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Journal of Nuclear Materials 266–269 (1999) 360–364

journal of nuclear materials

Transport of hydrocarbon molecules in the edge plasma of fusion experiments

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Abstract

The transport of emitted methane molecules has been analyzed with the 3D Monte Carlo code ERO. A *D*/*XB* coefficient is defined and allows a conversion of line-of-sight intensity of the integrated molecular CD band into the methane influx density by multiplication. This coefficient has been calculated for a wide range of plasma parameters (electron temperature and density). A strong dependence on the sticking probability of the different hydrocarbon molecules to the surface has been observed. The results are discussed in comparison with those obtained from a 0D reaction model where the transport is included by defining particle residence times. A calculation for ASDEX-Upgrade using a plasma background generated with the B2-Eirene code is presented.

Keywords: Chemical erosion; Methane breakup; Transport; Computer simulation; ERO code

1. Introduction

Carbon divertor targets near the strike zone have been chosen in the ITER design. The lifetime of these plasma facing components is largely determined by chemical erosion, especially at low electron temperatures. Up to now, the flux and energy dependence of erosion yields for energies less than 50 eV are not well established. In situ spectroscopic measurements of the CD molecular band emission offer the possibility to obtain these essential informations. However, in order to interpret the CD signals (relating them to the methane production) the break-up of the methane molecules in the near-surface plasma must be considered. A large number of dissociation processes, charge exchange reactions and transport effects, including redeposition, are of importance. In the next paragraph estimations concerning the reaction times and lengths are given for electron temperatures and densities of divertor plasmas in existing fusion experiments. The *D*/*XB*-coefficient is defined in Section 1.2. In Section 2 a reaction model is presented where the effect of transport is taken into account by assuming residence times. The ERO code [1] has been used to calculate the *D*/*XB*-coefficients for different plasma parameters in a simple geometry (Section 3.1). The simulation of the recently performed experiments concerning chemical erosion in ASDEX-Upgrade is described in Section 3.2.

1.1. Chemical erosion and reaction rates

Many uncertainties presently exist concerning the chemical erosion yield of graphite by hydrogen (deuterium) impact for low energy (<50 eV) and, especially, at high-flux densities ($>1 \times 10^{20}$ ions/m^2 s). At room temperatures yields of about 1% for ion impact energies in the region of 10–30 eV are measured for relatively low flux densities [2]. Recently, Roth has presented a semi-empirical formula for the yield calculation [3] which has been applied in the modelling with the ERO code. At lower ion energies, there will also be a greater production of C_2H_x (C_2D_x) and C_3H_x (C_3D_x) hydrocarbons

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PII: S0022-3115(98)00667-9

relative to CH_4 (CD_4). Due to the lack of reaction rate coefficients for these heavier hydrocarbon molecules only CD_4 has been assumed to be emitted in the present study.

Thirty-four reactions and their rate coefficients have been compiled by Ehrhardt and Langer [4] describing the break-up process of the methane molecules in the plasma. For electron temperatures $T_e < 6$ eV the most probable reaction chain is $CD_4 \rightarrow CD_4^+ \rightarrow CD_2 \rightarrow CD_2^+ \rightarrow CD$ where charge exchange reactions with the plasma ions dominate. For higher temperatures another channel $CD_4 \rightarrow CD_3 \rightarrow CD_2 \rightarrow CD$ has a higher probability. Note, that here the reduction of methane to CD occurs only via neutrals without molecular ions. For an energy of the emitted CD_4 molecules of 0.026 eV (corresponding to a surface temperature of 300 K) the average reaction time to break-up to CD is about 3×10^{-6} s for $T_e \approx 5$ eV. The reaction length is then $\approx$1.5 mm for an electron density of 1×10^{20} m^{-3}.

