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Modelling of carbide formation and chemical erosion at PISCES-B using the coupled ERO-SDTrimSP code

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Introduction. Erosion and re-deposition of beryllium (Be), tungsten (W) and carbon (C) will determine the life time of plasma facing components (PFC) and the tritium retention in ITER [1]. These processes will be largely influenced by the formation of mixed Be-W-C layers. Experimental investigation of these effects is underway and modelling of these layers is important to form a solid basis to predict their behaviour in ITER. Therefore, material mixing effects like carbide formation have been introduced in the ERO erosion/deposition and impurity transport code, which we use for plasma-surface interaction (PSI) simulations. A check of the reasonability of simplifications that are necessary and of the underlying data has been carried out by comparison of modelling with dedicated experiments in the PISCES-B divertor plasma simulator. This device can produce ITER-relevant plasma conditions and is equipped with an extensive set of diagnostics. The main aim of this work is to investigate whether the formation of Be-C carbides can be responsible for the non-linear dependence of the characteristic mitigation time of carbon chemical erosion on the Be concentration in plasma, as observed at PISCES-B [2, 3].

The 3D Monte-Carlo code ERO models PSI processes, the build-up of surface layers, the transport of plasma impurities and their light emission. A dedicated version of ERO for PISCES-B was developed earlier [5]. Recently a coupling of ERO and SDTrimSP (a version of TRIDYN) codes was provided [4]. SDTrimSP calculates depth resolved and dynamically changing concentration profiles of elements in the surface. In former ERO calculations a simple homogeneous mixing of elements in the interaction layer (IL) was assumed.

PISCES-B is a linear plasma simulator with the plasma chamber having a radius of 7.6cm whereas the plasma covers only a radius of about 2–3cm. An exchangeable circular target is located at the end of the plasma column. The deuterium plasma can be seeded with a pre-set amount of Be evaporated from an oven, which penetrates perpendicularly into the plasma at an axial distance of 15cm from the target. In the experiments discussed below the following plasma conditions were used: T_e~7eV, n_e~ $2*10^{12}cm^{-3}$ at the centre of the plasma column, T_{target}~450°C, T_{oven}~1300°C (determining the seeding rate). The chemical erosion of a carbon target is measured by the CD $A^2\Delta$-$X^2\Pi$ (λ~430nm) band emission. The most remarkable experimental observation at PISCES-B is that a small concentration of Be in plasma (1-0.01%) leads to a complete suppression of the C chemical erosion [2].

Modelling of Be transport in PISCES-B [5]. Before modelling of the PSI processes the transport of Be through the overall plasma volume to the target has to be modelled with ERO. As a test the experimental and simulated light intensity patterns of neutral Be (BeI at 457nm) and ionized Be^+ (BeII at 467nm) has been compared. The respective profiles along the plasma column were of particular interest, because they characterise the transport of Be from the oven to the target. It was found that a reasonable agreement with the experiment required the implementation of a number of physical effects into ERO. Most important are the following:

1) ***Elastic collisions with neutral gas*** – lead to broadening of the modelled Be density in PISCES-B volume. Without taking this effect into account the simulated light emission is always concentrated too much near the oven in contradiction to the observation.

2) ***“Effective reflection” of neutral Be from the chamber wall*** – this was also implemented for broadening of the Be density along the plasma column. The physical reason for this effect is still unclear and under further investigation and discussion. We have tried to reproduce using ERO a similar effect by implementing recombination and a drop of the neutral gas pressure (elastic collisions) just inside the plasma. However, the dedicated ERO simulations did not support this hypothesis.

