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Modelling of carbon transport in fusion devices: evidence of enhanced re-erosion of in-situ re-deposited carbon

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Abstract

The paper presents new Monte-Carlo transport simulations of methane $^{13}CH_4$ injected through a hole in a testlimiter and exposed to the edge plasma of TEXTOR. The results show that the spatial distribution of ^{13}C re-deposited locally on the testlimiter surface can be modelled if the parameter S for the sticking of returning hydrocarbons $^{13}CH_y$ is set to zero or almost zero. This is interpreted as a negligible effective sticking of the returning hydrocarbon radicals due to the instantaneous re-erosion caused by the hydrogen carried with the CH_y radicals ('self re-erosion'). However, the calculated local deposition efficiency of ^{13}C, remains too high compared with the observed value. Therefore, in addition an enhanced yield for chemical erosion caused by the background hydrogen for the fresh re-deposits has to be assumed. Similar assumptions can reproduce also the high amount of carbon deposition found on the inner louvers in the MkIIa divertor configuration of JET and on the plasma-shadowed areas of the MkIIGB divertor.

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1. Introduction

Carbon based materials are foreseen for the divertor target plates in ITER [1] since they do not melt during transient heat loads caused by ELMs or disruptions. In addition they possess excellent thermomechanical properties. Unfortunately carbon based materials suffer from chemical erosion by hydrogen (and oxygen) impact which is crucial for future fusion devices operating under much higher duty cycle and particle fluences. This can limit the lifetime but, even more serious, promote the formation and migration of chemically eroded hydrocarbons leading finally to the deposition of hydrogen rich carbon layers. For safety reasons the total amount of in-vessel tritium retention is not allowed to exceed 350 g. When this limit is reached the retained tritium has to be removed by special techniques, which are still under development. Reliable prediction of the tritium retention in future machines such as ITER is one of the most important issues. For this, model calculations have to be benchmarked against observations and experiments in present fusion devices.

In the following, simulation calculations are described which have been carried out with the Monte-Carlo codes ERO-TEXTOR [2] and ERO-JET, as appropriate, for two different experiments: (i) injection of methane into the scrape-off layer of TEXTOR and (ii) the transport of carbon in the JET divertor. The influence of the sticking parameter *S* assumed in the modelling for the hydrocarbon radicals returning to the surface is outlined. Also the evidence of an enhanced

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re-erosion of fresh deposits is discussed. Moreover, the impact of using different databases of rate coefficients for the dissociation and ionisation of methane is analysed.

In addition, the transport of beryllium in the JET divertor is modelled and compared with that of carbon. In contrast to carbon, the beryllium transport in the divertor of JET MkIIa shows no significant deposition on the louvers. This shows the important role of chemical erosion for the transport of carbon.

2. Local deposition of $^{13}CH_4$ injected into the SOL of TEXTOR

$^{13}CH_4$ methane molecules have been injected through a small hole of the surface of a testlimiter positioned at the last closed flux surface (LCFS) of TEXTOR. ^{13}C has been used to discriminate the deposition of injected carbon from the background carbon ^{12}C. Details about the experiment can be found in [3]. One of the most surprising results was the very low local deposition efficiency of ^{13}C on the testlimiter surface: less than 0.5% of the injected ^{13}C remained on the surface. First modelling calculations based on a sticking probability of returning carbon atoms and ions according to TRIM [4] calculations, zero sticking for neutral hydrocarbons ($S = 0$) and 50% sticking for charged ones ($S = 0.5$) revealed a much too high efficiency of about 40%. Assuming $S = 1$ for all hydrocarbons increases the ^{13}C deposition efficiency even to about 80%. Moreover, the ^{13}C deposition maximum is located very nearby the puffing hole. This is in contrast to the experimental observation which showed the maximum several cm away from the injection hole. However, the calculated ^{13}C deposition efficiency drops, to about 3% if the extreme assumption of zero sticking probability ($S = 0$) is made for all (charged and neutral) hydrocarbons CH_y returning to the limiter surface [3,5] whilst the sticking of carbon atoms and ions is still taken from TRIM. Thus, the deposition of carbon ^{13}C at the testlimiter is only due to the impact of carbon atoms and ions but not due to hydrocarbons. The calculations were done using the Ehrhardt–Langer database [6] for the dissociation of hydrocarbons. Chemical erosion by the background plasma was set to $Y_{chem} = 1.5\%$ following the recommended erosion yields for ITER and according to the measured yield for the surface temperature of the testlimiter present in the experiment [7,8]. Also the formula for Y_{chem} according to Roth [9] results in a chemical erosion yield between 1% and 2% using the values for the ion energy E_{ion}, flux Γ and surface temperature T_{surf} from the experiment ($E_{ion} \approx 300$ eV, $\Gamma \approx 2 \times 10^{22}$ $m^{-2}\,s^{-1}$ and T_{surf} between about 700 and 800 K). A parameter study including lower local electron temperature but increased local density and variations of the cross-field diffusion coefficient showed that the sticking assumption of the returning hydrocarbons is the most crucial parameter.

