.6). The experimental flux is divided by 2 to account for 50% of the recycled flux in form of  $\text{D}_2$  molecules decaying mostly to D and  $\text{D}^+$ [14], so only the first atom contributes to the lines mentioned. However, still the ERO simulated flux is about 50% lower than the measured one. As the Be light emission (Fig.5) is proportional to the flux, the deviation between ‘ERO simulations (assuming ‘ERO-min’) and experiment should be scaled from 1.5 to about a factor of two.

Basically the ‘ERO-min’ sputtering data produced in assumption of high D concentration in the surface interaction layer is a logical choice for the Be limiter wetted by plasma. However, though the deviation of the simulated intensities from the experiment does point to a necessity to reduce the ‘ERO-min’ low estimate, it is yet unclear whether the deviation comes just from uncertainties in plasma parameters and the Be concentration in plasma. The influence of certain effects like Be-D release [17] as additional erosion mechanism (increasing ERO deviation from the experiment) and



surface roughness [16] (could explain factor 2 yield reduction, although the surfaces were polished) also should be considered. It is also unclear if the reduction should be applied to the normal incidence part or to the angular factor in formula (1).

## **SUMMARY**

The Be sputtering yield determined at the Be limiters in JET-ILW by passive optical spectroscopy has been benchmarked with the ERO code implementing an extended set of plasma parameters restored in 3D, which include a fitting to the in-situ determined local Te at the location of BeII emission. This and the usage of effective integrated sputtering yields have considerably improved the modelling with respect to initial studies presented in [5]. It is demonstrated that for plasma-facing surfaces with shallow angle to the B-field the accounting of the angular factor of the sputtering yield is essential e.g. by the suggested integration procedure involving ERO simulations of angles and energies on impact.

The effective sputtering yields for Be determined experimentally by the S/XB approach lay between the high and low estimates produced using the ERO simulations. A deeper insight in the benchmarked integrated spectroscopic and the respective Be sputtering yields can be obtained by the underlying full 3D modelling with the ERO code, which mimics the volume integration made in the experiment.

This also allows transferring to ITER conditions, applying predicted ITER plasma and geometry condition [20] and detailed study of various effects. In the case of the JET-ILW limiter experiment, the ERO modelling reproduces well for Be and D the line ratios and line intensity trends measured during the density scan. However, even the lowest estimate for the Be sputtering yield ‘ERO-min’ applied the ERO code is about a factor 2 too high. However, this difference can be accounted to uncertainties in the input parameters including the Be impurity concentration in the plasma affecting the Be self-sputtering. Still, this indicates that ‘ERO-min’ estimate based on the high surface D concentration is the preferable assumption for plasma wetted areas.

Further modelling efforts aimed to study additional relevant effects like surface roughness [16], Be-D molecules release [17] and D concentration in the surface are necessary.

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## **REFERENCES**

- [1]. D.Borodin et al., *Physica Scripta* **T145** (2011) 014008
- [2]. S. Carpentier et al., *Journal of Nuclear Materials* **415** (2011) S165–S169

- [3]. H. P. Summers “The ADAS User Manual” (2004), version 2.6; <http://adas.phys.strath.ac.uk>
- [4]. G.F. Matthews et al., *Physica Scripta* **T145** (2011) 014001.
- [5]. D. Borodin et al., PSI-2012, *Journal of Nuclear Materials* (2013), <http://dx.doi.org/10.1016/j.jnucmat.2013.01.043>
- [6]. W. Eckstein et. al, IPP report 9/132, 2002
- [7]. W. Eckstein (2007) *Topics in Applied Physics*, 110, pp. 33-187; doi: 10.1007/978-3-540-44502-9-3
- [8]. K. Schmid et al., *Nuclear Fusion* **50** (2010) 105004
- [9]. M.F. Stamp et al., *Journal of Nuclear Materials* **415** (2011) S170–S173.
- [10]. A. Kirschner et al., *Physica Scripta* **T128** (2009)
- [11]. D. Borodin et al., *Contribution to Plasma Physics* **50** (3–5) (2010) 432–438.
- [12]. C. Silva et al., PSI-2012, *Journal of Nuclear Materials* (2013)
- [13]. J. Miettunen et al., PSI-2012, *Journal of Nuclear Materials* (2013)
- [14]. S. Brezinsek et al., EPS-2013
- [15]. A. Pospieszczyk et al 2010 *Journal of Physics B: Atomic, Molecular and Optical Physics* **43** 144017
- [16]. S. Dai Shuyu Dai et al 2013 *Plasma Physics and Controlled Fusion* **55** 055004
- [17]. C. Björkas et al., PSI-2012, *Journal of Nuclear Materials* (2013)
- [18]. C. Björkas, K. Nordlund/*Journal of Nuclear Materials* **439** (2013) 174–179
- [19]. A. Boboc et al., *Review of Scientific Instruments* **83**, 10E341 (2012); doi: 10.1063/1.4737420
- [20]. S. Lisgo et al., this conference. *Figure 1*.

