Modelling of Be Erosion in JET and Extrapolation of the Data for ITER

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Abstract. The paper provides an overview of Be erosion data validation which has been made during experiments with the ITER-Like Wall in JET [1] and demonstrates how this data can affect the predictive modelling of the erosion rates to be expected at the first wall in ITER [2, 3]. The key tool for this extrapolation is the Monte-Carlo simulation code ERO [4] which includes 3D impurity transport and plasma-surface interaction. Physical and chemical assisted physical sputtering were characterised by the Be I and Be II line and BeD A-X band emission in the observation chord measuring the sightline integrated emission in front of the inner shaped solid beryllium limiter at the torus midplane at constant plasma conditions in limiter configuration [5] and with variations in edge plasma conditions and impact energies. Revised analytical expression [6] for particle tracking in the sheath region and implementation of the BeD release into ERO improved the modelling and resolved discrepancies between modelling and experiments encountered in the previous studies [7, 8]. Reproducing the observations provides additional confidence in the 'ERO-min' fit for the physical sputtering yields of Be by deuterons for plasma-wetted areas. The same fit and other related data (e.g. atomic) and models are tested also in other experiments at JET and PISCES-B [11].

1. Introduction

In long pulse fusion devices at the reactor scale such as ITER, erosion will be one of the main factors determining the lifetime of the plasma-facing components (PFCs), particularly the low Z beryllium (Be) first wall (FW) in ITER. Estimating Be sputtering (physical and chemically assisted) by plasma ions and CX neutral is a key issue for general understanding of the plasma-wall interaction (PSI) [10, 11]. For instance it impacts on the tritium retention by co-deposition with Be, which must be kept within the nuclear safety limit of ITER.

The experimental campaign at JET equipped with the ITER-Like Wall (ILW) [1], with Be limiters and W divertor, included several experiments in limiter configuration dedicated to the determination of FW erosion. In the present paper we focus on three solid Be components ('tiles') of the poloidal guard limiter (GL) positioned at the inner wall (IW) close to the midplane. The limiter plasmas shifted towards the IW were used to have a single interaction point useful for the determination of Be yields. The magnetic configuration and plasma current was kept constant, just the D fueling was varied leading to the respective increase of electronic density with an opposite effect for its temperature and corresponding impact energy of sputtering ions. Passive spectroscopy of Be atoms, Be ions and BeD molecules were used for the characterization of erosion and its contributors. This work is a continuation and significant update of earlier studies [7, 8].

3D local transport modelling of eroded Be has been shown previously to be absolutely essential for the interpretation of sightline-integrated spectroscopy [7]. Similar to previous studies we utilize the Monte-Carlo (MC) code ERO [4] for this purpose. The code applies physical sputtering data based on molecular dynamics (MD) [12] and binary-collision approximation calculations [13]. This data is being benchmarked by comparison of the ERO synthetic results with the experimental observations.

A number of improvements have been carried out in comparison to the previous studies. The background plasma (ERO input) was revised including plasma conditions deduced from embedded Langmuir probes [14]. Moreover, the analytical expressions (AE) for the electric field in the sheath and for the very last part of the particle trajectory just before the ion collision with the surface were incorporated [6] providing more precise distributions of ion energies and angles with the surface on deuteron (D) impact. This affects the effective sputtering yield at each PFC surfaced point with varying local B-field angle with surface and local plasma temperature. The influence of the initial metastable population [15] after the physical sputtering on the light emission is studied. The contributions of self-sputtering and chemically assisted physical sputtering (CAPS) are assessed and discussed [16]. Since recent the new data [17] for Be molecular species decay in plasma including BeD_2, BeD_3 and molecular ions like e.g. BeD_2^+ is available (48 reactions), however incorporation in ERO is still ongoing.

The inclusion of the above mentioned effects and detailed benchmark of the simulations with experiments shall reduce uncertainties and give further confidence in the models and underlying data. From the other side it can lead to a correction of the earlier ERO predictions for ITER [3]. We discuss the possible effects in section 4.