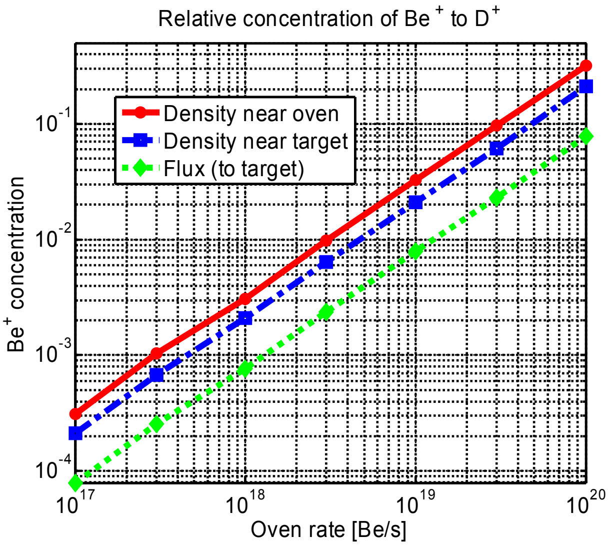

Fig.1. Simulated Be densities with respect to the oven seeding rate. T_e~7eV, n_e~ $2*10^{12}cm^{-3}$.

The dependence of Be flux impinging the target on the oven seeding rate was found to be linear (Fig.1), depending on plasma density and temperature. The spatial distribution of impinging Be along the target also depends on plasma conditions.

Modelling of carbon chemical erosion mitigation. The experiments at PISCES-B reveal a quadratic dependence of the characteristic time of carbon chemical erosion (emission of CD_4 near the target) mitigation on the Be concentration of plasma (ratio of BeII to Dγ emission) [2, 3]. There are indications from XPS post-mortem analysis that a large part of C in the target is bound to Be carbide, which possibly is the reason for the mitigation of chemical erosion.

Carbide formation has been implemented in ERO (also in coupled ERO-SDTrimSP version) in the following manner. The amount of Be_2C in any surface cell is defined by the amount of Be present there provided that there is enough C with respect to stoichiometric proportion 2Be:1C. It is assumed that carbon bound in carbide is not eroded chemically. This approximation is meant to investigate the direction and the order of magnitude of the effect.

In fig.2 the simulated time evolution of chemical erosion is shown. As in the experiment we start with a pure C target. At first the target is exposed to a plasma without Be. It is necessary to reach an equilibrium concentration of re-deposited C, which is assumed to experience 20 times larger erosion than bulk C. This assumption represents effectively the formation of “soft layers”. It was justified by modelling of a number of dedicated experiments at TEXTOR. After the start of Be seeding at t=0s there is an approximately constant flux of Be reaching the target. Re-deposition of Be eroded from target does not play a big role. As the concentration of Be in the surface IL grows, the concentration of C and therefore its chemical erosion hyperbolically decreases. The carbide formation causes an additional reduction. In the case of unrealistically large puffing rates (e.g. $3*10^{19}$Be/s corresponding to 10% of Be concentration in plasma) simulations show complete mitigation of C chemical erosion. ERO-SDTrimSP calculations with and without carbide lead to an even faster mitigation, because in this case all processes are localized inside the IL at the characteristic penetration depths.

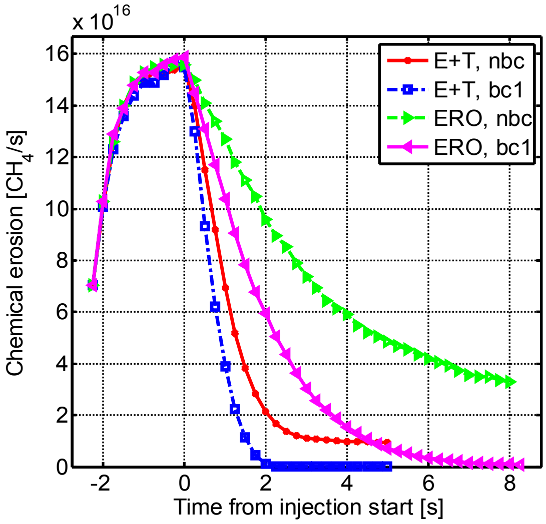

Fig.2. Simulated time evolution of C chemical erosion. Seeding rate 3e19Be/s. “E+T” – ERO-SDTrimSP calculations, “ERO” – conventional ERO calculations. “bc1” – all Be bound in carbide, “nbc” – none.