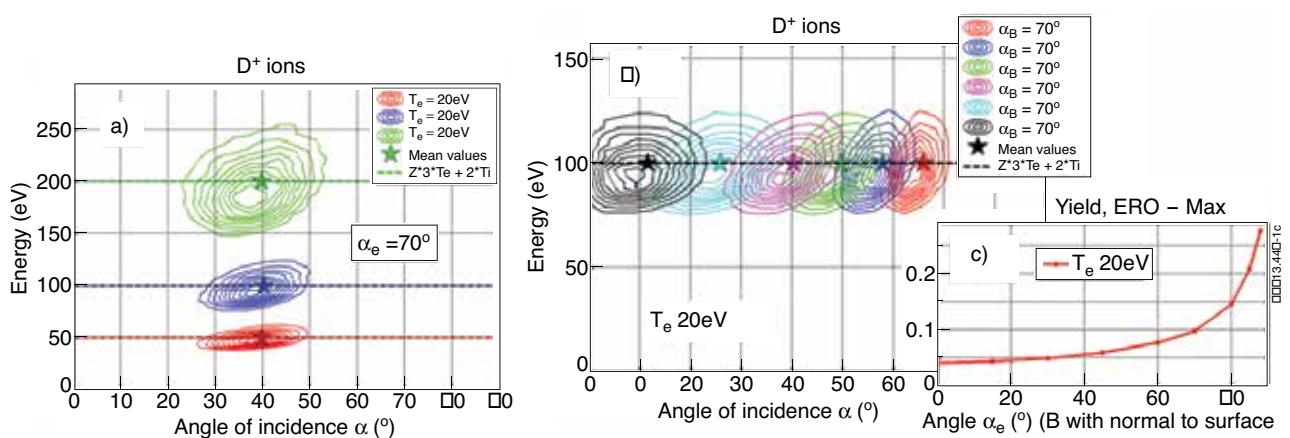


Figure 1: Histograms of impact angles and energies of  $D^+$  ions in dependence on plasma temperature (a) and B-field angle with normal to surface (b) and resulting effective sputtering yield (c) obtained with the ‘ERO-max’ assumption by integration of formula (1).