2. Simulation of physical and chemical sputtering in ERO

The Be physical sputtering yield has been shown to be well approximated by the multi-parameter expression given in [13] depending on ion impact angle α_{imp} and energy E_{imp} and can be factorized into a normal incidence part $Y(E_{imp}, 0)$ and an angular-dependent part $A(E_{imp}, \alpha_{imp})$ as

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

At normal incidence $A(E_{imp}, 0)=1$, but the term can be significantly larger (up to an order of magnitude) for the typical case of tokamak FW components, where the B-field is nearly parallel to the PFCs, leading to the most probable α_{imp} of about 50-60^o [6]. To compute accurate effective yields (expression (1) averaged over proper distributions of E_{imp} and α_{imp} on impact) we generate these distributions a) dedicated preliminary ERO runs [8] or b) in the analytical expressions [6] for the E-field and the trajectory of the particles in the sheath region. In both cases we generate pre-calculated tables of effective sputtering yields $Y_{eff}(\eta, T_e)$, where η is the angle between the surface normal and the magnetic field. These tables are interpolated to compute the sputtering yield for each point on a given PFC surface. As a consequence of the orders of magnitude scatter for Be sputtering data available in the literature, in this paper two fits to the form of eqn. (1) are used, both based on basic simulated data obtained in the binary collision approximation (BCA) [13] and from the molecular dynamics (MD) approach [12]. In general, BCA is more suitable for the higher and MD for the lower impact energy range. The two fits reflect the uncertainty in the D content in the surface interaction layer: 'ERO-max' is produced by assuming a pure Be surface, whereas 'ERO-min' implies a constant D content of 50%, leading to a yield decrease by a factor of about 3-4.