1.2. The D/XB-coefficient

The influx density of methane Γ^{CD_4} from a infinite surface is defined by the relation

$$\Gamma^{CD_4} = \int_0^\infty n^{CD_4}(x) n_e(x) \sum_j \langle \sigma v \rangle_{CD_4 \rightarrow j} \, dx, \tag{1}$$

where $n^{CD_4}(x)$ is the methane density at a distance x from the surface, n_e is the electron density and $\sum_j \langle \sigma v \rangle_{CD_4 \rightarrow j}$ is the sum of the rate coefficients for all possible loss reactions of CD_4 (dissociation and charge exchange reactions). The intensity of the molecular CD band emission I^{CD} (at 430 nm) measured for a line of sight orientated perpendicular to the surface becomes

$$I^{CD} = \frac{h\nu}{4\pi} B \int_0^\infty n_e(x) n^{CD}(x) \langle \sigma_{exc} v \rangle \, dx, \tag{2}$$

with n^{CD} being the density of the CD molecules. The excitation rate coefficients $\langle \sigma_{exc} v \rangle$ are given by Behringer [5] and can be approximated with $X = \langle \sigma_{exc} v \rangle \simeq 1.45 \times 10^{-14} \exp(-3.19/T_e)/T_e^{0.28}$ (T_e in eV, X in m^3/s) in the electron temperature range of $1 \leqslant T_e \leqslant 100$ eV. $B = 1$ is the branching ratio. A *D*/*XB*-coefficient (in anology with the *S*/*XB*-coefficient for atoms and ions) representing the ratio of the methane influx density to the intensity of the CD emission can be introduced

$$\frac{D}{XB} = \frac{h\nu}{4\pi} \frac{\Gamma^{CD_4}}{I^{CD}} = \frac{\sum_j \langle \sigma v \rangle_{CD_4 \rightarrow j}}{\langle \sigma_{exc} v \rangle B} \frac{n^{CD_4}}{n^{CD}}. \tag{3}$$

This relation is valid only for constant plasma parameters (T_e, n_e) along the line of sight. In all other cases an integration should be performed

$$D/XB = \Gamma^{CD_4} \Big/ \int_0^\infty n_e(x) n^{CD}(x) \langle \sigma_{exc} v \rangle \, dx \, B. \tag{4}$$

2. The zero-dimensional model

For a homogeneous plasma with given T_e and n_e, the ratio n^{CD_4}/n^{CD} can be determined by a set of reaction equations

$$\frac{\partial n^i}{\partial t} = -\frac{n^i}{\tau^i} - n_e n^i \sum_j \langle \sigma v \rangle_{i \rightarrow j} + n_e \sum_k n^k \langle \sigma v \rangle_{k \rightarrow i}, \tag{5}$$

where the index i denotes the eight different hydrocarbon molecules (CD_4, CD_4^+, CD_3, CD_3^+, CD_2, CD_2^+, CD, CD^+) being of interest; $\langle \sigma v \rangle_{i \rightarrow j}$ and $\langle \sigma v \rangle_{k \rightarrow i}$ are the rate coefficients for the loss and source reactions, respectively (taken from [4]). Such a reaction model has been also applied by Behringer [6] to determine the *D*/*XB*-coefficient. The effect of transport is introduced in this 0D model by the term n^i/τ^i with residence times τ^i for each molecule. Using the steady-state solution of (Eq. (5)) for the CD and the CD_4 densities the *D*/*XB*-coefficient has been calculated Eq. (3) for different T_e and $n_e = 1 \times 10^{20}$ m^{-3} (Fig. 1). In the first case (Fig. 1(a)) the assumed residence times are taken equal for all molecules – ions and neutrals. The results for the case where the neutrals are not lost by transport ($\tau_{neutrals} = \infty$) are shown in Fig. 1(b). With shorter τ the *D*/*XB*-coefficient increases. Many molecules are lost before they can dissociate up to CD which leads to lower CD than CD_4 densities. Note, that the results under steady-state conditions do not change if the product of electron density and residence time $n_e \tau$ remains constant.

3. ERO calculations

The reaction model of Ehrhardt and Langer is incorporated in the ERO code [1], where Monte Carlo techniques are used to determine which reactions occur in each time step. Neutral–neutral collisions are not considered, whereas the ions are the subject of electric, magnetic, ion and electron thermal forces. Friction with the plasma ions, parallel and cross-field diffusion (with a constant value of $D_\perp = 0.5$ m^2/s) are also taken into account. The methane molecules (CD_4) are launched with an initial energy of 0.026 eV, a cosine distribution in elevation angle and a uniform distribution in azimuthal angle.

