EUROFUSION WPPFC-CP(16) 15032

A Kirschner et al.

Modelling of prompt deposition of tungsten under fusion relevant conditions

Preprint of Paper to be submitted for publication in
Proceedings of 26th IAEA Fusion Energy Conference

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 No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Modelling of Prompt Deposition of Tungsten under Fusion Relevant Conditions

A. Kirschner[1], D. Tskhakaya[2,3], D. Borodin[1], S. Brezinsek[1], J. Romazanov[1], R. Ding[4], Ch. Linsmeier[1]

[1]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung – Plasmaphysik, Partner of the Trilateral Euregio Cluster (TEC), 52425 Jülich, Germany

[2]Fusion@ÖAW, Institute of Applied Physics, TU Wien, 1040 Vienna, Austria

[3]Institute of Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria

[4]Institute of Plasma Physics, Chinese Academy of Sciences, Hefei, Anhui, 230031, P.R. China

E-mail contact of main author: a.kirschner@fz-juelich.de

Abstract. The prompt deposition of sputtered tungsten has been simulated with the impurity transport and plasma-wall interaction code ERO. Parameter studies have been carried out for the two electron densities 1E12 cm^{-3} and 1E15 cm^{-3} and electron temperatures between 1 eV and 20 eV. Also, the effects of the magnetic field strength (3T or 1T) and the anomalous cross field diffusion (D_{perp} = 0.5 m^2/s or zero) have been analysed. The amount of promptly deposited tungsten reaches values of 100% at the highest electron temperature and density. However, at 1 eV and 1E12 cm^{-3} no prompt deposition occurs at all. The simulations show that the impact energy of promptly deposited tungsten ions can be larger than expected from the energy gain within the sheath potential. This is in particular the case at high electron densities in combination with small electron temperatures, where entrainment of returning ions due to friction with the background plasma ions is very effective. Thus, the self-sputtering by promptly deposited tungsten can become significant, though, under the conditions studied no runaway sputtering takes place. A first estimation of prompt deposition during ELM conditions typically occurring at JET has been done. For this, the so-called streaming model has been applied with a stream velocity of 3.1E7 cm/s, which corresponds to deuterium ion energy of 1 keV, and plasma density of 1E14 cm^{-3} and temperature of 20 eV. With these assumptions the simulations result in about 95% prompt deposition.

1. Introduction

Tungsten will be used in ITER as plasma-facing material for the divertor and is also a candidate material for future fusion devices like DEMO. Alongside its high melting temperature tungsten also shows relatively small physical sputtering due to its high atomic number. Moreover, the penetration of sputtered tungsten atoms into the plasma is limited owing to the large ionisation probability, which in combination with the large gyration radius can lead to significant amounts of deposition and therefore decreases the net-erosion. Usually in this context the term “prompt deposition” is introduced as deposition during the first gyration after erosion [1], which becomes effective if the ratio of ionisation length to gyration radius is smaller than one. Under certain conditions, e.g. very high electron density and temperature, the tungsten ions trajectories do not describe clear gyration motion anymore as the movement very near to the surface is dominated by the large electric field. Moreover, cross field diffusion can disturb the gyration. Thus the classical definition of prompt deposition as deposition during the first gyration radius becomes imprecise. Therefore, here

the term “prompt deposition” is used for ions, which after their ionisation need a time $t < t_{Gyro}$ for returning to the surface, where t_{Gyro} is the time required for the tungsten ion to fulfil one full gyration cycle.
The contribution at hand presents modelling results of prompt tungsten deposition carried out with the three-dimensional Monte Carlo code ERO [2]. A parameter study is given for different electron densities and temperatures, magnetic field strength and various assumptions for anomalous cross field diffusion. Also, the prompt deposition during ELM conditions will be addressed. Finally, the possible effect of runaway sputtering by self-sputtering due to returning tungsten ions is discussed.

