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D Borodin et al.

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ERO modelling of beryllium erosion by helium plasma in experiments at PISCES-B

D.Borodin[1], D.Nishijima[2], R.Doerner[2], S.Brezinsek[1], A.Kreter[1], A.Kirschner[1], J.Romazanov[1], I.Borodkina[3,1], A.Eksaeva[3], E.Marenkov[3], Ch.Linsmeier[1]

[1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich, Germany
[2]Center for Energy Research, University of California at San Diego, 9500 Gilman Dr., San Diego, CA, US
[3]National Research Nuclear University (MEPhI), Kashirskoe sh. 31, Moscow, RF

Abstract

The beryllium erosion by helium plasma irradiation is studied at PISCES-B linear plasma device and interpreted using the accompanying simulations by the ERO code. The influence of plasma conditions and varying negative biasing of the Be plasma target on BeI and BeII absolute line intensities are reproduced in detail by the simulations. The synthetic axial line intensity shapes and line ratios match with experiment indicates that atomic data are quite accurate. The initial population state of quasi-metastable ^{3}***P*** *level in BeI is found to be MS:GS=0.33 for all conditions. The determined by the modelling interpretation yields are compared to the SDTrimSP code simulations in the binary collision approximation.*

1. Introduction

The reliable data for beryllium (Be) erosion is a key for predictive modelling of ITER first wall duty cycle [ITER_SC]. The physical sputtering by hydrogenic species plays the main role, however the erosion due to the expected impurities like for instance helium (He) is also of importance. He is of importance not only because it will be a product of fusion, but also because it is proposed to use the He plasma at the starting (low activation) phase of the ITER operation [RP-He]. The 3D Monte-Carlo impurity transport and plasma-surface interaction (PSI) code ERO is often used for ITER predictions [ITER'11, ITER'07]. Because of that it is of importance to validate both the code and the underlying data at existing devices like PISCES-B [RD-GNE, EROPSC] capable to operate with Be. Recently ERO code was also extensively applied to various erosion experiments at JET ITER-like wall (ILW) [ILW'13, ILW'15, ILWRF] which have led to extensions and refinements of the model and data in ERO. Multiple improvements were implemented including the analytical treatment of the distributions of angles and energies on impact including additional surface biasing [AnMod]. The ERO application to the PSI-2 linear device has contributed in providing the initial angle distributions for physically sputtered species [PSI2] (for W erosion; operation with toxic Be is not allowed at PSI-2) . In parallel the empiric experience at PISCES-B has grown, for instance the indication for a rise of the electronic temperature (mostly a constant axial profile for T_e is assumed) just in front of the target was discovered [TeR].

In the present work the updated ERO code is applied to the benchmark of physical sputtering data by experiments at PISCES-B, the only alternative to JET for plasma operation with Be. PISCES-B provides unique opportunities for Be spectroscopy like continuous plasma operation and a possibility to observe the triplet 332nm line allowing to characterize the ***BeI*** $1s^22s2p\ ^3P$ quasi-metastable state (MS) population [MSEPS]. this particular study is aimed in understanding of the pure physical sputtering of Be by He plasma irradiation which allows excluding of any $\boldsymbol{Be\text{-}D_x}$ molecules release and respective uncertainties.

The experiment has provided an extensive spectroscopy and weight loss benchmark material. 2 BeI (triplet and singlet) and 2 BeII axial line intensity profiles were obtained in He plasmas in the vicinity of the Be target. The negative target biasing was scanned (from -50V to -125V) in 3 plasma conditions to study the influence of the sputtering ions impact energy. To provide an independent measurement several target weight loss measurements were performed at similar conditions.

The resulting from the experiment and ERO modelling interpretation physical sputtering yields $\boldsymbol{Y_{Be \leftarrow He}(E_{in})}$ for Be erosion by He ions as a function of impact energy $\boldsymbol{E_{in}}$ are compared with the SDTrimSP code simulations approximated by the Eckstein (2007) fitting formula [Eck07].

