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Hakola, A.; Airila, M. I.; Mellet, N.; Groth, M.; Karhunen, Juuso; Kurki-Suonio, T.; Makkonen, T.; Sillanpää, Heikki; Meisl, G.; Oberkofler, M.; ASDEX Upgrade Team ERO and PIC simulations of gross and net erosion of tungsten in the outer strike-point region of ASDEX Upgrade

Published in: Nuclear Materials and Energy

DOI: 10.1016/j.nme.2016.09.012

Published: 01/08/2017

Document Version Publisher's PDF, also known as Version of record

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Please cite the original version:

Hakola, A., Airila, M. I., Mellet, N., Groth, M., Karhunen, J., Kurki-Suonio, T., Makkonen, T., Sillanpää, H., Meisl, G., Oberkofler, M., & ASDEX Upgrade Team (2017). ERO and PIC simulations of gross and net erosion of tungsten in the outer strike-point region of ASDEX Upgrade. *Nuclear Materials and Energy*, *12*, 423-428. https://doi.org/10.1016/j.nme.2016.09.012

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Nuclear Materials and Energy 000 (2016) 1-6



Contents lists available at ScienceDirect



[m5G;October 8, 2016;6:24]

Nuclear Materials and Energy



journal homepage: www.elsevier.com/locate/nme

ERO and PIC simulations of gross and net erosion of tungsten in the outer strike-point region of ASDEX Upgrade

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ARTICLE INFO

Article history: Available online xxx

Keywords: ASDEX Upgrade Tungsten erosion ERO modelling PIC simulations Particle drifts Cross-field diffusion

ABSTRACT

We have modelled net and gross erosion of W in low-density L-mode plasmas in the low-field side strike point region of ASDEX Upgrade by ERO and Particle-in-Cell (PIC) simulations. The observed net-erosion peak at the strike point was mainly due to the light impurities present in the plasma while the noticeable net-deposition regions surrounding the erosion maximum could be attributed to the strong $\mathbf{E} \times \mathbf{B}$ drift and the magnetic field bringing eroded particles from a distance of several meters towards the private flux region. Our results also imply that the role of cross-field diffusion is very small in the studied plasmas. The simulations indicate net/gross erosion ratio of 0.2–0.6, which is in line with the literature data and what was determined spectroscopically. The deviations from the estimates extracted from post-exposure ion-beam-analysis data (~0.6–0.7) are most likely due to the measured re-deposition patterns showing the outcomes of multiple erosion-deposition cycles.

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1. Introduction

The limited lifetime of plasma-facing components (PFCs) can be a potential showstopper in future fusion reactors including ITER and DEMO [1]. Therefore, one has to fully understand the damage mechanisms and erosion behavior of different PFCs upon exposure to various plasma scenarios. Furthermore, quantifying the erosion rates requires distinguishing between gross and net contributions: these can differ considerably as a large fraction of the eroded material will be locally re-deposited [1].

Tungsten (W) has proven to be a suitable PFC material as demonstrated in several tokamaks like ASDEX Upgrade (AUG) [2] and JET [3]. Its main advantages are small erosion yield by plasma bombardment, good power-handling capabilities, and low accumulation of tritium in the material [4]. Re-deposition of W, for its part, is generally > 50% of gross erosion [5] and approaches 100% in high-density plasmas [6].

Here, we investigate steady-state gross and net erosion of tungsten and restrict our considerations to the low-field side (outer) strike point region of AUG. We numerically model the experimental net-erosion and re-deposition patterns by the ERO code [7] and by Particle-in-Cell (PIC) simulations [8], with the goal of identifying the contribution of various physical factors on the erosion characteristics. The starting point is an experiment, carried out at AUG in 2014 where W samples were exposed to a series of L-mode plasma discharges [9].

2. Review of experimental results

The experimental database is based on a dedicated experiment in which special W marker samples were exposed to 13 identical plasma discharges in deuterium in the outer strike point region of AUG [9]. A full poloidal row starting from about 50 mm below the strike point, in the private flux region (PFR), and extending ~150 mm in the scrape-off layer (SOL) of the divertor plasma was covered. The location of the samples and the strike line of the experiment are shown in the inset of Fig. 1. All the samples had a 20-nm thick W marker on graphite as well as a 0.2-mm deep, uncoated trench magnetically downstream of the marker and finally an inclined Mo marker (thickness 20 nm).