2. Modelling of prompt deposition of sputtered tungsten atoms

2.1. Modelling assumptions

To model the transport of sputtered tungsten atoms a roof like surface with 2° inclination angle relative to the magnetic field is used in ERO, see figure 1. The tungsten atoms are injected at the middle of the surface with cosine angular distribution and Thompson energy distribution around the tungsten surface binding energy (8.8 eV) to simulate physical sputtering. The electron and ion temperature and electron density are input parameters at the stagnation point, which is chosen to be 10 m away from the surface. According to the two point model for the scrape-off layer (SOL), the electron density n_e decreases by a factor of two when moving inside the SOL along the magnetic field lines from the stagnation point to the sheath entrance [3] and the plasma flow velocity v_{Flow} increases from zero to sound speed. The electron and ion temperatures (T_e, T_i) are assumed to be constant within the whole simulation volume. The plasma parameters within the electrical sheath in front of the surface are not resolved as its thickness – in the order of the Debye length λ_D or the deuterium gyration radius r_{Gyro} – is rather small. However, first ERO simulations considering Particle In Cell simulations of the sheath characteristics have been done to study the influence on the prompt deposition of tungsten [4]. For the plasma parameters studied therein (20 eV, 5 eV and 6E13 cm^{-3} at the stagnation point), the modelled amounts of prompt deposition with resolved sheath characteristics were about 5 to 10% smaller than the ones modelled without resolved sheath.

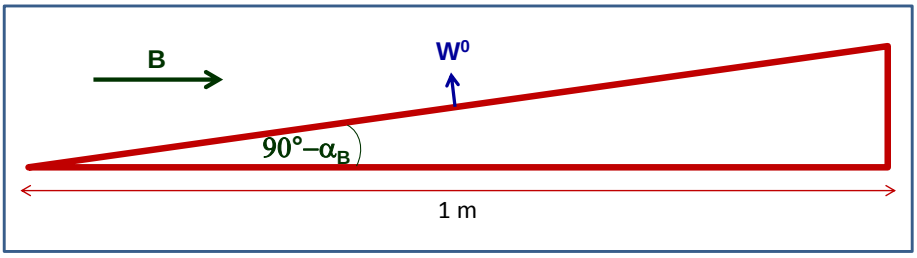

FIG. 1. Set up for the ERO simulations. For the magnetic field angle α_B a value of 88° is used. The toroidal length (parallel to the B field) of the surface is 1 m, the poloidal length 0.1 m. The observation volume above the surface has a height of 0.1 m.

The electrical potential U_S in front of the surface is described by the following formula, showing an exponential scaling along the distance z from the surface with the Debye length λ_D if the magnetic field is perpendicular to the surface and with the deuterium gyration radius r_{Gyro} for shallow magnetic field:

$$U_S(z) = U_0 \cdot f(\alpha_B) \cdot \exp(-z/(2\lambda_D)) + U_0 \cdot (1-f(\alpha_B)) \cdot \exp(-z/r_{Gyro})$$

Here U_0 is the sheath potential drop, $U_0 \approx 3 \cdot T_e$ for $T_e = T_i$ and neglecting secondary electron emission [5]. The function $f(\alpha_B)$ approaches zero for $\alpha_B = 90°$ and one for $\alpha_B = 0°$. For the total potential the pre-sheath potential drop of about $0.7 \cdot T_e$ is added.
The tungsten atoms leaving the surface move along straight lines until their ionisation. The ionisation probability of the atoms is calculated by means of rate coefficients from [6]. Further ionisation of the tungsten ions is determined by the Lotz formula [7] as no final data are available at present within the ADAS database. The charged tungsten ions interact with the plasma background ions via Coulomb collisions. In addition, anomalous cross field diffusion can be included in the simulations. The movement due to the Lorentz force within the electromagnetic field is calculated by means of the Boris method, which includes automatically possible drift effects. Finally, thermal forces are considered using formulae of the temperature dependence along the magnetic field and resulting thermal forces from literature [8]. Reflection of tungsten ions returning to the surface is not considered in the studies presented here.