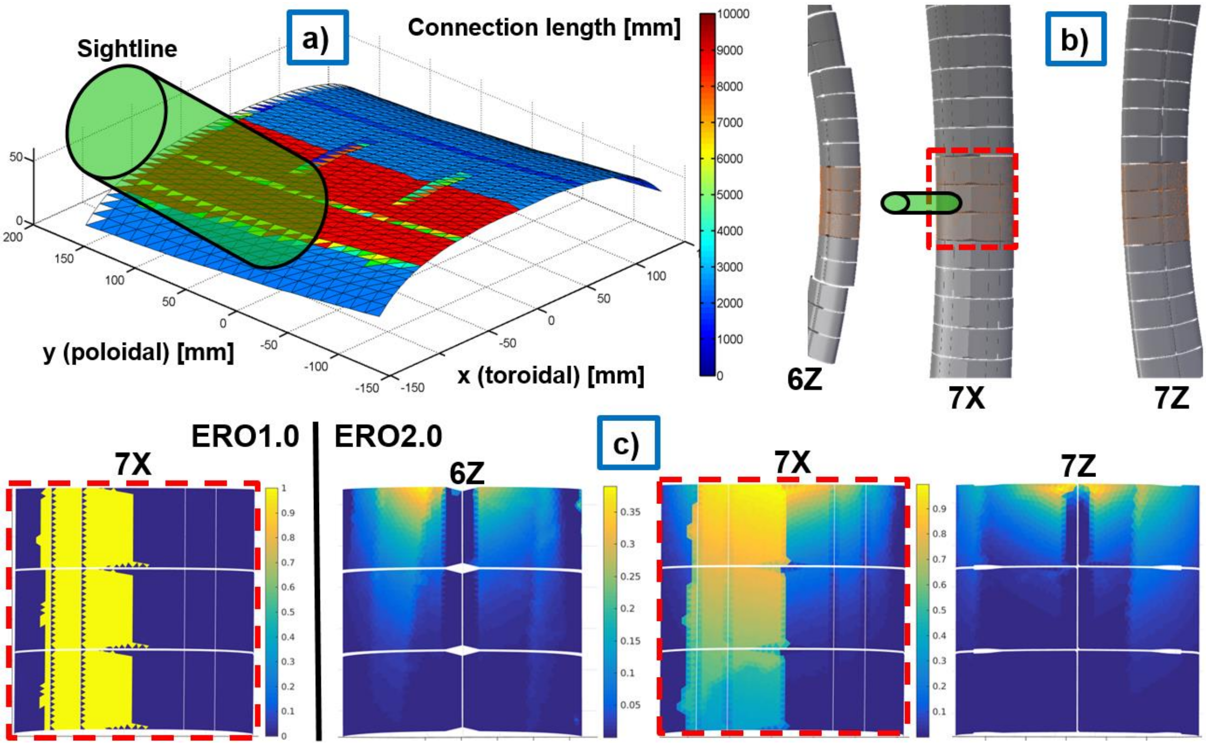

FIG.1. The passive spectroscopy at IW '7X' guard limiter: a) The connection length pattern simulated by the PFCFlux code [22] for the midplane part of the 7X limiter; b) The inner wall guard limiters '6Z', '7X' and '7Z' and the sighline location; c) shadowing patterns simulated with the crude ('ERO1.0') and the refined ('ERO2.0') assumptions [18].

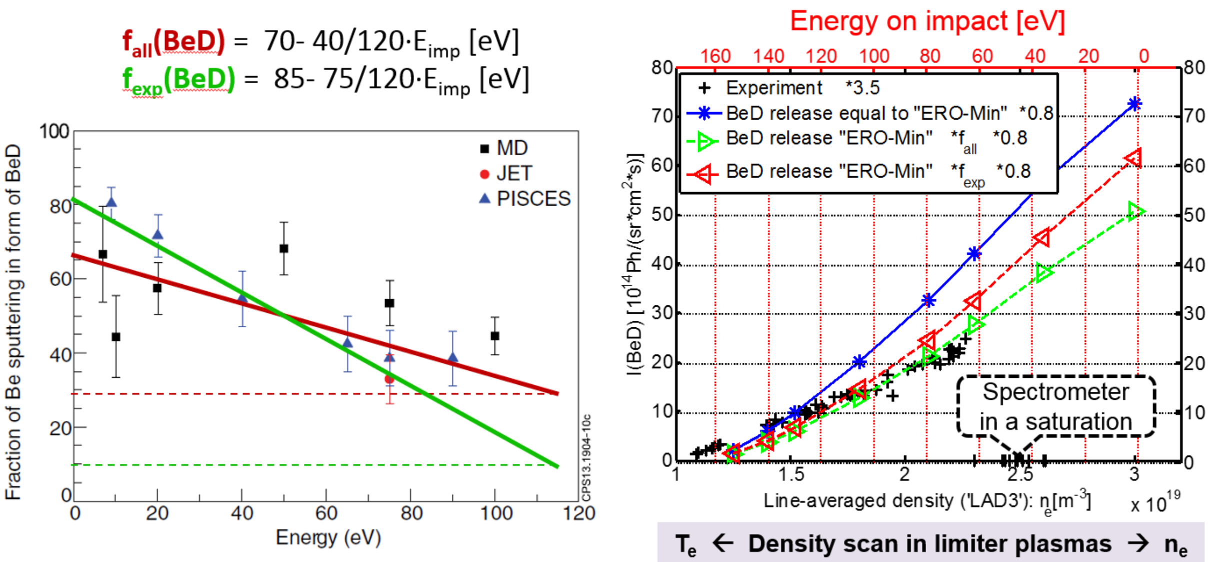

FIG.2. The BeD band emission simulated by ERO and observed in experiment (right) using the fits for the fraction of BeD release from obtained on the experimental ('PISCES', 'JET') and simulated ('MD') data from [5] (left graph). Measurements are multiplied by 3.5 to obtain the total band intensity whereas only a fraction of it depending on the vibrational and rotational temperatures is coming into the spectral window.