The above-described assumptions of $S = 0$ for all hydrocarbons and $Y_{chem} = 1.5\%$ reproduce fair agreement between calculated and observed deposition pattern but result in a ^{13}C deposition at the testlimiter surface which is still a factor of six too high. One possible uncertainty is the atomic database for the dissociation of the methane family. As mentioned above for the simulations, the data published by Ehrhardt–Langer had first been used. In the meanwhile revised data for the rate coefficients of the CH_4 reaction chain were published by Janev and Reiter [10]. These new data take into account many more reactions and the newest measurements available for the cross-sections. A comparison of these two databases and the impact on modelling of the transport of methane through a plasma are shown in [11]. With the Janev database instead of the formerly used Ehrhardt–Langer data the simulation calculations result in an even higher local deposition efficiency (14% versus 3%, assuming $S = 0$ for all hydrocarbons) whereas the two dimensional patterns of measured and simulated light emission of CH radicals (Fig. 1) and C^+ ions still show a good agreement. We conclude therefore, that the low deposition probability is determined by the erosion and deposition processes rather than by the transport of

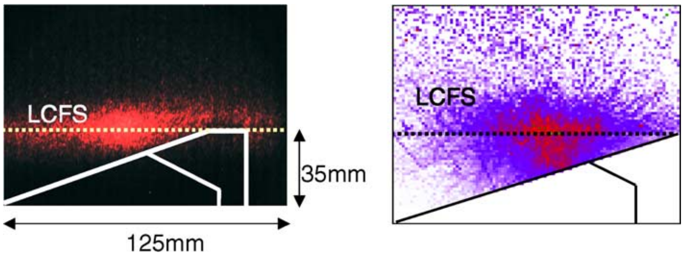

Fig. 1. Observed (left) and simulated (right) CH emission pattern during injection of $^{13}CH_4$ through a hole in an inclined testlimiter surface in TEXTOR.

hydrocarbons through the plasma. Since the extreme assumption $S = 0$ for all hydrocarbon radicals (corresponding to zero sticking) alone does not explain the observed low deposition efficiency, we speculate that an additional erosion process comes into play which affects only the freshly formed deposit. Observations made earlier in TEXTOR showed indeed an enhanced erosion rate of freshly formed a-C:D films and suggest a three to four times higher chemical erosion yield Y_e for those films [12]. Setting now in addition to the former assumptions ($S = 0$, $Y_{chem} = 1.5\%$ for substrate material) $Y_e = 8\%$ for the freshly formed carbon deposits, the simulated efficiency decreases from 14% to 0.5% and hence, results in a good agreement with the measured value. The calculated distribution of ^{13}C deposition remains unaffected because it is caused by the assumption $S = 0$. Fig. 2 shows the measured ^{13}C deposition pattern in comparison to the simulation using the Janev data, $Y_{chem} = 1.5\%$ for substrate material, $Y_e = 8\%$ for fresh deposits and $S = 0$ or $S = 1$. The deposition pattern cannot be modelled with the assumption of a noticeable sticking of hydrocarbons. The assumption of higher sticking together with an according higher erosion yield above 8% can also lower the deposition efficiency to 0.5% but the maximum of ^{13}C deposition becomes located at the puffing hole in contrast to the experiment.