2.2. Prompt deposition of tungsten for steady state plasma conditions

The simulations have been performed for two different electron densities, 1E12 cm^{-3} and 1E15 cm^{-3}, within a plasma temperature range of 1 eV to 20 eV. The ion temperature is assumed to be equal the electron temperature, $T_i = T_e$. Two different magnetic field strengths have been assumed, 3 T in comparison to 1 T. The effect of the anomalous cross field diffusion has been studied by assuming $D_{perp} = 0.5$ m^2/s in comparison to no cross field diffusion. Figure 2 shows exemplarily the distribution of W^0 atoms, W^+ and W^{2+} ions above the surface integrated in poloidal direction for (1E12 cm^{-3}, 20 eV) with no cross field diffusion and magnetic field of 3 T.

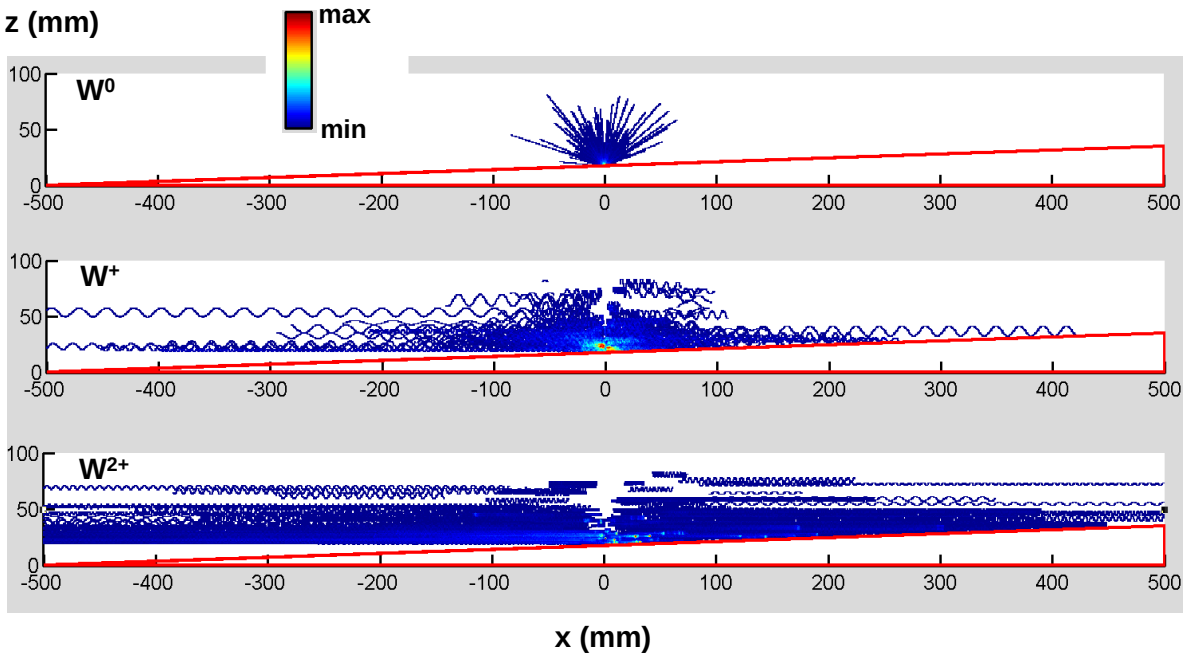

FIG. 2. Modelled two-dimensional spatial distribution of tungsten atoms and ions above the surface for n_e = 1E12 cm^{-3} and T_e = 20 eV. The colour scaling of each picture (W^0, W^+ and W^{2+}) corresponds to the respective maximum intensity wherefore the intensity of the different species cannot be compared with each other.

Prompt deposition of tungsten only occurs at or near to the source location. For the example of figure 2 about 21% of injected W atoms are deposited promptly. In addition, about 13% is deposited non-promptly on the inclined surface. However, this value is somehow arbitrary as it strongly depends on the size of the surface considered. Particles which are not deposited leave the simulation volume – for the example discussed, mainly in –x direction, which can be seen also in figure 2.