2. Experiment and benchmark material

The scheme of the PISCES-B linear device is given in fig. 1. The Be target is positioned inside the plasma column with the surface perpendicular to the axial B-field. ERO simulates the Be erosion, deposition and reflection as well as the local transport in the vicinity of the target. In Fig.1 one can see the ERO simulated side views of neutral BeI and ionized BeII emission. They are essentially different: the pattern of BeI is very much affected by the initial angle distribution of the sputtered Be, whereas BeII is more elongated along the device due to confinement of the ions by the axial B-field. Still, the plasma flow clearly pulls them back to the target. The light emission plume of eroded Be is characterized by axial line intensity profiles which are also useful for comparison of the experiment with the simulations.

The incidence of sputtering He ions on the target with a surface perpendicular to the electric field is nearly normal in particular that B-field in PISCES-B in these plasmas is relatively small ($\boldsymbol{B=0.0152T}$). The sheath electric field pulling the ions to the target is dominating in particular in the case of an additional negative biasing applied to the target like in the considered experiment. The sputtering yields at normal incidence are mostly dependent [Eck07] on the material parameters like e.g. surface binding energy and on the incidence energy of sputtering ions $\boldsymbol{E_{in}}$, which is determined by the biasing mentioned with the potential $\boldsymbol{U_{bias}}$ as $\boldsymbol{E_{in} = -Z_{ion}*U_{bias} - U_{plasma}}$, where $\boldsymbol{U_{plasma}}$ is the plasma potential. In some cases (mass loss experiment, section 5) the latter value was measured by the Langmuir probe, in case this was not available, it is assumed to be $\boldsymbol{U_{plasma}\sim T_e}$.

The scans of the target biasing ($\boldsymbol{E_{in}}$) were performed in three plasma conditions (table 1). The electron density $\boldsymbol{n_e}$ and temperature $\boldsymbol{T_e}$ were measured by the reciprocating Langmuir probe at the axis at 15cm distance from the target surface. It should be noted, that that $\boldsymbol{n_e}$ falls towards the target down to ~50% from the upstream value on a distance of about ~15cm [LBomb]. The $\boldsymbol{T_e}$ is assumed to be constant in the axial direction. The plasma column has a width of about 5cm with the Gaussian radial profile of $\boldsymbol{n_e}$ and a somewhat flatter (similar to pedestal) radial profile for $\boldsymbol{T_e}$. The target sample is a disk with a radius of 11mm fixed by the clamping ring also made of Be which increases the total radius up to 18mm.

Three He plasma exposures with the mass loss measurements at conditions related to spectroscopy were performed to provide an independent yield measurement for the benchmark.

2. Spectroscopy: simulations and experiment

It was of importance to reproduce the shape of the experimental profiles and the line ratios, because it confirms that the local transport simulations are feasible. Fig. 2 shows a typical example for condition ‘C2B3’ (table 1). The agreement for other conditions is very similar. The decay of BeI lines with a growing distance from the target is determined to certain part by ionisation, however it is much more affected by the angular distribution just after the sputtering, which determines how much neutrals leave the plasma volume to the sides. The perfect match between triplet and singlet lines in BeI demands metastable population tracking discussed below. The relatively good match of BeI to BeII ratio confirms the reasonability of plasma parameters and atomic data. The best match of BeII decay far from the target demands an additional assumption of a cut-off angle (COA) in the angular distribution of the sputtered Be atoms. This allows to get a larger BeII fraction far away from the target. It should be noted that the noise and error bars for BeII lines (in particular 313nm) are higher. Optimal COA determination is not very precise as the most critical part of the axial profile for that is the decayed signal far away from the target. Obviously it is mostly affected by noise and background subtraction assumptions. COA=30^{o} works well for conditions “C1” and “C2”, whereas the match of “C1” remains reasonable even in at COA=10^{o}. The physics behind the COA is discussed below.