Chemically assisted physical sputtering (CAPS) of Be in the form of various Be-D molecules can contribute significantly (up to ~50% under some conditions) to gross erosion [5]. It should be noted that unlike the extensively studied chemical erosion of carbon PFCs, CAPS requires a given energy of impinging ions and the yield varies with energy and surface temperature $\boldsymbol{T_{surf}}$. ERO uses MD simulated data [12] for molecular release and also reaction data of the further decay and ionization of Be-D species in plasma. These latter data have been recently significantly updated and extended [17]. The MD simulations for the surface release continue [21], they show significant release of BeD_2 and BeD_3 molecules, however cannot clearly reproduce for now the suppression of CAPS with $\boldsymbol{T_{surf}}$ rise from 200°C to 400-450°C [5]. We attribute this effect to the D outgassing from the surface (it leads to lower D concentration in the surface which can explain the less effective molecular formation). Coupled MD-KMC (kinetic Monte-Carlo) simulations aimed to reproduce this effect are ongoing.

3. Simulation of physical and chemical sputtering in ERO

Benchmarking ERO on experimental results from the JET ILW is critical for gaining confidence both in the modelling approach and in the underlying atomic and surface erosion data. Two Be erosion experiments have been performed in inner wall (IW) limited discharges [5]. The integrated spectroscopic intensity of the light emitted in the sightline depicted in the FIG.1 is used to characterise the erosion from the surface. Fortunately, the right slope of the limiter is quite shadowed (FIG.1a) and does not contribute much to erosion and the Be light emission inside the sightline.

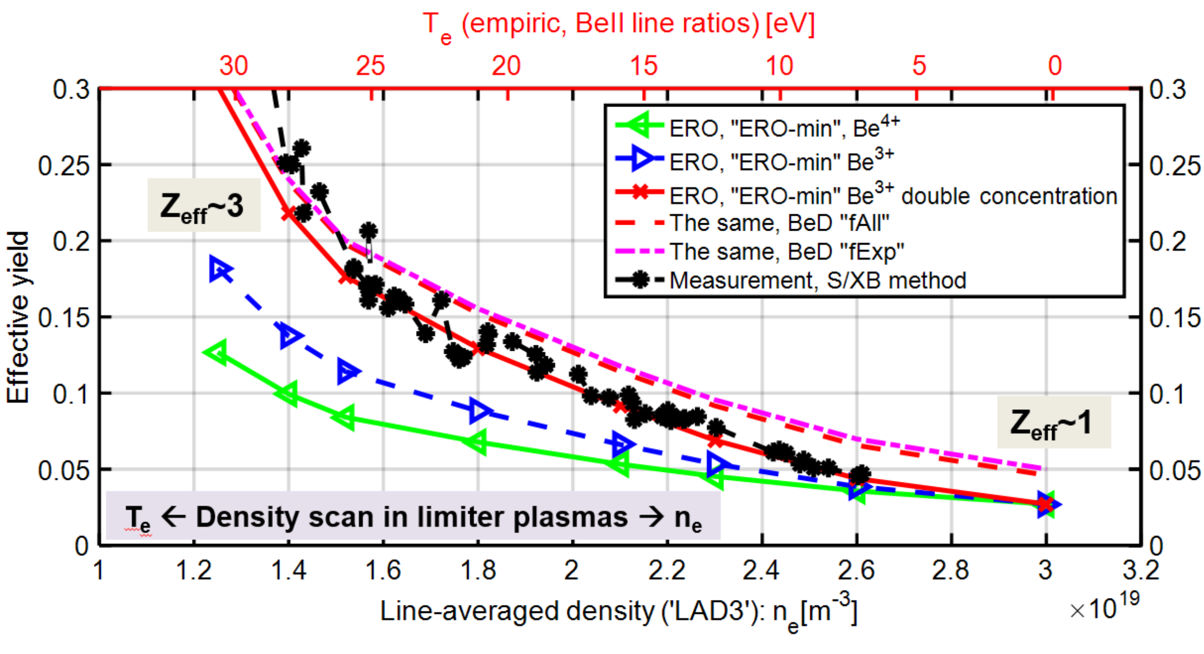

FIG.3. The effective sputtering yields in ERO and S/XB method measurements. The physical sputtering yield fit for Be with 50%D in the interaction layer ('ERO-min') is used [7]. The effect of self-sputtering assumptions (all Be ions charge and concentration) is illustrated. The analytical expressions [6] are used to produce the effective yields. The remaining uncertainties in the influence of CAPS and the intrinsic Be impurity concentration (leading to self-sputtering) are illustrated. The BeD release fractions "fAll" and "fExp" are explained in FIG.2 (left).

