

# Revised scaling equation for the prediction of tritium retention in beryllium co-deposited layers

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## Abstract.

The prediction of tritium retention in ITER relies on the extrapolation from present data. An empirical equation was proposed in (*De Temmerman G. et al 2008 Nucl. Fusion 48 075008*) to account for the influence of the beryllium deposition rate, the substrate temperature and the average energy of the deuterium neutrals on the deuterium retention. However, the beryllium deposition rate observed in PISCES-B is much lower than that expected in the ITER divertor. On the other hand, the flux ratios of deuterium and beryllium are comparable in magnitude. Therefore, a revised scaling equation is proposed here to take into account the flux ratio of deuterium to beryllium arriving at the co-depositing surface and to match the validity range of the scaling equation with the ITER parameters.

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## 1. Introduction

The issue of tritium retention is critical for the realization of burning plasma reactors. In ITER, the in-vessel tritium retention is to be limited to 1 kg of mobilizable tritium for safety reasons. In order to prevent this limit being reached and operations stopped, the tritium retention needs to be understood and recovery methods developed [1]. Co-deposition of tritium with material eroded from the plasma-facing components (PFCs) is expected to be the main process of tritium accumulation in the vessel, as was already observed in the JET and TFTR tokamaks [2].

Some progress has recently been made on the understanding of the co-deposition process and the parameters influencing the retention levels in such layers. A scaling equation has been proposed in [3] to predict the deuterium retention in beryllium co-deposits formed in PISCES-B as a function of the beryllium deposition rate, the energy of the incident D particles and the substrate temperature during deposition. Such an approach has allowed a significant reduction of the large scatter observed in the literature for expected values of the D/Be ratio in beryllium co-deposits. Therefore, a similar procedure has been applied for tungsten [4] and carbon [5] co-deposits.

Extrapolation of these results to the ITER case poses the problem of the parameter range over which those equations have been validated. In particular, the beryllium deposition rate in PISCES-B is about 50 times lower than the predicted deposition rate at the inner divertor of ITER [6]. On the other hand, the deuterium fluxes in ITER are also about 100 times higher than in PISCES-B. It, therefore, appears that predictions in terms of flux ratios of deuterium and beryllium atoms arriving at the co-depositing surface ( $\Gamma_D/\Gamma_{Be}$ ) would make the step between the PISCES-B and ITER cases smaller and increase the confidence in the extrapolation. Such an approach has been successfully applied to the case of tungsten co-deposited layers [4]. In this paper, data presented in [3] and [7] are revisited in order to express the dependence of the D/Be ratio on the flux ratio  $\Gamma_D/\Gamma_{Be}$ , the substrate temperature and the energy of the incident deuterium particles.

## 2. Influence of the deposition conditions on the deuterium retention

A systematic study of the influence of the deposition conditions (substrate temperature, deposition rate, energy of the incident particles) on the deuterium retention in co-deposited beryllium layers has been carried out in the PISCES-B linear plasma device [3]. The mechanism by which deuterium co-deposits with beryllium appears to be a combination of co-deposition and implantation. Indeed the retention decreases with increasing deposition rate, which indicates a co-deposition process, and increases with the energy of the impinging deuterium particles, which is a trend usually observed during implantation. In addition, the retention decreases with increasing substrate temperature during deposition. An empirical equation has been proposed in [3] to account for the influence of those three parameters on the deuterium retention expressed as the ratio of

deuterium to beryllium (D/Be) in the co-deposited layer:

$$\frac{D}{Be} = 2.94 \cdot 10^{-5} \times r_d^{-0.59 \pm 0.1} \times E_n^{1.34 \pm 0.15} \times e^{\frac{1306 \pm 190}{T}} \quad (1)$$

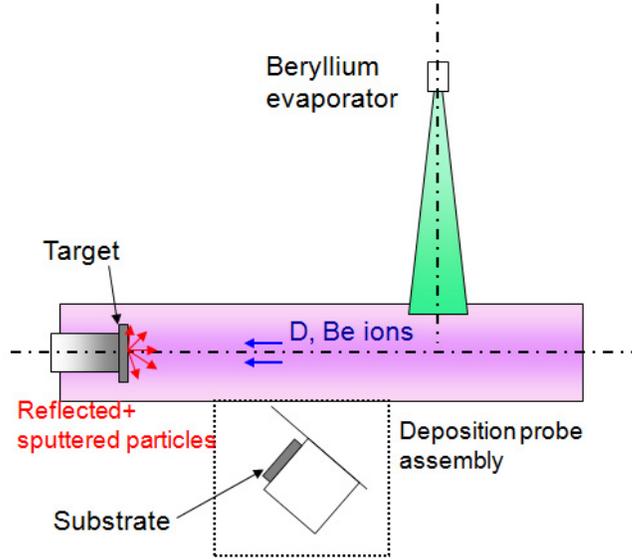
where  $r_d$  is the beryllium deposition rate in units of  $10^{15} \text{at} \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$ ,  $E_n$  in eV is the average energy of the deuterium particles bombarding the growing layer, and with  $T$  in K the substrate temperature, with  $293 \text{ K} \leq T \leq 600 \text{ K}$  and  $15.6 \text{ eV} \leq E_n \leq 62 \text{ eV}$ . In addition, in [7], the influence of the neutral pressure during deposition and of the addition of argon in the plasma on the deuterium retention were studied. It was found that eq. 1 was still able to reproduce the experimental observations.