It was shown earlier in [TeR] that the BeII and He line ratios as well as probe measurements indicate the rise of a $\boldsymbol{T_e}$ towards the target in its vicinity which depends on the pressure of neutral gas filling the PISCES-B volume. This effect was introduced in ERO as a correction factor based on BeII line ratio measurements interpreted with the help of ADAS’96 [ADAS] data. Fig. 2, right shows that the assumption of this rise improves agreement for BeII lines, however the profile agreement for BeI just in front of the target gets somewhat worse. This may be explained for instance if the radial distribution of this rise is not constant. The main aim of the present paper is to determine the absolute sputtering yields from spectroscopy and values just in front of the target are fogged by the described uncertainty. The simulations have shown, that the part of the BeI 457nm line profile between z=20mm and z=60mm is much more suitable for integration of absolute intensities, because its shape is independent on assumption concerning $\boldsymbol{T_e}$ rise and COA. The integration along the 40mm of profile increases signal to noise ratio. In all figures below all values including the line rations are produced on the basis of the integrated in the explained way values for both BeI lines.

To get the nearly perfect match for relative intensities of the singlet 457nm and triplet 332nm lines one can see in Fig. 3 (left) the MS tracking should be used [MSEPS]. In general words the tracking of the ***BeI 1s^{2}2s2p ^{3}P*** population (this quasi-MS state is the lowest in the triplet system) allows ERO to follow the relative total population of all triplet states against the total population of the singlet system. It can be shown that relaxation between the systems due to intercombinational transitions is much slower than inside each system. Naturally, the contributions to the spectral line photon efficiency coefficients [ADAS] from the states belonging to the same spin are usually the largest. Sputtered particles leave the surface with an unknown initial internal state, which however can be determined from the line ratio mentioned. In Fig. 3 ERO simulations based on various assumptions are presented alongside with the experiment for all experimental conditions available (table 1). The initial population of MS:GS=0.33 seems to fit best (fig. 3, right) independent on plasma conditions and surface biasing. The quantum mechanical reasons for this interesting fact are not yet studied, however this is out of the scope of the present paper.

The number of photons emitted by each Be specie depends on the described above factors whereas their amount is proportional to the gross erosion fully determined in the case at hand by physical sputtering. This process is known to depend on the angle and energy [ILW'15] of the sputtering ions, however due to the nearly normal incidence of sputtering He^+ ions in PISCES-B the angular factor in the Eckstein'2007 formula for the sputtering yields [Eck07] is equal to unity. The energy of incidence $\boldsymbol{E_{in}}$ distribution can be of importance also, therefore in the case at hand it was investigated (Fig. 4, left) by dedicated ERO simulations as well as analytical approach [AnMod]. Both approaches does not agree fully with each other in particular in the high density condition "C1" which is difficult for ERO from numerical point of view. However, the main outcome is absolutely the same: the $\boldsymbol{E_{in}}$ distribution is relatively narrow around the average value determined by biasing. Fig. 4, right shows that the effective yield averaged by any of these distributions nearly exactly matches the normal incidence yield, thus the energy distribution can be neglected.

The integrated between ***z=20mm*** and ***z=60mm*** intensities mimic the absolute sputtering yields. Fig. 5 presents the ERO simulations in comparison with experiment for the BeI 457nm line for all conditions (table 1). The singlet line intensity is not that much influenced by the MS tracking as the triplet one, however it clearly improves the agreement with the experiment. One can see that the dependence on target biasing is reproduced well for conditions "C2" and "C3". The agreement for "C1" is not that perfect but also good. The effect of plasma conditions is reproduced as well. The absolute values are overestimated in ERO simulations by a factor of about 2, which is however constant for all considered conditions.

The bottom part of fig.1 shows the dependence on the cut-off angle. Obviously the focussing of the initial velocity distribution along the PISCE-B axis leads to less side losses and more Be light. It increases the fraction of BeII light and changes the shape of profiles – they go deeper into the plasma. The latter allows speculating about the reason behind this effect. It is a usual observation at PISCES-B that the profiles are initially, just after switching on the plasma, are shorter. The penetration depths rise significantly during first minutes of the plasma exposure. It was shown earlier that this process is correlating with the growth of the multiple cone-like structures [RD-Cones, AK-Cones]. It is easy to imagine that these very steep structures collimate the beam of the eroded particles. They also affect the angle of incidence which would be normal for a flat surface, however it can become very shallow for a cone side. The deeper understanding of these surface morphology issues is not available for now. The most relevant for the task MD simulations does not allow including even a single cone, not speaking about a group of those, into the simulation box which is measurable for the realistic simulation times; the construction of a He-Be potential for MD has also been found nontrivial and just ongoing [CBKN] For the present study it is sufficient that this speculation allows considering the COA as an uncertainty.