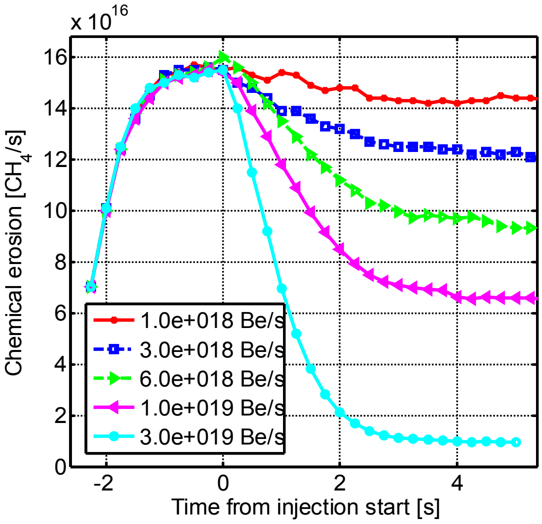

Fig.3. The ERO-SDTrimSP (no carbide) simulated time evolution of C chemical erosion for different seeding rates (legend).

The SDTrimSP code calculates surface evolution with the physical time scale. In the ERO calculations a homogeneous mixing of elements in the interaction layer is assumed. Erosion/deposition/reflection of each surface element is calculated using the according yields multiplied with the concentration. Thus, the concentration of e.g. Be in the surface deposited from plasma depends on the choice of interaction layer depth. While the resulting flux balance in the final equilibrium is independent of the thickness, the characteristic times in calculations by ERO without SDTrimSP coupling grow with the increase of the IL depth.

The speed of chemical erosion mitigation depends on the seeding rate defining the concentration of Be in the plasma (fig.3). At first stage, the decay can be approximated with an exponent ~exp(-t/τ) as seen in the experiment. Later the chemical erosion becomes constant. This happens due to the saturation of the Be concentration in the surface when the removal of Be by physical sputtering compensates the Be deposition from plasma. The simulated characteristic times τ are in the order of several seconds.

In the experiments at PISCES-B an exponential decay of carbon chemical erosion was observed in a wide range of Be seeding rates (oven temperatures). The characteristic time of the mitigation depends as $1/\tau \sim f_{Be}^2$ on the Be concentration in plasma f_{Be}. The principal disagreement with the modelling results is that at any f_{Be} the measured chemical erosion is mitigated completely (CD light falls down to the background level) while a saturation is reached in the modelling. The characteristic time of the mitigation is in the order of minutes or even hours. The first short period of about 10s after opening the shutter for the Be oven is difficult to follow up experimentally due to initial plasma instabilities. This period is therefore not studied experimentally. However, probably the fast decay modelled in ERO happens. The mitigation that is observed at later times in PISCES-B is obviously due to physical processes that are not accounted fully for in ERO. The experimental continuous mitigation of C chemical erosion indicates a further increase of Be and Be carbide content in the surface which is not seen in the modelling. This indicates that there is an additional mechanism, which leads to a prevention of Be sputtering, or to a deeper penetration of Be into the surface, e.g. diffusion. The surface analysis [3] shows that cone-like structures appearing on the C surface due to plasma exposure are dramatically reduced after Be seeding. So, the effect may be also connected to a slow changing of the surface morphology.

Summary. The ERO code modelling for PISCES-B has been further improved and tested. The possibility to use coupled ERO-SDTrimSP calculations is provided. The achieved understanding of transport pattern (proved by comparison of simulated and observed light emission) allows to begin the modelling of the PSI processes on the PISCES-B target.

With the present assumptions the ERO modelling can not reproduce the experimentally observed slow, however complete, C chemical erosion mitigation. The implementation of carbide formation in ERO leads to a stronger mitigation in line with the observations, but cannot resolve fully the other contradictions. Therefore, other mechanisms like diffusion or the change of the surface morphology should be implemented into the surface model of ERO.

The new effects introduced in ERO can also affect the predictions for ITER.

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[1] A.Kirschner et.al., J.Nucl.Mat. 363–365 (2007) 91–95
[2] D.Nishijima et.al., J.Nucl.Mat. 363–365 (2007) 1261–1265
[3] M.Baldwin et al., Nuc. Fusion 46 (2006) 444
[4] S.Droste et.al., Contrib. Plasma Phys., U46U (2006) 628-634
[5] D.Borodin et.al., Phys.Scr. T128 (2007) 127–132