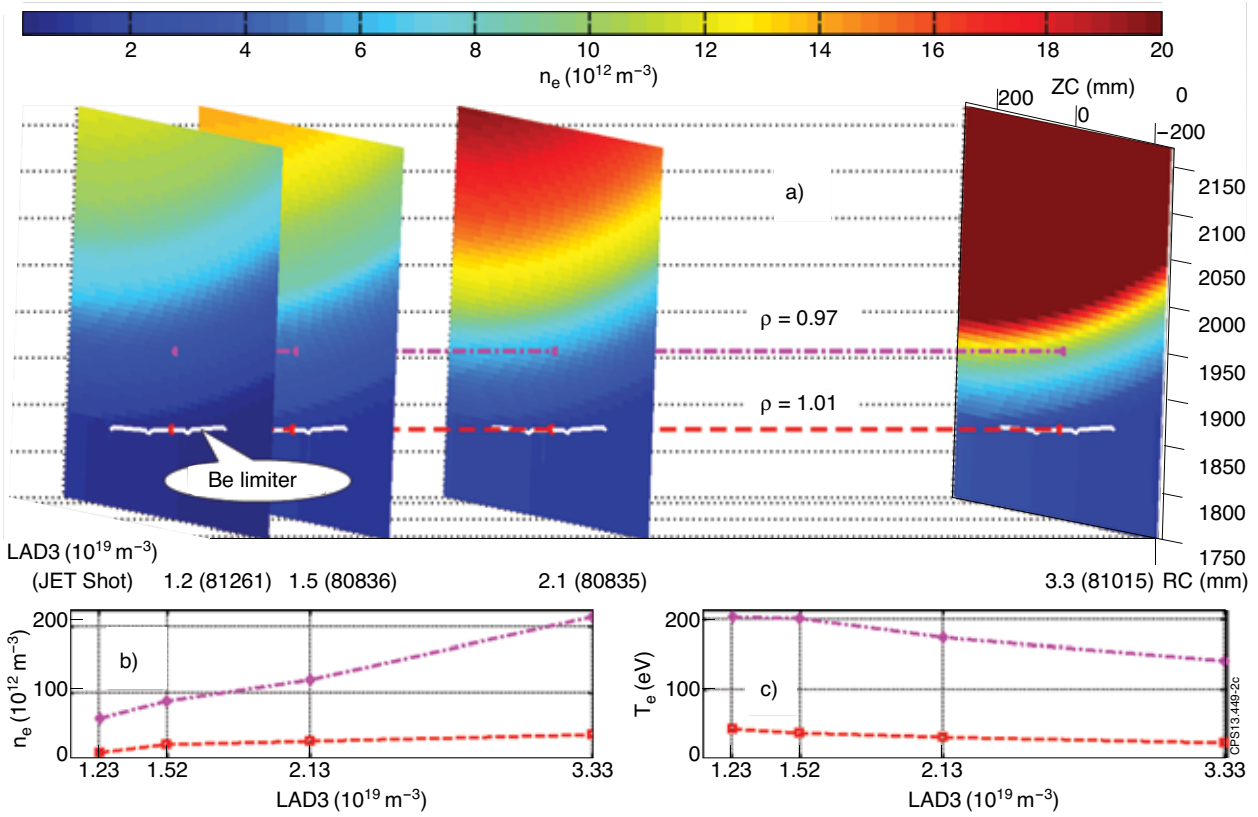


Figure 2: Plasma parameters mapped in 2D [13] for 4 JET-ILW limiter discharges. a) electron density maps b) density at the midplane ( $Z_C = 0$ m) very close to the Be limiter surface and deeper in the plasma, respective effective radii  $\rho$  are given c) electron temperature for the same locations.

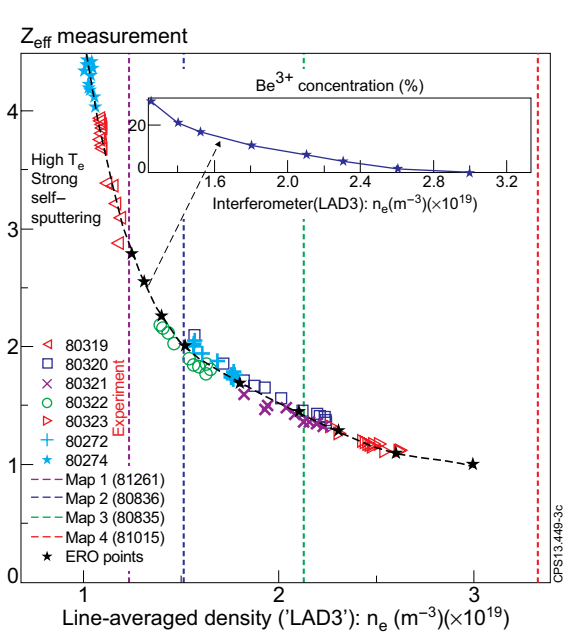


Figure 3: Z-effective measurements used for the  $\text{Be}^{3+}$  concentration estimation. Density scan discharges are shown ('experiment'). The poloidal 'maps' (Fig.2) are marked illustrating the plasma parameter interpolation range. The low density discharges have larger plasma temperature leading to strong self-sputtering and larger Be plasma impurity concentration.