Low-density L-mode plasmas were used such that the electron temperatures around the outer strike point were 20–40 eV.

http://dx.doi.org/10.1016/j.nme.2016.09.012

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Fig. 1. (a) Experimentally determined poloidal net deposition/erosion profile of the W marker as well as poloidal re-deposition profiles for W on the graphite and Mo markers. Negative values denote net erosion, positive net deposition and PFR corresponds to the poloidal distance being negative. Inset shows schematic illustration of the AUG divertor and the target tile (red). The magnetic field points towards the viewer. (b) Photograph of the marker samples on the target tile after their exposure to plasma discharges together with a schematic drawing of one of the samples and its geometry. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



Fig. 2. (a,b) Experimental Langmuir-probe data and simulated OSM profiles for the poloidal profiles of (a) electron density and (b) electron temperature around the strike point. (c) Poloidal profiles for the two electric field components (E_x and E_z) used in the ERO simulations together with the definitions for the ERO co-ordinate system.

The poloidal profiles of n_e and T_e , as measured by fixed Langmuir probes, are shown in Fig. 2a and b together with their modelled counterparts that were used in subsequent ERO and PIC simulations. The net erosion of the W markers as well as re-deposition of W on the trench and on the Mo marker were determined using Rutherford backscattering spectroscopy (RBS) and the resulting erosion and deposition rates (nm/s) are collected in Fig. 1.

The main observations are a noticeable net-erosion zone, coinciding with the location of the strike point, and clearly distinguishable deposition-dominated regions on both sides of the erosion maximum. On the SOL side, the deposition peak is almost 40 mm wide and matches with the location of the main deposition peak of light impurities boron (B), carbon (C), and nitrogen (N) (see [9]). These observations hint towards a strong influx of material, however, in the absence of direct measurements of the fluxes of different impurity ions in the plasma (B, C, N, W) this hypothesis cannot be experimentally verified.

The shape of the W re-deposition profile on the graphite and Mo markers in Fig. 1 is, unexpectedly, quite similar to the net erosion/deposition curve for the W marker. If graphite and Mo were efficiently shadowed from direct contact with plasma during the experiment, the deposition rate should peak close to the most prominent source, i.e., the strike point, and gradually diminish further away from it. According to Fig. 1 this is not the case.

If we estimate the ratio between net erosion, N, and gross erosion, G, close to the strike point, assuming that G = N + R, where R stands for re-deposition, we obtain N/G~0.6–0.7. However, literature values indicate much larger re-deposition, corresponding to N/G < 0.5 (see [3,6]). Thus, especially the trench and Mo marker appear to show the outcomes of multiple erosion-deposition cycles. An independent estimate for gross erosion by spectroscopic

measurements of the neutral WI line at 400.9 nm supports the conclusion: a relatively sharp erosion profile with N/G = 0.4-0.6 around the strike point emerges [9].

3. Simulation setups

3.1. ERO modelling of net and gross erosion

To understand the physics behind the features observed in Fig. 1, we have modelled the erosion and deposition processes using ERO. ERO is a 3D Monte Carlo code that simulates the transport of test particles in the SOL [7]. We used the divertor version of the code and carried out the simulations in a computational volume illustrated in Fig. 3a. The entire toroidal ($\Delta y = 70$ mm) and poloidal ($\Delta x = 300$ mm) extent of the target tile were covered, and the box was $\Delta z = 50$ mm high in the direction normal to the surface. A 5-mm spacing was used for the simulation grid, and in the toroidal direction periodical boundary conditions were established to prevent unphysical losses of particles. This is in line with full W coverage of the AUG divertor in the toroidal direction. The solid black line in Fig. 3a denotes the simplified wall geometry of AUG that was used in background-plasma calculations.

For simplicity, only the W marker was considered and implemented as bulk material. The overall simulation time was 1 s at 0.01 s steps and the number of test particles was 10^4 per time step. This was enough for equilibrium to be reached and accumulate enough statistics for reliable profiles. Losses through the poloidal and perpendicular side faces of the simulation box were generally < 0.1% of the primarily sputtered atoms.