The specification of the reflection model for hydrocarbon molecules reaching the surface, i.e. being redeposited, is a critical question. In the absence of models

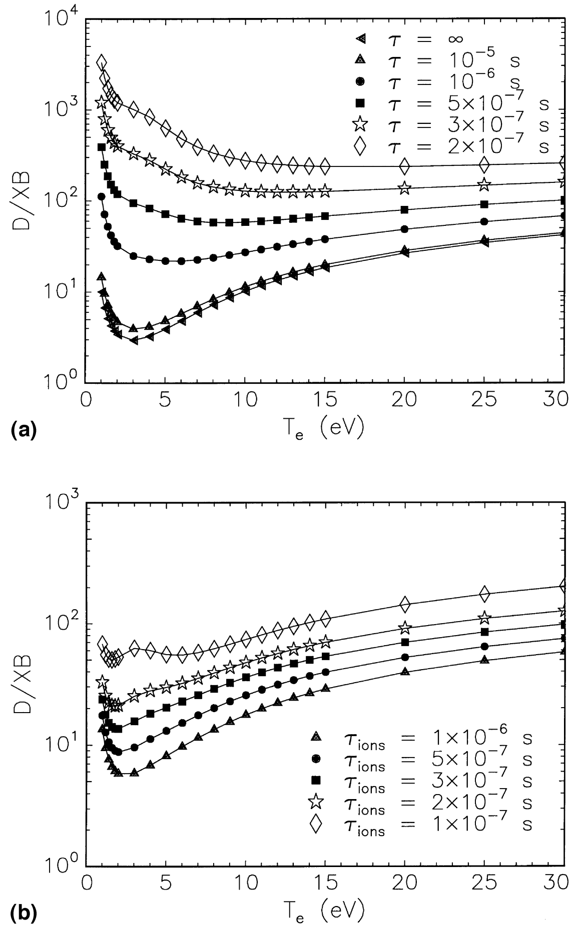

Fig. 1. Electron temperature dependence of the *D/XB*-coefficient as calculated with the reaction model (Section 2). The different residence times assumed in the model are indicated: (a) $\tau = \tau_{ions} = \tau_{neutrals}$, (b) $\tau_{neutrals} = \infty$.

confirmed by experiments, four different models have been applied in the modelling. Firstly (A), the model of total adsorption. Secondly (B), the molecules (ions and neutrals) are assumed to be dissociated at the surface. The C atom sticks, whereas the released deuterium atoms (for example three D atoms in the case of a redeposited CD_3^+ ion) react chemically with the graphite. New methane molecules are emitted with a specified yield Y_{chem}. Thirdly (C), the redeposited neutral molecules are simply reflected, whereas the redeposited ions have enough energy (due to the acceleration in the electric sheath) to undergo the dissociation/chemical erosion process as described in model B. Fourthly (D), all redeposited molecules (ions and neutrals) initiate an emission of a methane molecule with a probability corresponding to the number of D atoms bonded on the C atom (0.25 for CD, 0.5 for CD_2, 0.75 for CD_3, 1.0 for CD_4 [7]). The model C seems to be the more realistic one. The redeposited neutrals have predominantly energies below the binding energies of the molecule and, probably, do not dissociate.

3.1. Variation of the plasma parameters

The density $n^{CD}(x)$ as a function of the distance x from a surface that emits methane molecules has been calculated with the ERO code. For a given flux density Γ^{CD_4} the *D/XB*-coefficient is determined using Eq. (4). Table 1 summarizes the results for the different reflection models A–D, where the average residence times for each molecule are also quoted. The plasma parameters ($T_e = T_i, n_e$) above the surface are assumed uniform. For the inclination angle of the magnetic field lines with respect to the target surface a value of 2° has been chosen. The calculated *D/XB*-coefficient depends strongly on the reflection model applied in the simulation.