3. Mass loss results and Discussion

For the spectroscopic observations discussed in previous section the clamping ring (also from Be) was included into the ERO simulations to account for the common ring and target surface (re)erosion, reflection and re-deposition. However, the mass loss measurements were performed only for the sample with 11mm radius. The corresponding experimental and simulated results are compared in the table 2. The exposure time was varied in the experiment 500-1000s to keep the target fluence about the same.

One can see that ERO accounting for net erosion and self-sputtering (much less meaningful in this particular case) along the target surface helps to come somewhat closer to the experimental results. However, the deviations are too high to be explained by this kind of ERO modelling with any assumptions. In fact ERO simulations based on Eckstein fitting formula applied to every surface cell deviate from the Eckstein value for the characteristic E_{imp} up to ~30%, whereas weight loss indicates factor 5-9 difference with ERO and even larger with the Eckstein fit applied to the E_{imp} in the centre of the target. It should be noted that systematically smaller by about an order of magnitude than SDTrimSP data sputtering yields are not a new result [RD-f5]: it seems to be rather a rule for the sputtering by small mass species line H, D and He [TSchwSel].

Returning back to the spectroscopy we see that ERO simulations show that Eckstein's yields also seem to be overestimated by a factor of 2 or may be even more due to the uncertainty in the COA. the real yield seems to be proportional to the Eckstein fit $Y(0, E_{in})$ with a diminishing factor. This indicates that probably the physical sputtering itself happens in the similar way, so that the BCA simulations remain relevant. Another option is that the reduction occurs due to the prompt processes just after the sputtering.

Both spectroscopy and weight loss approaches indicate the overestimation of the BCA physical sputtering yields. However spectroscopy gives much smaller reduction factor of about ~2-4 whereas mass loss ~5-9 making the methods agree within a factor of 2.5. Partially it can be explained by the remaining uncertainties in both approaches. Still, it is important to note that spectroscopy is characteristic for the gross erosion, whereas the weight loss rather for the net erosion. ERO simulations does not show significant difference between the net and gross erosion, however it may mean that not all related physics in included [RD-GNE] for instance the effect of the surface roughness which can change local erosion/deposition balance on a microscopic scale. While spectroscopy is quite proportional to the Ecktein's fit, the deviation factor for mass loss measurements (table 2) is quite scattered. This indicates either large error bars or some unaccounted effect. It is clear that until the surface effects on atomistic level including the nano-level morphology are not understood it is necessary to continue the gathering of the experimental facts with systematic modelling interpretation: the ERO modelling of similar experiment in D plasma is ongoing, Ar plasma irradiation experiments at PISCES-B are proposed [TSchwSel].

4. Conclusion

The physical erosion of Be by He plasma in PISCES-B was charachterised by spectroscopy and weight loss measurements with interpretation by the PSI and local transport ERO code. Both methods indicate that the Eckstein'2007 [Eck07] fit for the sputtering yields based on SDTrimSP code simulations in BCA approximation overestimate the sputtering yield.

The simulation of radial intensity profiles and their ratios for BeI and BeII proves the feasibility of the simulations and the underlying ADAS [ADAS] atomic data. The spectroscopy simulated by ERO deviates by factor 2-4 and reproduces very well the observed trends of the absolute intensities on during the plasma parameter and target biasing (sputtering ion impact energy) scan. The uncertainty of about factor of 2 is associated with the COA in the angle distribution of sputtered ions which seems to be related to the changes in the surface morphology (cone-like structures) due to the He plasma irradiation. The MS tracking [MSEPS] has somewhat improved the results. Remarkable fact that initial population just after sputtering was found to be MS:GS=0.33 independent on plasma conditions and target biasing.

The weight loss results confirm an overestimation of the Ekstein'2007 yields, however the deviation factor is scattered ~5-9 without a clear system, which can partially be explained by quite large error bars in these measurements.