The background deuterium plasma was produced by the DI-VIMP code with its Onion Skin Model (OSM, SOL option 22) ac-

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Fig. 3. (a) Schematic illustration of the ERO simulation box and the applied co-ordinate system. (b) ERO results for the poloidal net deposition/erosion profile in the base case (blue circles, $c_W = 0.005\%$, $c_B = c_C = c_N = 0.5\%$) and in the cases with $c_W = 0.01\%$, $c_B = c_C = c_N = 0.5\%$ (red rectangles) and with $c_W = 0.01\%$, $c_B = c_C = c_N = 1.0\%$ (black asterisks). Also the experimental profile has been reproduced. (c) Poloidal gross erosion (blue circles) and re-deposition (red rectangles) profiles for the base case. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

tivated [10]. The code returns values for electron density, electron and ion temperatures, and flow velocity along magnetic flux surfaces of the OSM grid, which were then interpolated to obtain corresponding plasma data in the ERO volume. The resulting profiles for n_e and T_e along the target surface (z=0) are shown in Fig. 2a and b together with the experimental ones. Different fits for the experimental profiles were used as input for the OSM simulations. Deep in the private flux region, where the OSM background was missing, a cold plasma approximation with $n_e = 10^{17}$ m⁻³ and $T_e = T_i = 0.1$ eV was used. The T_e profile has a somewhat longer decay length in the SOL side and the peak is lower than the Langmuir-probe data suggests, while the n_e peak is overestimated at the strike point. These may have had an influence on the shape and absolute levels of the simulated erosion and deposition profiles.

In the simulations, the type and concentration of typical light impurities in the AUG divertor plasma (here B, C, and N) and W originating from other parts of the torus than the simulation box were varied such that the effective charge, Z_{eff} , remained within reasonable limits (between 1.5 and 2.6) and that the concentrations of individual impurities agreed with previous measurement results from AUG, i.e., c_B , c_C , and $c_N < 1.0\%$ and $c_W < 0.01\%$ [11,12]. One should note that the measurements are from the core while in the divertor region the concentrations can locally be much larger. From coronal equilibrium [13], we obtain for the average charge states of the impurities $q_{\rm B} = 3$, $q_{\rm C} = 4$, $q_{\rm N} = 5$, and $q_{\rm W} = 13$ in the simulation volume. The anomalous diffusion coefficient was varied from 0 to 1.0 m²/s with $D_{\perp} = 0.2 \text{ m}^2/\text{s}$ being the nominal value. No pre-calculated, integrated sputtering yields existed for the projectile-target combinations at higher charge states (q > 2) to describe background plasma sputtering. Instead, we estimated the missing data by the Bohdansky-Yamamura formalism (see [14,15]).

The effect of $\mathbf{E} \times \mathbf{B}$ drift was investigated by including the electric field in the plasma background [16,17]. Since the OSM solution did not contain the electric field, nor the plasma potential, we created plausible profiles for the poloidal (E_x) and normal (E_z) components of the field by assuming the potential Φ being directly proportional to T_e , i.e., $\Phi = 3k_BT_e/e$; the electric field is then evaluated by $\mathbf{E} = -\nabla \Phi$ [18]. By assuming that the plasma potential remains the same along all the lines that are parallel with the magnetic field in the *xz* plane, one obtains a profile shown in Fig. 2c.

3.2. PIC simulations

To further study the role of re-deposition on the erosion/deposition behaviour of tungsten we carried out simulations based on the magnetic sheath potentials calculated selfconsistently with a 1D PIC code introduced in [19]. Impurities were injected into the plasma as test particles and assumed not to influence the evaluated electric field as described in [8]. The required profiles for plasma parameters were again taken from the OSM solution (see Section 3.1) and also the impurity mix of the plasma was varied similarly to the case of the ERO runs.

The 2D profiles for the normal (E_z) and poloidal (E_x) components of the calculated electric field are shown in Fig. 5a and b. The field was determined by interpolating the potentials resulting from PIC calculations for a set of parameters that include the density, the angle of the magnetic field with respect to the surface, and the ion/electron-temperature ratio. The component E_z reaches much larger values than E_x and the profiles used in ERO simulations (see Fig. 2c), but only in the immediate vicinity of the surface, within the magnetic sheath; further away, the two components are comparable. Note also that the sheath electric field towards the surface extends the farthest into the plasma where the temperature is the highest. A correction for the potential drop was introduced to compensate for the drift induced by the poloidal field so that ambipolarity was maintained.