Although the use of eq. 1 has allowed to significantly reduce the large scatter of D/Be values observed in the literature, its use for the prediction of the tritium retention in ITER co-deposited layers is only valid within the ranges of parameters studied. For example, recent numerical modeling of layer deposition in the ITER divertor [6] indicate a beryllium deposition rate in the range  $10^{-4} - 1 \text{ nm} \cdot \text{s}^{-1}$ . On the other hand, in PISCES-B, the beryllium deposition rate could only be varied in the range  $5 \cdot 10^{-3} - 5 \cdot 10^{-2} \text{ nm} \cdot \text{s}^{-1}$ . At the same time the deuterium/tritium fluxes in the ITER divertor are also 100 times higher than in PISCES-B. It therefore appears predictions in terms of flux ratios of deuterium and beryllium atoms arriving at the co-depositing surface ( $\Gamma_D/\Gamma_{Be}$ ) would make the step between the PISCES-B and ITER cases smaller and increase the confidence in the extrapolation.

### 3. Estimates of $\Gamma_D/\Gamma_{Be}$

Experimental details about the preparation of the samples can be found elsewhere [3, 7]. Figure 1 schematically shows the arrangement used. Targets made of beryllium and tungsten are exposed to a deuterium plasma containing beryllium ions injected in the plasma by an evaporative atomic beam source. The beryllium fraction in the plasma is controlled by adjusting the effusion cell temperature and is determined spectroscopically. Co-deposits are collected on polished tungsten substrates installed with a line-of-sight to the target. The substrate is shielded from cross-field plasma transport.

In order to estimate the particle fluxes to the substrate during the co-deposit formation, it is important to identify the mechanisms contributing to these particle fluxes. The flux of deuterium neutrals is assumed to be due to the reflection of deuterium ions from the target. The contribution from charge-exchange processes is neglected here as the samples are largely shielded from direct line-of-sight to the plasma. With the plasma conditions used in this study, ( $n_e \sim 2\text{-}3 \times 10^{18} \text{m}^{-3}$ ,  $T_e \sim 6\text{-}10 \text{ eV}$ ), the ion flux to the target consists of a mix of molecular ions which can be determined from a 0-D model [8] and is found to be  $(D^+, D_2^+, D_3^+) = (0.25, 0.47, 0.28)$ . Once a molecular ion,  $D_3^+$  for example, strikes a surface it dissociates into 3 D atoms with each 1/3 of the incident energy. If  $\Gamma_{ion}$  is the ion flux measured by the reciprocating Langmuir probe,  $R_{eff}^{D \rightarrow M}$  is the effective particle reflection coefficient of deuterium ions scattered from the



**Figure 1.** Experimental setup used to collect deuterium and beryllium atoms eroded/reflected from a metallic target exposed to a PISCES-B plasma.

target surface, and  $\Gamma_D$  the neutral flux to the substrate one thus has:

$$R_{eff}^{D \rightarrow M} = 0.25 \cdot R^{D \rightarrow M}(E_0) + 2 \cdot 0.47 \cdot R^{D \rightarrow M}(E_0/2) + 3 \cdot 0.28 \cdot R^{D \rightarrow M}(E_0/3) \quad (2)$$

$$\Gamma_D = \Gamma_{ion} \cdot R_{eff}^{D \rightarrow M} \quad (3)$$

where  $R^{D \rightarrow M}(E_0)$  is the particle reflection coefficient of deuterium ions with energy  $E_0$  scattered from the target surface. In case of a beryllium target the flux of beryllium atoms to the co-depositing surface comes from:

- sputtering of the target by D ions
- sputtering of the target by Be ions
- reflection of Be ions from the target

In the case of simultaneous bombardment of a surface by deuterium and beryllium ions, the effective sputtering yield of the material (Be here) can be expressed as:

$$Y_{eff} = (Y^{D \rightarrow Be} \cdot f_D + Y^{Be \rightarrow Be} \cdot f_{Be}) \quad (4)$$

where  $f_I$  is the concentration of the element I in the plasma and  $Y^{D \rightarrow Be}$  is the sputtering yield of beryllium by deuterium ions,  $Y^{Be \rightarrow Be}$  is the self-sputtering yield of beryllium.