It is obvious that further progress demands a deeper understanding of the erosion processes on the atomistic level including the influence of surface morphology evolution by plasma exposure e.g. using the MD simulations [BeDCaro]. Further similar experiments (e.g. Be in D and Ar plasma) accompanied by the ERO modelling interpretation can be useful to understand the effects on the phenomenological level.

5. Acknowledgement

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Figures and tables

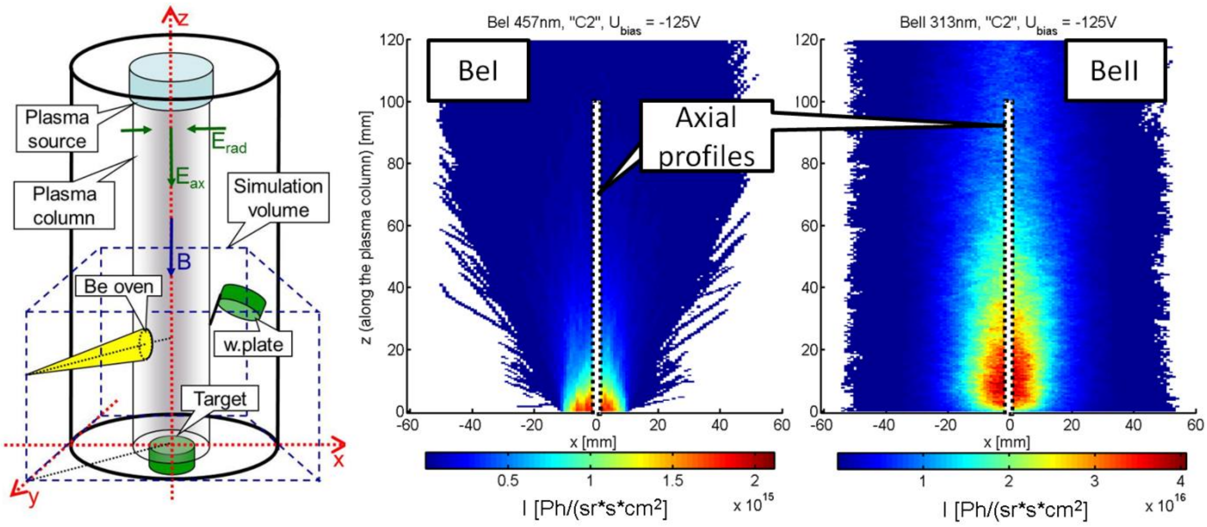

Fig. 1. *The schema of the PISCES-B linear device including ERO simulation volume and coordinate system (left). Be effusion cell ("oven") and witness plate ("w.plate") are shown though they are not in use in the experiment discussed in the present paper. ERO simulated light emission if BeI and BeII are shown (middle and right), the position of the axial profiles measured in experiment and synthesized by ERO are shown.*

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'

Table 1. *The plasma and biasing conditions in the experiment and the respective reference names used in the following figures.*