Physical sputtering was treated according to the Eckstein's formulas [20] or, in the case of B and C, to the revised Bohdansky– Yamamura formalism [14,15]. Re-deposition was computed by injecting atoms with cosine angular and Thomson energy distributions. Altogether 10⁶ tungsten atoms were injected in each run. We also used at least 1000 iterations for each Larmor gyration once the particle was ionised. The simulation domain covers the same size box as the one used in ERO, which is much larger than the region shown in Fig. 5a and b.

4. Results

4.1. ERO modelling

Light impurities are responsible for almost all the observed net erosion in the vicinity of the strike point (see Fig. 3b). Here, poloidal net erosion profiles resulting from ERO simulations with $c_{\rm B}$, $c_{\rm C}$, and $c_{\rm N}$ varied from 0.5–1.0% and the W concentration within the range $c_{\rm W} = 0.005$ –0.01% are shown. For comparison, the experimental net erosion profile of Fig. 1 is reproduced in the figure. If only W was included in the simulations, net erosion would be almost two orders or magnitude smaller unless unrealistically high $c_{\rm W}$, of the order of a few %, was used.

One should note that it is mainly the effective charge, Z_{eff} , that influences the maximum of the main erosion peak: the exact impurity composition plays a minor role. The peak scales roughly as Z_{eff}^{-1} within the investigated range of $Z_{\text{eff}} = 1.5-2.6$. According to [11], the typical impurity content of the AUG SOL plasma would result in $Z_{\text{eff}} \sim 1.5-2.0$, albeit $Z_{\text{eff}} > 2.0$ can locally exist in divertor plasmas. This leads us to select a *base case* with $c_{\text{B}} = c_{\text{C}} = c_{\text{N}} = 0.5\%$ and $c_{\text{W}} = 0.005\%$ for follow-up simulations, cor-

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Fig. 4. (a) ERO results for the poloidal net deposition/erosion profile in the base case both with (red triangles) and without (blue circles) the electric field. (b) Poloidal gross erosion (blue circles) and re-deposition (red rectangles) profiles for the case with the electric field being switched on. (c) Influence of cross-field diffusion on net deposition/erosion: $D_{\perp} = 0$ (black diamonds), $D_{\perp} = 0.2m^2/s$ (red triangles), and $D_{\perp} = 1.0m^2/s$ (orange stars). In (a) and (c) also the experimental profile has been reproduced. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

responding to $Z_{\text{eff}} = 1.81$. According to Fig. 3b, maximum net erosion would then be underestimated by about a factor of three. Increasing Z_{eff} improves the match but the simulated erosion rate is still off by ~25%. Besides the net-erosion peak, the simulations qualitatively predict the formation of a broad net-deposition plateau on the SOL side of the strike point, though the deposition rates are 3–5 times smaller than the experimental values. In addition, a deposition notch is seen to emerge in the PFR but the remarkable narrow peak around x = -20 mm remains far from being reproduced.

The net erosion region clearly coincides with the peak of the T_e profile (see Fig. 2b), while the occurrence of net deposition zones is best explained by a large fraction of the eroded particles returning on the surface a few mm off from the location from which they were sputtered. This we can see in Fig. 3c where poloidal gross erosion and re-deposition profiles of W are illustrated for the base case. The simulated erosion and re-deposition rates are 2–5 times larger than the net-erosion rates, indicating that indeed the net/gross erosion ratio would be N/G~0.2–0.5 in contrast with N/G~0.6–0.7 reported in [9]. This gives support for the hypothesis that the measured amounts of W at the bottom of the graphite trench and on the Mo marker have been subjected to significant plasma-surface interactions during the experiment.