The modelled amounts of prompt deposition for the plasma parameter range studied are summarised in figure 3 for magnetic field of 3 T and 1 T and neglecting cross field diffusion (D_{perp} = 0). For all conditions, prompt deposition at 1 T is larger than for 3 T, which can be explained with the larger gyration radius of tungsten ions at the smaller magnetic field strength. Also, prompt deposition is significantly larger at the higher electron density due to smaller ionisation length of the sputtered tungsten atoms. At the high density of 1E15 cm^{-3} prompt deposition of 100% is simulated for high enough electron temperature whereas maximum prompt deposition of only about 47% is reached at 1E12 cm^{-3} in combination with 20 eV and 1 T. The amount of prompt deposition even goes to zero at the small electron density in combination with small electron temperatures.

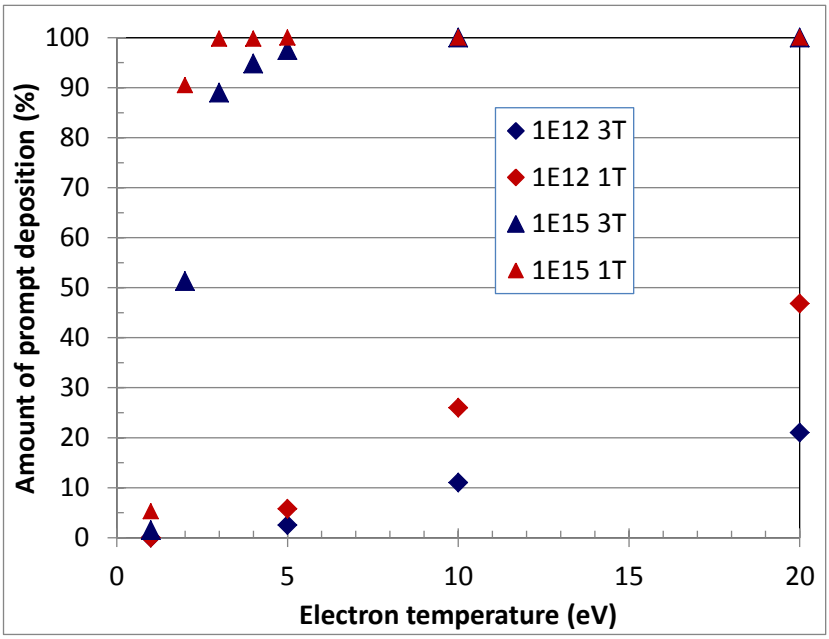

FIG. 3. Modelled prompt deposition for two different electron densities (1E12 and 1E15 cm^{-3}) and magnetic field strengths (3 T, 1 T) in dependence on the electron temperature. Cross field diffusion is not included in the simulations (D_{perp} = 0).

The simulations including anomalous cross field diffusion with D_{perp} = 0.5 m^2/s lead to slightly larger prompt deposition in particular at the lower electron temperatures (≤ 5 eV), whereas at the higher electron temperatures no significant differences occur.

For the estimation of self-sputtering due to returning tungsten ions the energy and angular distribution of these ions have to be known. The ERO simulations deliver this information taking into account the energy gain due to the sheath potential and friction with the background plasma ions via Coulomb collisions. For the above-presented parameter study, figure 4 shows the resulting mean impact energy (E_{mean}) and mean impact angle (α_{mean}) of promptly deposited tungsten ions. The impact angle is given relative to the surface normal, i.e. an impact angle of zero would correspond to normal incidence of the ion.