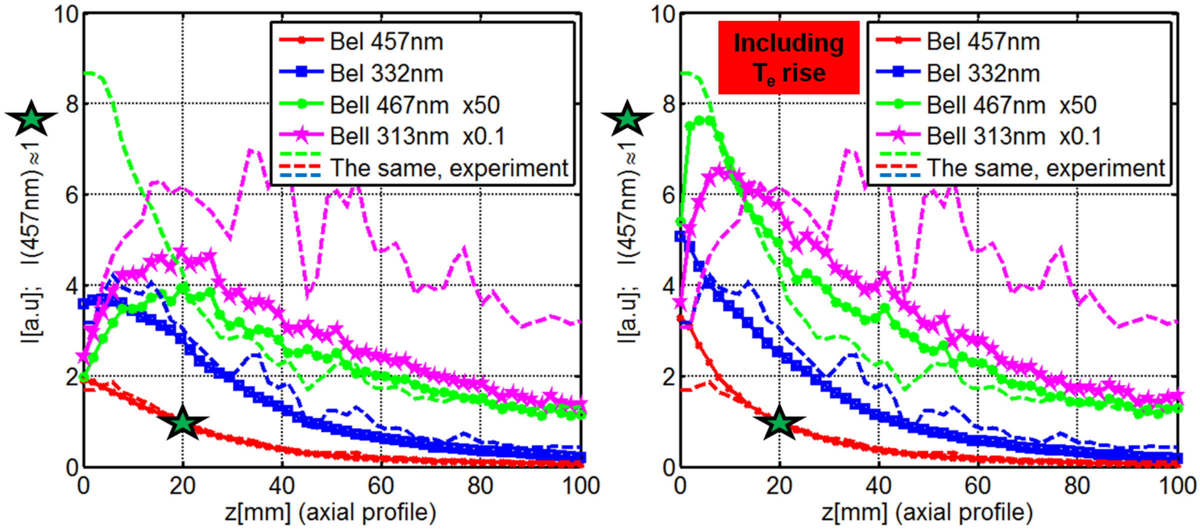

Fig. 2. *The axial line intensity profiles of various BeI and BeII lines measured at PISCES-B during the Be target exposure to He plasma and the corresponding ERO simulations (dashed lines of the same color).*

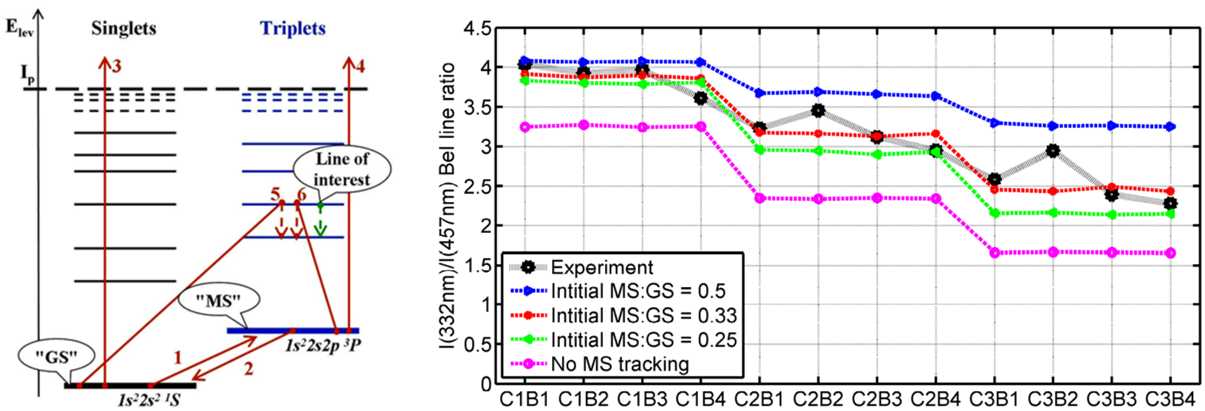

Fig. 3. *The triplet (332nm) to singlet (457nm) line ratios in BeI as obtained in the experiment (black stars) or simulated by ERO using various assumptions about the initial population just after sputtering or with switched off MS tracking.*