The T_{surf} rise in consecutive identical discharges was used to study its influence on the molecular release fraction, which was found to decrease to negligible values at T_{surf}~400^oC. The simulation of this effect with ERO is dependent on the progress with MD simulation of these data [21] which has difficulty to reproduce this effect.

The E_{imp} was scanned by varying the scrape-off layer plasma temperature (and density) whilst simultaneously monitoring the spectroscopic emission of Be I, Be II and BeD in the vicinity of the solid Be IW guard limiter. 3D ERO modelling allows the surface erosion to be characterized by the line-of-sight integrated emission. Two benchmark approaches were used [5]: a) the calculated $Y_{eff}(\eta, Te)$ were averaged over the relevant surface area and compared with experimental values obtained by the S/XB [23] method (FIG.3), and b) the absolute experimental brightness (of various lines) was compared to synthetic results from ERO (the details are given in [16]). Both methods show that the 'ERO-min' (high D concentration) sputtering assumptions lead to the best match between modelling and experiment, which is to be expected (high D surface content) for the plasma-wetted limiter surface.

The BeD light emission trend (FIG.2, right) and absolute value during the E_{imp} scan agree within 20% assuming a BeD fraction fit based only on empirical data points from PISCES-B, and slightly worse if MD data points are included.

The approach b) involves detailed ERO simulation of the erosion along the shaped surface, 3D local transport in the context of 3D plasma and electromagnetic field configuration, atomic and molecular processes and, finally, simulating and integrating in the sightline light emission. It gives deeper insight, however it demands much more input data. The main uncertainties are connected with the plasma parameter background for ERO reconstructed in 3D from various diagnostic results (reciprocating and embedded Langmuir probes, spectroscopy, Thomson scattering). Post-processing for the embedded probe data [14] has led to the significant correction of the plasma background used in newest simulations [16]. The T_e was corrected by factor of about 2 and was found to be of about 15eV at the limiter tip limiting the plasma. Nevertheless, the credibility of this important input for ERO was confirmed by reproducing the experimental line ratios in Be II, D spectroscopy and the branching ratio of Be-D reactions. At large densities and low impact energies (Z_{eff}~1) the trends for various Be I and Be II lines are well reproduced. Still, the simulations overestimate the Be II light nearly by a factor of 2. Partially it can be explained by the remaining uncertainties in the plasma backgrounds and BeD data and assumptions e.g. is was supposed that BeD release does not affect physical sputtering. The details can be found in [16].

Several additional effects were considered in the calculations, e.g. the influence of the metastable state population [9, 15] and, most important, magnetic shadowing. Unlike the crude geometrical procedure used in the earlier ERO runs for ITER [3] to determine the shadowed areas, the current version of the code uses the connection lengths calculated by the PFCFlux field tracing code [22]. However the first application of the new massive-parallel 'ERO2.0' code [18] demonstrates that there is a room for improvement. Including larger simulation volume leads to a significant increase of the amount of the traced particles returning to the surface and contributing up to 40% more to the self-sputtering. Another 15% of the self-sputtering increase comes from the neighbour limiters erosion (FIG.1b). One should note that self-sputtering by the intrinsic plasma impurity discussed below is dominating over the locally eroded particles traced by ERO. More refined treatment of the shadowing (FIG.1c) can obviously also be of importance though in the case at hand it is not very significant (for '7X' IW guard limiter).