Besides the discrepancies discussed above, the simulated net erosion poloidally far away from the strike point approaches zero independent of the applied impurity content of the plasma while experimentally it should saturate towards a value of ~0.04 nm/s. The reason may be connected with the OSM solutions for T_e and n_e deviating from the measured profiles (see Fig. 2a and b), which may further contribute to the erosion/deposition balance. In addition, the approximations we made to obtain the missing integrated sputtering yield data (see Section 3.1) may have led to underestimated gross erosion at low T_e . However, also other factors than the impurity content need to be considered.

The clearest contribution comes from the $\mathbf{E} \times \mathbf{B}$ drift. To this end, we ran simulations using the field profile of Fig. 2c and the impurity content of the base case above. The net erosion peak at the strike point becomes more pronounced and the deposition maxima surrounding it more peaked such that a relatively good qualitative match with the experimental curve within the strikezone region x = -30...20 mm is obtained. This is illustrated in Fig. 4a where the resulting net erosion/deposition profiles for ERO simulations with and without the drift term are shown, together with the experimental ones. Especially, the deposition peak in the PFR has become much more noticeable than in the no-drift case of Fig. 3b. This is caused by altered transport of the particles: gross erosion is not affected by the field but the re-deposition profile is largely shifted towards the SOL in the poloidal direction as we notice from Fig. 4b. However, both gross erosion and re-deposition remain at the same level as in Fig. 3c, which sets the net/gross erosion ratio to $N/G \sim 0.5-0.6$. This is close to the experimental values in [9] but still smaller and subject to large error bars induced by the shape of the electric field profile.

The normal component of the field, E_z , affects the distribution of W atoms on the surface by driving them poloidally either towards or away from the strike point, e.g., in the geometry of Fig. 3a downwards if $E_z < 0$. The other field component, E_x , influences the erosion/deposition picture only indirectly. The more negative E_x is, the more particles will drift away from the surface and in addition to being re-deposited further away from their origin escape from the simulation box; positive values for E_x will keep the eroded atoms more tightly close to the surface.

The effect of thermal gradient forces parallel to the magnetic field [17] on the erosion/deposition profiles (not shown) was observed to be negligible but cross-field diffusion played an important role in the balance between erosion and deposition. By reducing the perpendicular diffusion coefficient, net erosion and deposition peaks were both sharpened whereas larger values for D_{\perp} re-distributed the particles on the surface, thus smearing out all the prominent features of the profiles. This becomes evident from Fig. 4c where the simulations at $D_{\perp} = 0$, 0.2, and 1.0 m²/s are presented with the $\mathbf{E} \times \mathbf{B}$ drift switched on.

We conclude that the locations and magnitudes of the deposition maxima are largely attributed to the poloidal transport of particles and diffusion across the field lines. Since in our model the electric field is proportional to the gradient of the electron temperature, it is clear that even small changes in the T_e profile can result in large changes in the **E** profile, when also inaccuracies in determining the exact value for the T_e peak are taken into account. Besides, also the field component induced by parallel Pfirsch-Schlueter current would need to be taken into account [21] but this is beyond the scope of the present work.

4.2. PIC modelling

Three PIC simulations were performed: one with the full electric field of Fig. 5a and b, the second with only the E_z component turned on, and the last one without any electric fields. The case with only E_z being active was selected to study transport purely in the poloidal direction, according to the discussion above (in Section 4.1).

The poloidal erosion/deposition profiles are shown in Fig. 5c. Additionally, Fig. 5d shows the comparison between the re-deposition and gross erosion profiles in the full electric field case. Qualitatively, the PIC profiles have many similarities with the ERO results of Figs. 3 and 4 but the net erosion maximum at the strike point is deeper and the deposition peak on the SOL side is almost non-existent. The situation without the electric field

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Fig. 5. (a,b) 2D profiles for (a) E_z and (b) E_x used in the PIC simulations. The field had been generated by interpolating the magnetic sheath potentials calculated by the PIC code. (c,d) PIC results for (c) net deposition/erosion computed using the test-particle in three cases: no electric field (blue), only the E_z component activated (blue) and the full electric field (black) and (d) poloidal gross erosion (blue) and deposition (red) profiles in the full electric field case. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



Fig. 6. PIC results for 2D re-deposition profiles of the prompt (a,c) and long-range (b,d) fractions. Two models have been compared: only E_z (a,b) and the full electric field (c,d). Superimposed in (d) is re-deposition taking place toroidally outside of the original box.

is even more extreme – only large net erosion with rates more than 2 times the experimental values is observed. This we can understand by noting that now only Larmor gyration influences re-deposition, which will shift the entire re-deposition distribution poloidally upwards. In the PFR, the experimentally observed net-deposition peak starts to be formed when the electric field is switched on - but only for the full electric-field case a good correspondence with the experimental and simulated profiles is obtained in this region.

