Simulation Study on Effects of Chemically Eroded Methane and Ethylene Molecules on Carbon Impurity Transport and Net Erosion of Carbon Materials

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Abstract
Effects of chemically eroded CD$_4$ and C$_2$D$_4$ molecules on local transport of ionized C impurities and net erosion of the C target are studied using a simulation code for plasma surface interactions. The calculated C$^+$ emission profile reproduces the experimental one, which indicates a stronger contribution of CD$_4$. For C$^{2+}$ and C$^{3+}$, the contribution of C$_2$D$_4$ is stronger near the target. For their penetrations, however, the contribution of CD$_4$ is essential. For a high density and low temperature plasma, there is a significant influence of the charge transfer reactions of C$_x$D$_y$ with D$^+$, by which the penetrations as well as the net erosion rates for CD$_4$ and C$_2$D$_4$ are suppressed with their local redeposition. The net erosion rate for C$_2$D$_4$ is higher if $Y_{CD4} = Y_{C2D4}$. If the temperature becomes high, however, the rate for C$_2$D$_4$ is suppressed by its local redeposition, and approaches that for CD$_4$.

Keywords:
chemical erosion, carbon, methane, ethylene, carbon impurity transport, net erosion

1. Introduction
Because of a high thermal shock resistance, C material will be used as a plasma facing material of ITER divertor target plates. However, there is a crucial issue in net erosion relevant to the divertor lifetime, namely, chemical sputtering of C material. This causes penetration of hydrocarbons, such as methane (CD$_4$) and ethylene (C$_2$D$_4$), to the core plasma [1]. The impurity penetration contaminates the plasma, which results in a degradation of the plasma performance. Thus, effects of the chemically eroded CD$_4$ and C$_2$D$_4$ molecules on the impurity penetration and the net erosion rate need to be clear to improve the plasma performance and the divertor lifetime.

In this study, the effects on the penetrations of ionized C impurities are studied using a simulation code for plasma surface interactions, ERIm [2]. The result is compared with experimental data [3]. Also, the effects on the net erosion rates for a variety of plasma parameters and for the normal ITER divertor plasma predicted by B2-EIRENE [4] are studied. The paper discusses how the penetration depth from the C target to the core plasma and its net erosion rate are changed by chemical erosion (release) of CD$_4$ and C$_2$D$_4$ each.

2. Simulation code and model
On the basis of the Monte-Carlo impurity transport model [5] and the binary collision model [6], ERIm simulates the penetration depth of ionized C impurities from a C target exposed to the plasma/impurity ions and its net erosion rate. Only the important features of the code for this study are described here (see ref. [2] for details). For the penetration depth, the eroded impurities are assumed to be subject to the Lorentz and friction forces [5]. The impurity penetration contaminates the plasma, which results in a degradation of the plasma performance. Thus, effects of the chemically eroded CD$_4$ and C$_2$D$_4$ molecules on the impurity penetration and the net erosion rate need to be clear to improve the plasma performance and the divertor lifetime.

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Here, a word “deposition” is used for impurities transported by a plasma from other wall targets, and “redeposition” is used for those locally returned back to the target. The energy of the impinging ions is given by the Maxwellian distribution with an acceleration energy due to the electrostatic sheath potential, \( V_S = T_i/2\pi m_i m_e(1 + T_i/T_e) \), and the flux is given by \( n_i(T_i + T_e)/m_i^{1/2} \) \[10\]. Here, \( T_i \) and \( T_e \) are the plasma electron and ion temperatures in front of the target, respectively, \( m_e \) and \( m_i \) are the electron and ion masses, respectively, and \( n_i \) is the ion density. \( CD_4 \) and \( C_2D_4 \) molecules are assumed to be released from the C target according to their chemical release yields, \( Y_{CD_4} \) and \( Y_{C_2D_4} \), respectively. For the physically released \( C^0 \) atoms, their release is based on the binary collision model \[5\]. In this study, there are no differences in chemical properties between the deposited layer and the bulk target.

3. Results and discussion

3.1 Carbon impurity transport

The simulation of the penetration depth is performed based on the TEXTOR-94 edge plasma \[11\]. The electron density and temperature profiles used in this study are the exponential functions fitted to those measured by the Li- and He-diagnostics. They are given by \( n_e(r) = n_{e_{LCFS}} \exp(-(r - 0.46 m)/0.02 m) \) and \( T_e(r) = T_{e_{LCFS}} \exp(-(r - 0.46 m)/0.025 m) \), where \( n_{e_{LCFS}} = 10^{18} \ \text{m}^{-3} \) and \( T_{e_{LCFS}} = 30 \ \text{eV} \) are the density and temperature at the last closed flux surface (LCFS), at a minor radius of \( r \approx 0.46 \text{ m} \), respectively \[3,12\]. For the impinging ions, \( D^+ \) (\( 98 \% \)) and \( C^+ \) (\( 2 \% \)) are used assuming \( T_i = T_e \) \[12\].