The fast transport of the ions to the surface leads to shorter residence times in the plasma in comparison with the neutrals. The residence times of the molecular neutrals are mainly defined by the reaction times. Such a clear distinction between the reaction and the residence times as done in Eq. (5) is not possible in the ERO calculations. In the modelling – and in the experiment – the two processes occur simultaneously. But, assuming a value of $\tau = 1.8 \times 10^{-7}$ s for all molecular ions and $\tau = \infty$ for the neutrals the same value for the *D/XB*-coefficient (*D/XB* = 34.7 for model C, Table 1) can be obtained with the 0D reaction model (see also Fig. 1(b)).

Table 1
Calculated *D/XB*-coefficients and average residence times for $n_e = 1 \times 10^{20}$ m^{-3}, $T_e = T_i = 6$ eV, $B = 2$ T

Model	A	B	C ($Y_{chem} = 0.01$)	D
D/XB	57.5	54.2	34.7	12.2
τ^{CD_4}(s)	3.1×10^{-7}	6.1×10^{-7}	3.2×10^{-7}	3.5×10^{-6}
$\tau^{CD_4^+}$(s)	3.8×10^{-8}	4.0×10^{-8}	4.7×10^{-7}	4.0×10^{-8}
τ^{CD_3}(s)	2.4×10^{-7}	2.4×10^{-7}	3.5×10^{-7}	2.4×10^{-7}
$\tau^{CD_3^+}$(s)	1.3×10^{-7}	1.2×10^{-7}	2.7×10^{-7}	1.2×10^{-7}
τ^{CD_2}(s)	3.4×10^{-7}	3.3×10^{-7}	4.1×10^{-7}	3.3×10^{-7}
$\tau^{CD_2^+}$(s)	2.5×10^{-7}	2.4×10^{-7}	2.1×10^{-7}	2.3×10^{-7}
τ^{CD}(s)	4.0×10^{-7}	4.0×10^{-7}	4.5×10^{-7}	4.0×10^{-7}

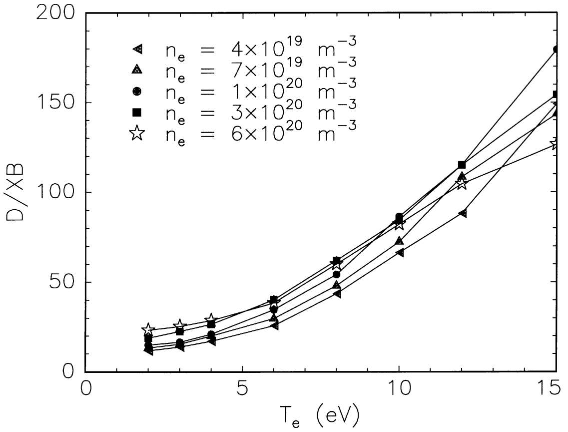

Fig. 2. Electron temperature dependence of the *D*/*XB*-coefficient as calculated by the ERO code for different electron densities.

Fig. 2 shows the calculated *D*/*XB*-coefficients (with reflection model C) for different plasma parameters. The calculated dependence on the electron temperature is stronger than the dependence on the electron density in the parameter range under consideration.

3.2. Modelling for ASDEX-Upgrade

A strong hydrogen flux dependence of chemical erosion has been observed in ASDEX-Upgrade [8]. To model these experiments a 2D plasma background as generated by a B2-Eirene run [9] has been adopted to the 3D ERO simulation assuming toroidal symmetry. The magnetic configuration and the divertor shape are also taken from B2-Eirene. For a high-recycling discharge the electron density and temperature (Figs. 3 and 4), the ion temperature, their gradients and plasma flow velocity are calculated by B2-Eirene and used in ERO. Only chemical erosion due to plasma ions (and emission only of CD_4) has been considered using the relation for the yield proposed by Roth [3].