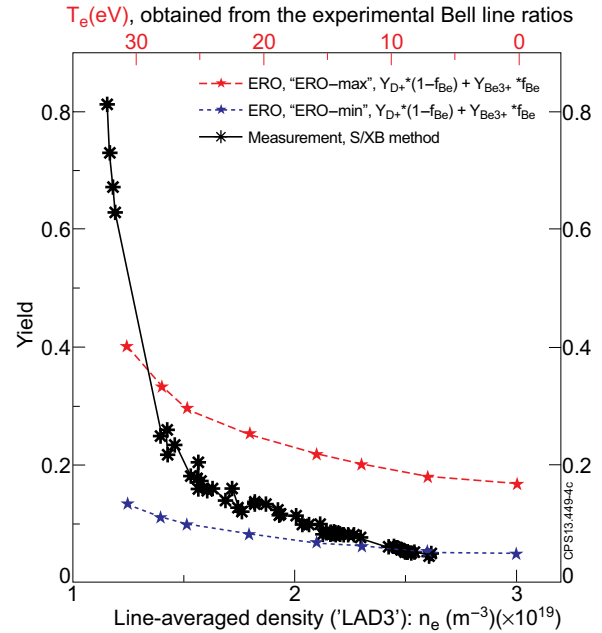


Figure 4: ERO simulated effective sputtering yields and spectroscopic measurements [14]. Plasma temperature is fitted to the observed BeII line ratios.

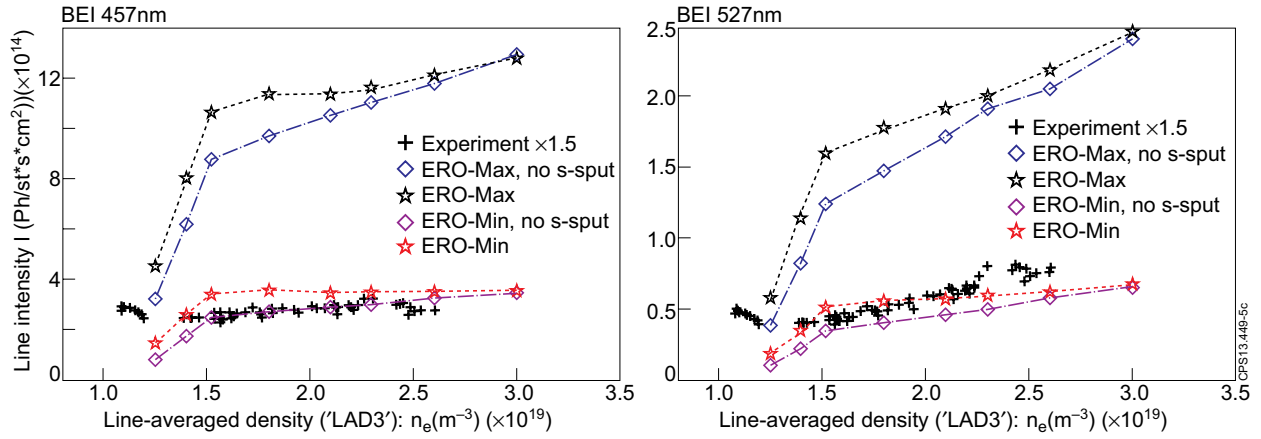


Figure 5: ERO simulated line intensities for ‘ERO-min’ and ‘ERO-max’ assumptions compared to the corresponding absolute experimental data. BeI 457nm line (left) and BeII 527nm line (right). Self-sputtering is calculated according to Be plasma impurity concentrations estimated from the Z-effective measurements (Fig.3).

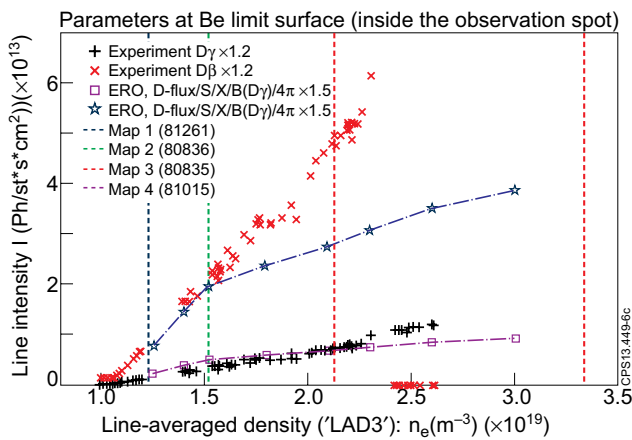


Figure 6:  $D^+$  ion surface flux benchmark. ERO simulated flux divided by the respective  $S/XB(n_e, T_e)$  [3] is compared to the respective measured of D and D line intensities.