The negligible 'effective' sticking of hydrocarbons cannot be understood as a high reflection probability from the surface. Measurements [13,14] and calculations [15] of the sticking probability of hydrocarbons show a non-negligible sticking depending on the conditions and the hydrocarbon species. Our findings should therefore be understood in terms of an effective self re-erosion of the carbon deposits formed by hydrocarbons having incorporated the hydrogen in the species itself. This large self re-erosion might be triggered by a synergism caused by the energetic background hydrogen ions. Synergism effects of ions enhancing the chemical erosion are discussed in [16]. Energetic ions can create dangling bonds, active sites and kinetic release of loosely bonded hydrocarbons and therefore cause an increased erosion. This means that the hydrocarbon species are only transiently re-deposited and do not contribute to the formation of a deposit. Therefore, within this model only carbon ions and atoms hitting the surface contribute to the build-up of a layer. However, this layer also suffers from an 'enhanced' chemical erosion ($Y_e \approx 8\%$) caused by the background hydrogen. Laboratory experiments of the chemical erosion of (soft, hydrogen-rich) a-C:H layers show much higher erosion yields compared to graphite [17].

The majority of the injected $^{13}CH_4$ escapes the local re-deposition and is transported inside the last closed flux surface where it is completely dissociated. The ^{13}C ions are then transported back into the scrape-off layer (SOL) and hit the wall surface as energetic ions with an average charge state $Q = 4$ similar to the 'usual' background carbon ^{12}C in TEXTOR. The deposition efficiency of these $^{13}C^{4+}$ ions is much higher (compared to carbon or hydrocarbon radicals which directly return to the limiter surface) due to their high impact energy of several hundred eV (acceleration in the sheath potential to about $3QT_e$ plus thermal energy $2T_i$). Thus it is no surprise that the injected ^{13}C could be found on other wall elements in the SOL of TEXTOR and at the side-wall of the testlimiter with a fixed ratio to the ^{12}C deposition.

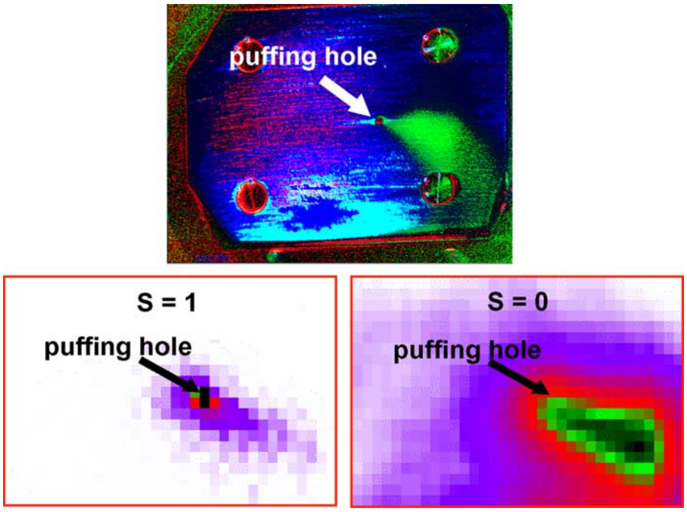

Fig. 2. Measured and simulated (assuming sticking parameters of $S = 1$ or $S = 0$ for hydrocarbons) spatial distribution of ^{13}C deposition from external injection of $^{13}CH_4$ through the inclined testlimiter surface in TEXTOR.

3. Transport of hydrocarbons and beryllium in the divertor of JET

Large amounts of carbon deposition at JET are especially found at areas not directly wetted by plasma. In the MkIIa divertor configuration, the carbon is found at remote areas at the water-cooled louvers of the entrance to the inner pump [18]. In the MkIIGB geometry, which includes a dome, the majority of the carbon layers was formed in the private flux region on the horizontal targets and on the dome [19].

As in TEXTOR, also for the case of JET the carbon deposition cannot be modelled if a noticeable sticking of hydrocarbons and $Y_{\mathrm{chem}} \approx 2\%$ are assumed [20,21]. To approach the observations by modelling an enhanced erosion of re-deposited carbon species in combination with a negligible 'effective' sticking of hydrocarbons ($S = 0$) at plasma wetted areas have to be assumed. At the high flux areas the re-deposited carbon is eroded effectively by the hydrogen atoms incorporated in the returning hydrocarbons in addition to the erosion due to the D^+ ions and atoms from the background plasma. By this, the carbon is transported successively to plasma-shadowed areas where the D^+ flux is small. The self re-erosion (corresponding to $S = 0$) and the erosion by D^0 is only enhanced in the presence of D^+ ions. This point of synergism effects was discussed in Section 2.