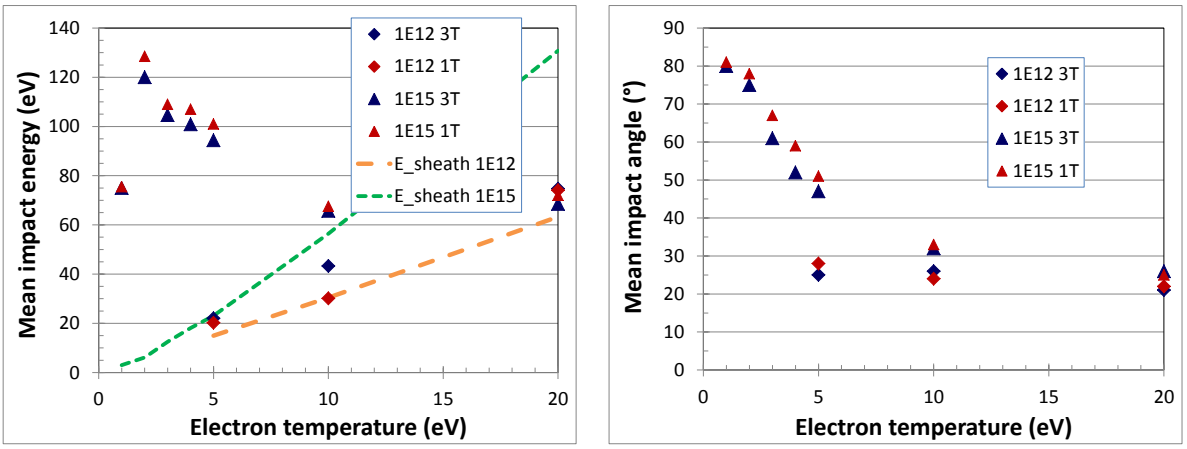

FIG. 4. Modelled mean impact energy (left) and mean impact angle (right) of promptly deposited tungsten ions. Cross field diffusion is not included in the simulations (D_{perp} = 0). The dashed lines in the left figure indicate the energy gain $3 \cdot Q_{meean} \cdot T_e$ within the sheath potential.

The simulated mean energies of promptly deposited tungsten ions do not significantly depend on the magnetic field strength. In contrast, the electron density and temperature strongly influence the resulting impact energy. It is seen that the small density of 1E12 cm^{-3} leads to mean impact energies near or slightly larger than the energy $E\_sheath = 3 \cdot Q_{mean} \cdot T_e$ expected from ions passing through the sheath potential. The mean charge state Q_{mean} is taken from the simulations and is equal to one for the low density cases. For the high density of 1E15 cm^{-3} the picture is different. Now at large electron temperatures the impact energy is smaller than expected from the sheath potential. For instance, at 20 eV the mean charge state of promptly deposited ions is about 2.2 resulting in E_sheath ≈ 130 eV compared to the modelled mean impact energy of only about 70 eV. Obviously the ionisation length at (1E15 cm^{-3}, 20 eV) is smaller than the dimension of the sheath potential. At low electron temperatures and high electron density, however, the modelled mean impact energy is significantly larger than E_sheath. This can be explained by an effective entrainment under these conditions between the tungsten ions and the background deuterium plasma flow due to Coulomb collisions. The maximum impact energy of about 125 eV occurs at 2 eV and 1E15 cm^{-3}, which is clearly larger than E_sheath ≈ 6 eV with $Q_{mean} = 1$.

The modelled mean impact angle of promptly deposited tungsten ions is rather insensitive on the magnetic field, compare figure 4 (right). Between 10 eV and 20 eV a mean impact angle of 20 – 30° occurs for both studied electron densities. For 1E12 cm^{-3} this does not change much when decreasing the electron temperature to 5 eV. For even smaller electron temperatures at this small density, prompt deposition becomes negligible or even zero. For the high electron density of 1E15 cm^{-3} an increase of the mean impact angle occurs when decreasing the electron temperature reaching a maximum mean value of about 80° at 1 eV. Also here the effect of entrainment becomes significant leading to an impact of tungsten ions, which is oriented along the magnetic field lines.

Figure 5 shows the resulting sputtering yield Y of tungsten due to promptly deposited tungsten ions. The sputtering yield has been calculated by means of the so-called Eckstein fit formula with necessary fit parameters taken from [9]. The estimated sputtering yield considers the individual yield of each returning tungsten ion and therefore is not equal to $Y(E_{mean}, \alpha_{mean})$ using the mean impact energy and angle of promptly deposited ions as input for the fit formula.