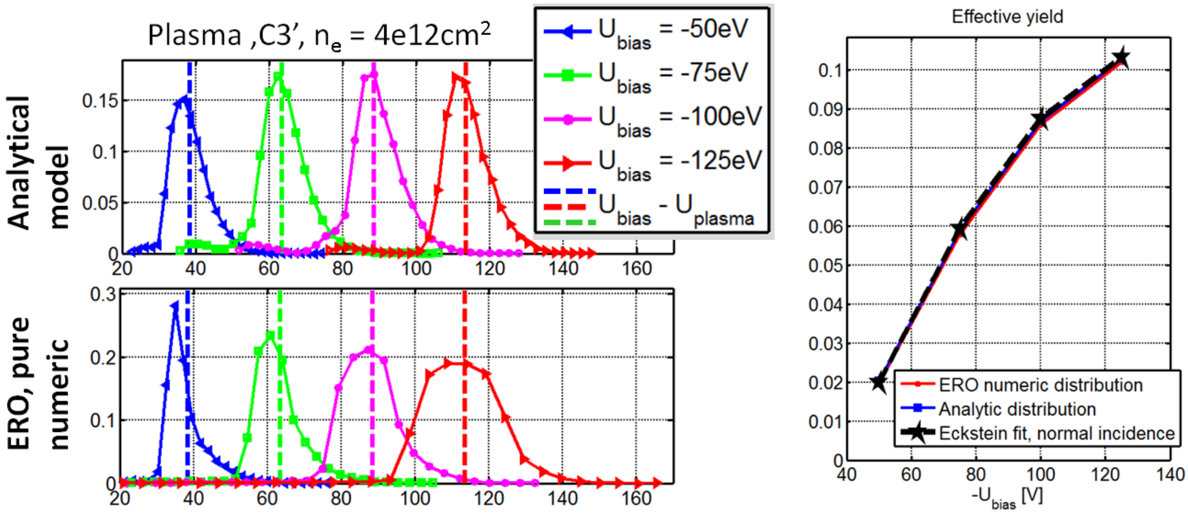

Fig. 4. *The axial line intensity profiles of various BeI and BeII lines measured at PISCES-B during the Be target exposure to He plasma and the corresponding ERO simulations (dashed lines of the same color).*

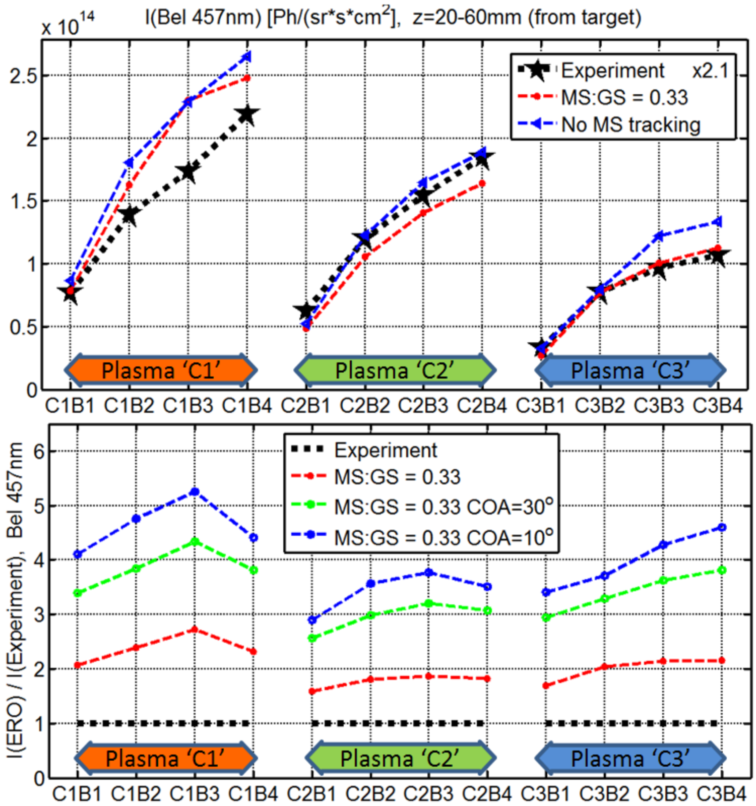

Fig. 5. *Integrated light emission values near the Be target at various plasma and biasing conditions (table 1). The absolute intensity values ERO with and without MS-tracking and the experimental ones (top). The ratios to the experimental values of simulations with various cut-off angle assumptions (bottom).*

Case NN	E_{in} *[eV]*	*Exposure time [s]*	*Eckstein yield*	*ERO yield*	*Experimental yield*	*ERO / Experiment*
1	*37*	*1000*	*1.78e-02*	*1.38e-02*	*2.84e-03*	*5*
2	*93*	*550*	*9.12e-02*	*6.21e-02*	*7.04e-03*	*9*
3	*92*	*500*	*9.05e-02*	*5.90e-02*	*7.34e-03*	*8*

Table 2. *Three Be target irradiation by He plasma experiments at PISCES-B and various estimations (or ERO simulations) for sputtering yields. ERO accounts for re-deposition and (found to be much smaller) self-sputtering giving up to 30% reduction to the utilized also by this code Eckstein's yields. Still, the experimental results are 5-9 times smaller. Fluence was about ~3.2e25cm*$^{-2}$ *in all cases.*