Simulations of the CIII light emission in the divertor of JET MkIIGB in an H-mode discharge (#53070) show a good agreement with the experiment (Fig. 3). Differences in the CIII pattern between the inner divertor (which is most of the time detached from the target plates) and the outer divertor (attached) can be well reproduced. The agreement between simulation and experiment shows that modelling with the ERO-JET code reasonably well reproduces the local transport of impurities.

The transport of beryllium in the inner divertor MkIIA can also be described well by the simulations. Beryllium is evaporated at JET from time to time in the main chamber and partly transported as impurity into the inner divertor region where a certain fraction is

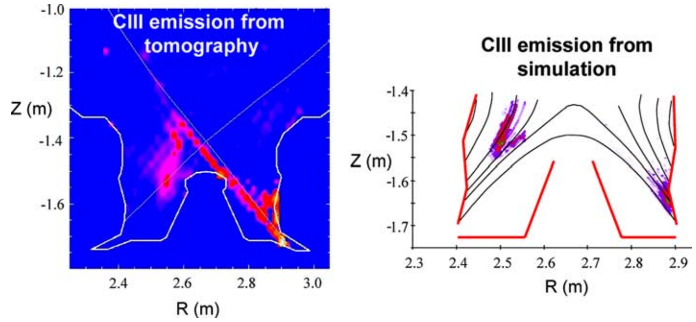

Fig. 3. Measured (left) and simulated (right) two-dimensional emission pattern of C^{2+} ions (CIII) in the divertor MKIIGB of JET during an H mode discharge. The co-ordinates R and Z refer to the geometric center of the JET device.

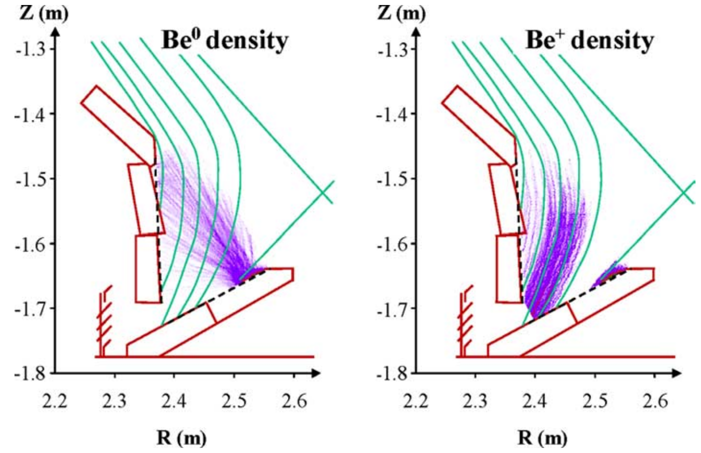

Fig. 4. Simulated two-dimensional distribution of neutral beryllium (Be^0) and beryllium ions (Be^+) after physical sputtering along the horizontal target in the inner divertor MkIIa of JET.

deposited at the horizontal target plate (in the simulations the strike point is located at the horizontal divertor plate). Main beryllium erosion takes place at the location of the strike point. Due to the absence of chemical erosion and the high density and temperature near the strike point most of the beryllium ($\approx$80%) is re-deposited locally at areas of ion flux impact (plasma wetted areas) adjacent the strike point. The remaining part moves through the plasma and finally ends up at the vertical divertor targets where the plasma temperature is only several eV. When the electron temperature is too low for physical sputtering the transport is inhibited. This may explain that the transport into the louver region is suppressed for beryllium as observed experimentally (Fig. 4). In contrast to carbon the formation of beryllium layers is mainly seen on the plasma-wetted divertor targets (at locations with low plasma temperature) and not on plasma shadowed areas like the louvers.

4. Conclusions

$^{13}CH_4$ injection in TEXTOR results in a very low local deposition efficiency, which suggests a high re-erosion of the in-situ, transiently built-up carbon layers. The high re-erosion leads to a negligible effective sticking of hydrocarbons returning to the surface. It can be understood as a self re-erosion due to the deuterium contained in the hydrocarbon returning to the surface. In addition to the process of self re-erosion also the erosion caused by the background deuterium ions seems to be enhanced for freshly formed deposits compared to pure graphite ($Y_e \approx 8\%$ vs. $Y_{chem} \approx 1.5\%$). These chemical erosion processes are probably triggered via a synergism effect by the deuterium plasma ions. The low effective sticking (less than 0.5%) would therefore not be in contradiction with measured sticking probabilities revealing in general a noticeable sticking with the absence of plasma ion impact. At JET significant carbon layer formation is observed at areas shadowed from ion impact. According to our assumptions, re-deposited layers suffer from large re-erosion at areas wetted by plasma ion impact. They seem to exist only transiently. However, it should be noted that this model needs further confirmation by additional experiments. In particular the effect of transient heat loads due to ELMs on the thermal stability of the layers and their possible thermal decomposition should be considered.