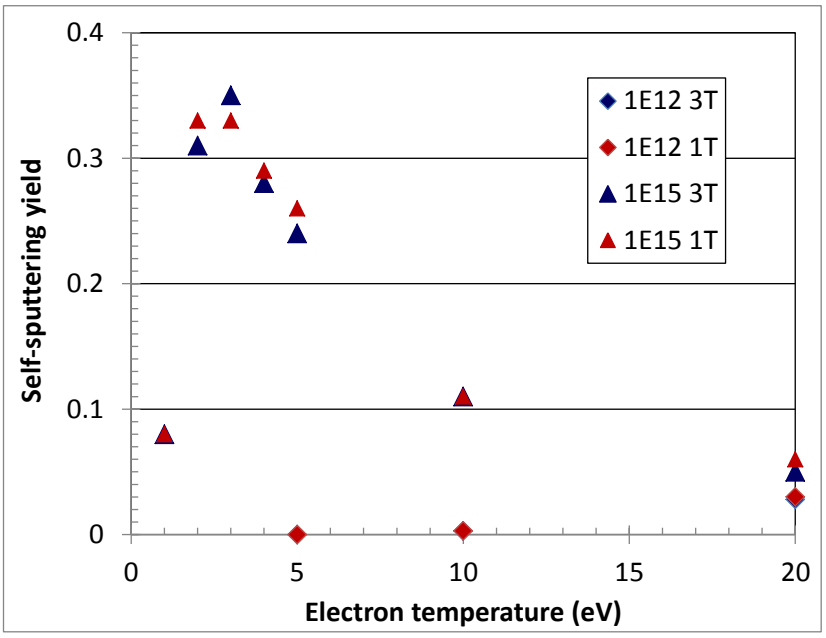

FIG. 5. Estimated self-sputtering yield of promptly deposited tungsten ions. Cross field diffusion is not included in the simulations (D_{perp} = 0).

As seen before for the mean energy and angle, the magnetic field strength has no significant effect on the resulting self-sputtering yield. For the parameter studied, largest sputtering yield is obtained for the high electron density of 1E15 cm^{-3} and an electron temperature of 2–3 eV. However, the maximum yield about 0.3 is clearly below one wherefore runaway erosion due to self-sputtering does not occur. A more detailed discussion about runaway erosion will follow in section 2.4.

The simulations shown so far focused on the assumption of neglecting anomalous cross field diffusion. Further simulations assuming D_{perp} = 0.5 m^2/s instead have been performed for the same parameter range of electron density, temperature and magnetic field strength. There is a slight effect on the amount of prompt deposition, see discussion of figure 3. The modelled mean impact energies tend to be smaller when cross field diffusion is considered, which consequently also results in smaller self-sputtering yields. Particularly, the diffusion reduces the efficiency of the entrainment, which clearly reduces the impact energy at the high electron density in combination with small electron temperatures. As for the non-diffusion case the maximum self-sputtering yield appears at 1E15 cm^{-3} and 2–3 eV. However, considering diffusion leads to clearly reduced maximum yield of about 0.1 compared to 0.3 at these conditions but without diffusion.

2.3. Prompt deposition of tungsten for ELM conditions

To study the effect of ELMs on the prompt deposition of sputtered tungsten an ERO simulation has been performed with plasma conditions based on observations of high power unseeded H-mode discharges at JET [10]. According to these experiments the deuterium ion impact energy is in the keV range whereas the electron temperature is around 20 eV. The high ion energy can be understood in the frame of the so-called “Free Streaming Model” in which the electrons transfer most of their parallel energy to the ions, see e.g. [11]. For the ERO modelling the deuterium ion energy is set to 1 keV resulting to a velocity of 3.1E7 cm/s, which is assumed to be the plasma flow velocity along the magnetic field lines. For the electrons a temperature of 20 eV and density of 1E14 cm^{-3} is assumed. These plasma conditions result in prompt deposition of sputtered tungsten of about 95%. For comparison,

typical inter-ELM conditions (~10 eV, ~1E13 cm^{-3}) lead to prompt deposition of about 60%. The mean impact energy of promptly deposited tungsten ions during the ELM is about 70 eV with a mean charge state of about 1.5. Obviously, under the ELM conditions considered here the entrainment effect is not very effective and thus the impact energy of promptly deposited tungsten ions is not very large. Together with rather low impact angles (in average 25°) this consequently also leads to relatively low self-sputtering yield of about 0.05.