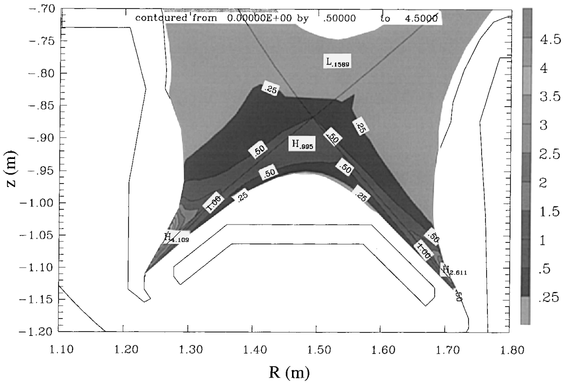

Fig. 3. Contours of the electron density (in $10^{20}\ m^{-3}$) in the divertor region of ASDEX-Upgrade calculated with the B2-Eirene code.

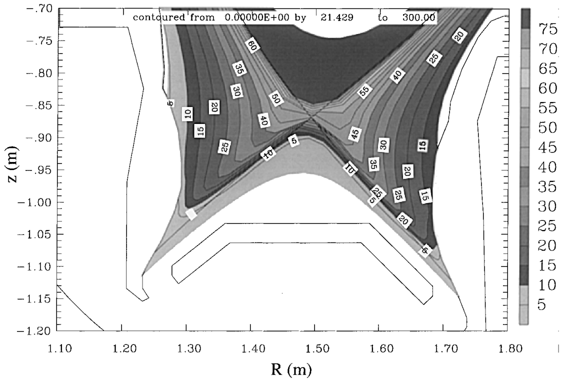

Fig. 4. Contours of the electron temperature (in eV).

The calculated CD density along the line of sight ROV15 of the ASDEX-Upgrade spectroscopy system is shown in Fig. 5 together with the outer divertor geometry. For these high-electron densities the break-up process of the methane molecules is localized near the divertor plate, and therefore is determined by the plasma parameters close above the surface. For the molecular ions the strong electric field in the sheath plays a significant role. A *D*/*XB*-coefficient of 45.5 is obtained using the reflection model C.

Taking the values at the strike point of the line of sight ROV15 on the outer divertor target: $n_e \simeq 1.4 \times 10^{20}\ m^{-3}$ and $T_e \simeq 7$ eV nearly the same value can be estimated from the ERO results for an uniform plasma (Fig. 2).

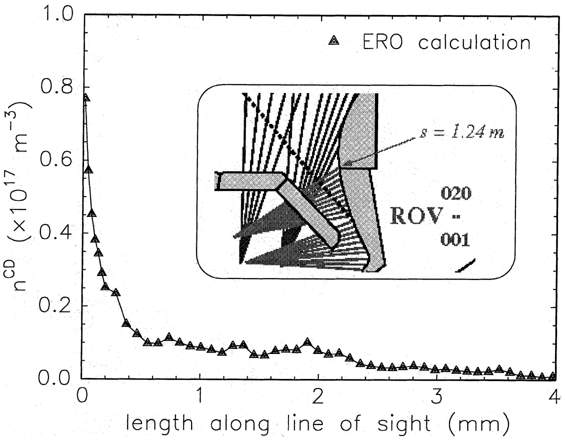

Fig. 5. Calculated CD-density distribution along the line of sight ROV15 of the ASDEX-Upgrade divertor spectroscopy system starting from its strike point ($R = 1.6929$ m, $z = -1.075$ m) on the outer divertor plate.

4. Conclusions

The influx density of methane can be related to the intensity of the CD band emission measured in fusion experiments by the a *D*/*XB*-coefficient. This value has been calculated using the 3D impurity Monte Carlo code ERO varying the main plasma parameters, n_e and T_e. The dependence on the electron temperature appears to be stronger than the dependence on the electron density in the studied parameter range and should be taken into account.

The influence of the reflection model for the redeposited molecules is found to be strong. Further experimental investigations are clearly required to confirm which model should be applied. The contribution of the heavier hydrocarbon molecules C_2D_x and C_3D_x could not be estimated in the presented study due to the lack of corresponding rate coefficients. The ERO code has been extended to use B2-Eirene generated plasma backgrounds which allows a more realistic modelling. As an example an ASDEX-Upgrade experiment dedicated to chemical erosion [8] has been simulated and the corresponding *D*/*XB*-coefficient has been evaluated.

Acknowledgements

The authors like to thank A. Kallenbach and C.H. Wu for helpful discussions and encouragement.

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