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References

[1] ITER Technical Basis, ITER EDA Documentation Series No. 24 (2002) IAEA, Vienna.

[2] A. Kirschner, V. Philipps, J. Winter, U. Kögler, Nucl. Fusion 40 (2000) 989.

[3] P. Wienhold, H.G. Esser, D. Hildebrandt, A. Kirschner, M. Mayer, V. Philipps, M. Rubel, J. Nucl. Mater. 290–293 (2001) 362.

[4] W. Eckstein, Computer Simulation of Ion Solid Interaction, Springer, Berlin, 1991.

[5] A. Kirschner, A. Huber, V. Philipps, A. Pospieszczyk, P. Wienhold, J. Winter, J. Nucl. Mater. 290–293 (2001) 238.

[6] A.D. Ehrhardt, W.D. Langer, Report PPPL-2477, Princeton University, 1987.

[7] G. Federici, R.A. Anderl, P. Andrew, J.N. Brooks, R.A. Causey, J.P. Coad, D. Cowgill, R.P. Doerner, A.A. Haasz, G. Janeschitz, W. Jacob, G.R. Longhurst, R. Nygren, A. Peacock, M.A. Pick, V. Philipps, J. Roth, C.H. Skinner, W.R. Wampler, J. Nucl. Mater. 266–269 (1999) 14.

[8] A. Pospieszczyk, V. Philipps, E. Casarotto, U. Kögler, B. Schweer, B. Unterberg, F. Weschenfelder, J. Nucl. Mater. 241–243 (1997) 833.

[9] J. Roth, J. Nucl. Mater. 266-269 (1999) 51, and private communication.

[10] R.K. Janev, D. Reiter, Report Jül-3966 (2002) ISSN 0944-2952.

[11] A. Kirschner, J.N. Brooks, V. Philipps, P. Wienhold, A. Pospieszczyk, R.K. Janev, U. Samm, J. Nucl. Mater. 313–316 (2003) 444.

[12] P. Wienhold, M. Rubel, M. Mayer, et al., Phys. Scr. T94 T94 (2001) 141.

[13] C. Hopf, T. Schwarz-Selinger, W. Jacob, A. von Keudell, J. Appl. Phys. 87 (2000) 2719.

[14] M. Mayer, V. Rohde, T. Pütterich, P. Coad, P. Wienhold, JET-EFDA contributors, ASDEX Upgrade Team, Phys. Scr., in press.

[15] D.A. Alman, D.N. Ruzic, Phys. Scr., in press.

[16] E. Vietzke, K. Flaskamp, V. Philipps, J. Nucl. Mater. 111&112 (1982) 763.

[17] E. Vietzke, A.A. Haasz, in: W.O. Hofer, J. Roth (Eds.), Physical Processes of the Interaction of Fusion Plasmas with Solids, Academic, San Diego, 1996.

[18] J.P. Coad, N. Bekris, J.D. Elder, S.K. Erents, D.E. Hole, K.D. Lawson, G.F. Matthews, R.-D. Penzhorn, P.C. Stangeby, J. Nucl. Mater. 290–293 (2001) 224.

[19] J.P. Coad, P. Andrew, D.E. Hole, S. Lehto, J. Likonen, G.F. Matthews, M. Rubel, Contributors to the EFDA-JET work-programme, J. Nucl. Mater. 313–316 (2003) 419.

[20] A. Kirschner, J.N. Brooks, V. Philipps, J.P. Coad, Contributors to the EFDA-JET Workprogramme, Plasma Phys. Controlled Fusion 45 (2003) 309.

[21] J.N. Brooks, A. Kirschner, D.G. Whyte, D.N. Ruzic, D.A. Alman, J. Nucl. Mater. 313–316 (2003) 424.