The re-deposition picture is, however, more complicated than what can be concluded from the analyses above. To this end, we separated re-deposition into two components: prompt redeposition where tungsten ions end up on the surface within their first Larmor radius and long-range re-deposition where they undergo several gyrations before returning on the surface. The 2D redeposition profiles are displayed in Fig. 6a and b for both these contributions in the case $E_x = 0$ and in Fig. 6c and d for the full model. In both cases, prompt re-deposition (Fig. 6a and c) is local, the profiles have an extent of some 10-20 mm from the strike point, and the effect of E_x is weak. The pattern, however, changes drastically when long-range deposition is considered (Fig. 6b and d). In the case $E_x = 0$, a significant part of re-deposition occurs poloidally downwards of the strike point and can be attributed to the **E** × **B** drift induced by large and negative E_z (see Fig. 6b). This we also notice from Fig. 5c. In the full model, however, the relatively strong **E** × **B** drift towards the plasma due to E_x competes with the effect of the magnetic field to bring the particles towards the wall and results in re-deposited W travelling several meters in the toroidal direction. This suggests that the peak in the PFR in Fig. 5c could originate from bulk divertor material - or from material originating from other PFCs of the AUG torus - as the inset of Fig. 6d illustrates. Simultaneously, the number of particles accumulating poloidally upwards to the strike point (where E_x is oppositely oriented) is increased. Unlike the case $E_x = 0$, particles can be re-deposited in the direction opposite to the magnetic field as the projection of E_x on **B** is oriented in that direction (**B** being not fully toroidal).

5. Discussion and conclusions

We have numerically modelled the experimentally determined net and gross erosion of W in the outer strike point of AUG by ERO and PIC simulations. The strong net-erosion peak at the strike point was reproduced by adding a realistic mixture of light impurities (a few at.%) in the plasma while the noticeable deposition peaks poloidally on both sides of the strike point could be explained by the strong $\mathbf{E} \times \mathbf{B}$ drift on the targets.

The determined net/gross erosion ratio was 0.2–0.6, which is to be compared with the experimentally determined value of \sim 0.6– 0.7. The discrepancy is attributed to the re-deposited material having been in contact with plasma during the rest of the experiment. Indeed, independent, spectroscopic estimate for the net/gross erosion ratio of 0.4–0.6 supports this hypothesis.

The $\mathbf{E} \times \mathbf{B}$ drift is the most significant individual factor contributing to the shape of the erosion/deposition profile. ERO simulations indicate that both the erosion and deposition peaks become sharper when the drift terms are activated. On the other hand, PIC simulations indicate that also transport of material along the magnetic field lines has to be taken into account: the particles originating from other regions of the divertor or main chamber can travel several meters in the toroidal direction and increase the W inventory in the private flux region. On top of the drifts, our results suggest a very small value for D_{\perp} in low-density plasmas, thus crossfield diffusion plays a minor role.

The remaining shortcomings in the reproduction of the two experimentally observed deposition peaks are currently being adJID: NME

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dressed by WallDYN simulations [22] which use computational grids covering a large volume. Based on the analysis of the erosiondeposition patterns of W in medium-density L-mode plasmas, local W migration can lead to such a two-peak structure [22]. Also, our ERO simulations indicate that at least part of the observed discrepancy is caused by a loss of eroded W at the boundary of the computational grid. However, a more detailed analysis of these simulations, the preparation of background plasmas that better reproduce the n_e and T_e profiles, using more realistic electric-field profiles, and the evaluation of the missing integrated sputtering yields on the basis of data by Eckstein [19] are still pending. Finally, new experiments with modified geometry of the material samples are considered to eliminate one source of uncertainty.

Acknowledgements

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014–2018 under grant agreement number 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission. Work performed under EUROfusion WP PFC.

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