2.4. Runaway sputtering

To study the conditions for runaway sputtering to occur, a simplified examination is done. If the exposure time is divided into time steps one can calculate the gross erosion N_n at time step *0* and each succeeding time step *n* as follows:

$$n = 0: \quad N_0 = N_{BG} + N_{BG} \cdot Ret \cdot Y_{SZ}$$

$$n \geq 1: \quad N_n = N_{n-1} + N_{BG} \cdot (Ret \cdot Y_{SZ})^{n+1}$$

Here N_{BG} is the number of particles eroded by the background plasma flux per time step, *Ret* is the ratio of particles promptly returning to the surface relative to the amount of sputtered particles and Y_{SZ} the self-sputtering yield. Reflection of returning ions is not considered. Figure 6 illustrates the resulting time evolution of gross and net erosion for *Ret* = 0.8 and three different values of Y_{SZ}. The value for N_{BG} has been set to 10.

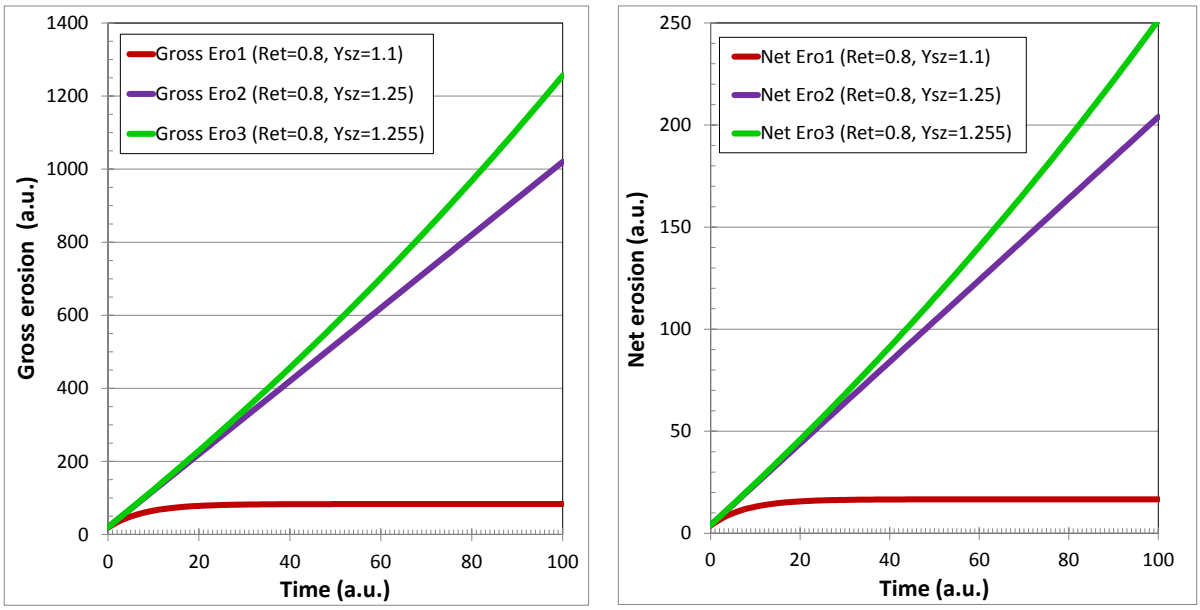

FIG. 6. Illustration of gross (left) and net (right) erosion for different assumptions of the amount of returning species (Ret) and self-sputtering yield (Y_{SZ}).