Another uncertainty arises from the concentration of the Be plasma impurity. It can be illustrated well by the benchmark with the simpler S/XB [23] approach (FIG.3). One can see good agreement of all simulations at small T_e meaning less sputtering due to small E_{imp}

leading to negligible Be concentration in plasma confirmed by Z_{eff}~1. In general the self-sputtering is treated using the formula

$$Y_{total} = Y^{Eff}_{Be \leftarrow D} * (1-f_{Be}) + Y^{Eff}_{Be \leftarrow Be} * (f_{Be}), \qquad (2)$$

where $Y^{Eff}_{Be \leftarrow D}$ and $Y^{Eff}_{Be \leftarrow Be}$ are the effective sputtering yields for D and Be ('self-sputter') eroding species. The f_{Be} is estimated from the measured effective charge Z_{eff}. Be impurity comes partially from the closest PFCs, but also from the core as Be^{4+} (Z_{Be}=4), which however can also recombine e.g. to Be^{3+} on its way. Self-consistent modelling would demand including a much larger volume, with all relevant impurity sinks and sources and self-consistent tracking of Be ions. For now we can just assume that all Be ions come for instance as Be^{4+} or alternatively Be^{3+}. The charge Z_{Be} has no influence on the sputtering yield by itself, however it affects the charge-dependent acceleration in the sheath, though the yield dependence on energy is stagnating. Thus the erosion upon assumption of 3+ charge is larger due to the amount of atoms deduced from Z_{eff} (fig. 6). The assumption of Z_{Be} =3 charge and double concentration (not illogical for the erosion location) leads to a perfect match with the experiment. This is of course more an indication than a proof that we interpret the self-sputtering correctly.

The uncertainties do not allow a direct benchmark of the self-sputtering yields, although no unexplainable contradictions were found. The 'ERO-min' basic fit (1) for 'Be by Be' sputtering as well as distributions on impact and the corresponding effective yields are produced in exactly the same way as for 'Be by D' sputtering, leading us to expect similar accuracy.

The 'ERO-max' fit based on (mostly BCA) simulations for pure Be surface would lead to about 4 times larger sputtering [7] than 'ERO-min' which matches well the experiment. The contribution of CAPS is also illustrated in FIG.3. It increases the effective total yield, but not significantly, probably within our uncertainties in particular for the Be-D/Be release fraction. The 'ERO-min' with the old pure numeric approach for generating distributions on impact would lead to ~30% smaller results than the experiment.

It should be mentioned that a very similar work goes in parallel for the OW of JET where Be erosion at certain location is affected by the RF-power of the ICRH antenna [19] which was interpreted by ERO using further development of the AE mentioned above [20]. It allows testing the maximum of the sputtering yield and indirectly confirms the 'ERO-min' assumptions. The Be data used in ERO are also tested by experiments the PISCES-B linear plasma device [9] again indicting that BCA simulations for pure Be overestimate the yield.

4. Possible effect of the recent findings on the ITER predictions

Earlier ERO predictive modelling results [3] for the erosion of ITER FW panels should be re-visited in the light of the new input on erosion yields. The ILW benchmark leads to the conclusion that the previously calculated upper limit (based on the 'ERO-min' assumption) of the lifetime estimation due to steady state erosion of ~4200 full burn ITER discharges for the FW panels in the vicinity of the secondary X-point at the top of the main chamber is the most appropriate. However, the analytical approach [6] for treating of ion-surface impacts leads to an increase (*FIG.4*) of effective yields (section 2). In [3] it was shown that the maximal erosion at the critical location (limiting the lifetime) is linear dependent on the effective yield, however all these simulations were done with the same version of the code. The contribution of CAPS can lead to a further contribution to the erosion, depending on the T_{surf}. The influence of the self-sputtering due to Be plasma impurity has also been investigated, however despite the yields are much larger the influence of this effect for ITER can be expected to be significantly low due to the much lower Be impurity concentration.

It is important to point out, however, that these estimates are based on the most conservative assumptions regarding the both a) background plasma parameters expected on ITER under burning conditions with QDT = 10, and b) magnetic equilibria in terms of separation between the primary and secondary separatrix. In reality, the Be FW panel lifetime due to steady state erosion is expected to be far greater.

In [3] it was shown that the maximal erosion at the critical location (limiting the lifetime) is linear dependent on the effective yield, however all these simulations were done with the same version of the code. The significantly updated with JET experience model and data can lead to qualitatively different results. It should also be noted, that factors like for instance plasma shadowing or re-deposition of Be plasma impurity lead to a decrease of the net erosion. The interplay of various factors demands the re-calculation with the updated code to make responsible predictions. Such re-visiting makes sense in the near future after fixing remaining uncertainties in the CAPS yields [21] and incorporation of Be-D reaction data [17].