In the case of a beryllium target, the total flux of beryllium atoms to the co-depositing surface is then:

$$\Gamma_{Be} = (Y_{eff} + f_{Be} \cdot R^{Be \rightarrow Be}) \cdot \Gamma_{ion} \quad (5)$$

In the case of a tungsten target, since no Be layer was found to have grown on the target, it is assumed that all incoming beryllium ions are reflected or sputtered on the surface, so that:

$$\Gamma_{Be} = f_{Be} \cdot \Gamma_{ion} \quad (6)$$

In addition, the energy of the incoming ions was below the sputtering threshold for tungsten.

Values of the reflection coefficients and sputtering yields have been extracted from [9]. It is assumed that both the sputtered and reflected particles have the same cosine angular distribution which is usually the case for a smooth surface [9, 10]. Applying the described method to all the data presented in [3, 7],  $\Gamma_D/\Gamma_{Be}$  was found to vary in the range 10-2000, which is relatively close to the range 15-10000 predicted for the ITER divertor [6].

#### 4. Modified scaling equation for the prediction of D/Be in co-deposited layers

Having estimated the arrival flux ratio for all the studied co-deposited layers, it is proposed to modify the scaling equation proposed in [3] such as:

$$\frac{D}{Be} = C \cdot \left( \frac{\Gamma_D}{\Gamma_{Be}} \right)^\alpha \cdot E_n^\beta \cdot \exp\left(\frac{\gamma}{T}\right) \quad (7)$$

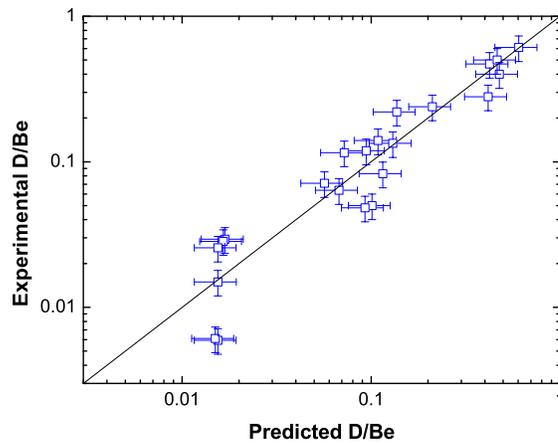
A regression analysis has been done on all of the data to determine the constant C and the parameters  $\alpha, \beta$ , and  $\gamma$ . This allows the dependence of the D/Be ratio on each individual parameter to be taken into account. The full scaling equation derived from fitting all of the data is then:

$$\frac{D}{Be} = 5.82 \cdot 10^{-5} \cdot \left( \frac{\Gamma_D}{\Gamma_{Be}} \right)^{-0.21 \pm 0.1} \cdot E_n^{1.17 \pm 0.2} \cdot e^{\frac{2273 \pm 311}{T}} \quad (8)$$

where  $E_n$  is in eV and  $T$  in K, and with  $293 K \leq T \leq 600 K$  and  $15.6 eV \leq E_n \leq 62 eV$  and  $10 \leq \frac{\Gamma_D}{\Gamma_{Be}} \leq 2000$ .

A comparison of the experimentally measured D/Be ratios, found in [3, 7], with the D/Be ratio predicted by equation 8 is shown in figure 2. A relatively good agreement is observed for the different datasets.

Nevertheless, the accuracy of 0.1 in the exponent of the flux ratio term appears to be larger than that of the deposition rate term in eq. 1. The deposition rate used in eq. 1 was experimentally determined by dividing the film thickness determined by nuclear reaction analysis (NRA) by the exposure time, those values for which the accuracy is relatively good. On the other hand, the estimates of the flux ratios rely on some of the assumptions described above. In addition, deuterium neutrals bombarding the witness plate have been assumed to originate solely from the reflection of ions incident on the target. The witness plate is shielded from cross-field plasma transport, but depending on the working gas pressure, dissociated deuterium atoms (with energies 1-2 eV) will also collide the target and be reflected. Although the reflection coefficient of these low energy particles can be non negligible [11], the mean free path of these reflected particles will be much shorter than that of the reflected ions, which is of the order of the distance target-witness plate. The contribution of those low energy neutrals to the global deuterium flux to the witness plate is therefore expected to be negligible compared to neutrals from reflection of incident ions.



**Figure 2.** Comparison between experimentally determined D/Be ratio and the values of the scaling expression.

## 5. Conclusions

In order to increase the confidence in the extrapolation of present data to the ITER case, a revised scaling equation has been presented to express the dependence of the D/Be ratio on the flux ratio  $\Gamma_D/\Gamma_{Be}$ , the substrate temperature and the energy of the incident deuterium particles. A reasonable agreement is found between the experimental and the predicted values.

## 6. Acknowledgments

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