It is seen that the erosion reaches a steady state value for $(Ret \cdot Y_{SZ}) < 1$, increases linearly with exposure time for $(Ret \cdot Y_{SZ}) = 1$ and increases exponentially for $(Ret \cdot Y_{SZ}) > 1$. The latter two cases thus would lead to runaway sputtering. The product of prompt deposition amount and self-sputtering yield is always well below one for the tungsten sputtering cases studied in the previous sections wherefore no runaway sputtering occurs. According to the Eckstein fit formula, tungsten self-sputtering yields larger than one occur at impact energies larger than about 300 eV and impact angles around 60°. For example Y_{SZ}(300 eV, 60°) ≈ 1.1. For runaway sputtering to occur with this yield, the amount of prompt deposition must be larger than 91%. Whereas such large amounts of prompt deposition have been observed within the

presented parameter study, the modelled impact energy of promptly deposited tungsten was always smaller than about 130 eV leading to Y_{SZ} well below one. Therefore, runaway sputtering is not expected for the parameter range studied within the present contribution.

3. Conclusions

The prompt deposition of sputtered tungsten has been modelled with the ERO code. For the electron temperature range (1 eV to 20 eV) and magnetic field strengths (1T vs. 3T) studied, the amount of modelled prompt deposition varies between 0% and 47% for an electron density of 1e12 cm^{-3} and between 2% and 100% for 1E15 cm^{-3}. Thus, at plasma temperatures and densities not too small prompt deposition in principal significantly can reduce the net erosion and by this increase the life time of plasma facing components. However, self-sputtering by returning tungsten ions has to be considered, which reduces the positive effect of prompt deposition. Tungsten self-sputtering yields calculated with the Eckstein formula for the studied parameter range vary between 1E-5 and 0.4 with the maximum values obtained at the large electron density and small electron temperatures. It should be noted that these yields could be enhanced for the sputtering of deposited tungsten as reported earlier, see e.g. [12].
As next step the simulation of tungsten erosion and deposition at JET and along the ITER divertor plates is foreseen. Besides the local prompt deposition such simulations then also includes the non-prompt deposition of tungsten ions, which could have larger impact energies (in particular at high electron density and small electron temperature) due to the entrainment after longer travelling paths. These returning tungsten ions could lead to significant erosion at the location of their impact.

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 No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission. This work has been done under WP PFC. It has been supported by the Sino-German Center for Research Promotion under Contract No. GZ769.

References

[1] NAUJOKS, D., et al., J. Nucl. Mat. 210 (1994) 43
[2] KIRSCHNER, A. et al., Nucl. Fus.40 (2000) 989
[3] STANGEBY, P.C., "The plasma boundary of magnetic fusion devices", IOP, Bristol and Philadelphia (2000), ISBN 0 7503 0559 2
[4] KIRSCHNER, A., Contrib. Plasma Phys. 56, No. 6-8, 622 (2016)
[5] STANGEBY, P.C., McCRACKEN, G.M., Nucl. Fus. 30 (1990) 1225
[6] VAINSHTEIN, L.A., et al., J. Phys. B: At. Mol. Opt. Phys. 44 (2011) 125201
[7] HIGGINS, M., et al., "Atomic and molecular data for fusion, Part III: recommended cross sections and rates for electron ionisation of light atoms and ions: copper to uranium", Tech. Rep. CLM-R294, Culham Laboratory, Abingdon, Oxfordshire, UK (1989)
[8] STANGEBY, P.C., ELDER, J.D., Nucl. Fus 35 (1995) 1391
[9] BEHRISCH, R., ECKSTEIN, W., "Sputtering by particle bombardment, experiments and computer calculations, from threshold to MeV energies", Springer, 2006
[10] GUILLEMAUT, C., et al., Phys. Scripta T167 (2016) 014005
[11] FUNDAMENSKI, W, et al., Plasma Phys. Control. Fus. 48 (2006) 109
[12] KIRSCHNER, A., et al., J. Nucl. Mat. 438 (2013) S723