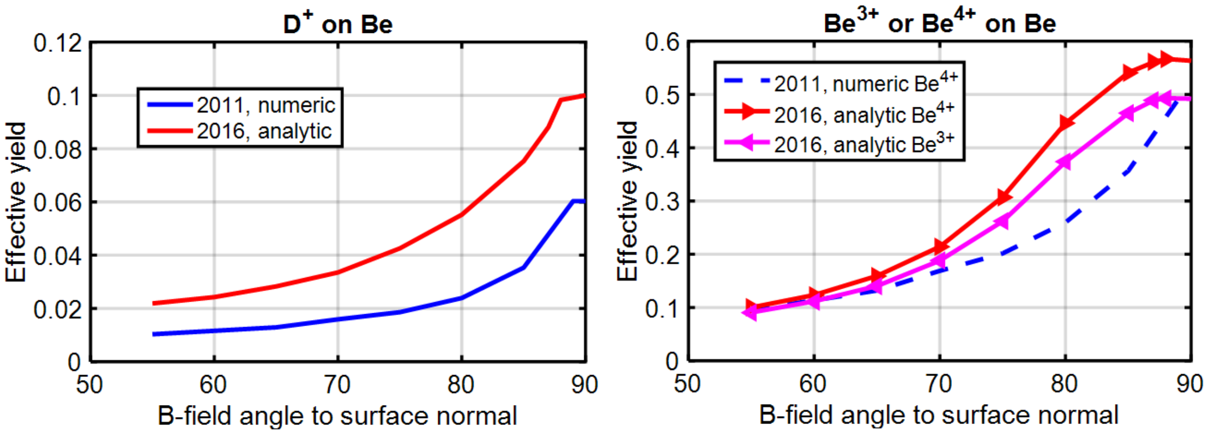

FIG.4. The effective yields $\mathbf{Y_{eff}(\eta)}$ integrated on the basis of the pre-calculated angle and energy distributions of the sputtering ions on impact. The older pure numeric ERO simulations used in [3] and recent simulations on the basis of analytic expressions [6]. $\mathbf{T_e}$ *=10,* $\mathbf{T_i}$*=20 are constant for the whole surface of the ITER blanket module considered in [3] in the assumed 'high density' conditions.*

5. Conclusions

A significant update for modelling [8] of Be erosion at JET ILW characterized by the passive spectroscopy [5] is carried out. The plasma parameters input was revisited [16] (correction of formerly overestimated $\boldsymbol{T_e}$). New analytical expressions [6] were applied to generate the energy and angle sputtering ion distributions on impact determining the effective sputtering yields. The AE-based distributions lead in general to the increase of the sputtering yield depending on the basic yields (1), B-filed orientation and plasma conditions at the PFC. The benchmark with the ILW experiment using the S/XB approach indicates that 'ERO-min' fit (averaged over the impact angle and energy distributions to get the effective yields) can be recommended for plasma-wetted areas as the limiter surface considered in this work. The corresponding BeD A-X band intensity trend during the $\boldsymbol{E_{imp}}$ scan is reproduced well and the absolute value within 20%. The ERO application to Be exposure to helium plasma at PISCES-B [11] also indicates lower effective yields than BCA calculations (SDTrimSP code) [13] for the pure Be surfaces. The same comes from the PISCES-B experiments with D plasma [24].

The ERO modelling of BeD release, local transport and respective surface and reaction data should be further improved. For that a detailed simulation of the surface temperature scan experiment [5] would be useful as well as further experimental studies. The shadowing treatment and self-sputtering assumptions should also be refined (more powerful massive parallel ‘ERO2.0’ version of ERO [18], which allows including larger simulation volume, more of the relevant PFCs and more detailed geometry). After that the simulations for ITER life time [3] should be re-visited. It is easy to see from the work at hand that ERO modelling is very useful for extrapolation of the Be erosion data from the experiments at existing devices (JET with ILW, PISCES-B) for ITER.

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