The radial penetrations of \( C^{1+} \), \( C^{2+} \) and \( C^{3+} \) generated through the reaction chains of \( CD_4 \), \( C_2D_4 \) and \( C^0 \) released from the target at \( r = 0.47 \text{ m} \) are simulated as shown in Fig. 1. In the result, \( Y_{CD_4} = 3.6 \% \) and \( Y_{C_2D_4} = 0.9 \% \) are assumed, which are based on the experimental data for C targets exposed to the TEXTOR-94 plasma \[11\] and 200 eV \( D^+ \) beam \[1\]. As shown in Fig. 1(a), the \( C^{1+} \) penetration is in good agreement with the measured CII light emission profile \[3\] (this means that their decay lengths are the same). The agreement indicates that the contribution of \( CD_4 \) is stronger than that of \( C_2D_4 \) near the target. For \( C^{2+} \) and \( C^{3+} \), however, the opposite results occur as shown in Figs. 1(b) and 1(c), which indicate the stronger contribution of \( C_2D_4 \) near the target. However, the contribution of \( CD_4 \) is found to be essential for the penetration of highly ionized C impurities under the low density and high temperature plasma \( n_{e_{LCFS}} = 10^{19} \ \text{m}^{-3} \) and \( T_{e_{LCFS}} = 30 \ \text{eV} \).
Comparison in the C$^+$ and C$^{2+}$ penetrations between the reaction chain of CD$_4$ and C$_2$D$_4$ with e$^-$, (a) and (b), and that with e$^+$ plus D$^+$, (c) and (d), under a high density and low temperature plasma ($n_{LCFS} = 10^{19}$ m$^{-3}$, $T_{LCFS} = 3$ eV).

### 3.2 Net erosion of carbon material

The simulation of the net erosion rate (including the redeposition rate) for different plasma densities and temperatures is also performed based on the same TEXTOR-94 edge plasma as described in the previous subsection [11] (contribution of physical sputtering is included in this result). In order to clarify a difference in the results between CD$_4$ and C$_2$D$_4$ chemical erosions, the same erosion yields are assumed: $Y_{CD4} = Y_{C2D4} = 4.0\%$. A change in the net erosion rate of the C target at $r = 0.47$ m with $n_{LCFS}$ and $T_{LCFS}$ is calculated as shown in Fig. 3 (if there is no chemical erosion, net deposition of the impinging carbon occurs at a low temperature, see ref. [14] for details).

At a low density ($n_{LCFS} = 10^{18}$ m$^{-3}$), there is a difference in the results between the CD$_4$ and C$_2$D$_4$ reaction chains with e$^-$. The net erosion rate for C$_2$D$_4$ is higher [Fig. 3(a)], although its redeposition rate is higher [Fig. 3(a')] This is simply because the gross erosion for a molecule of C$_2$D$_4$ is equivalent to that for two C atoms. On the other hand, they have a similarity that they increase with $T_{LCFS}$ due to an increase in the physical erosion. However, if the density increases ($n_{LCFS} = 10^{19}$ m$^{-3}$), there is a drastic change in the net erosion rate for C$_2$D$_4$ [Fig. 3(b)]. With increasing $T_{LCFS}$, the net erosion rate for C$_2$D$_4$ increases, and then decreases at $T_{LCFS} > 5$ eV. The further increase in $T_{LCFS}(> 40$ eV) makes it increase again, but it is almost the same as that for CD$_4$. The drastic change is because the redeposition rate for C$_2$D$_4$ increases rapidly with $T_{LCFS}$ [Fig. 3(b')]. In this calculation, the redeposition comes from the friction forces on the impurity ions in the direction parallel to the magnetic field (no thermal forces are taken into account). Thus, at the high density and temperatures, the net erosion rate for C$_2$D$_4$ is found to be significantly suppressed by its local redeposition.

If the charge transfer reactions with D$^+$ are added (black and gray solid curves), both of the net erosion rates are suppressed at the high density [Fig. 3(b)]. Due to this addition, for example, both of the redeposition rates at $T_{LCFS} < 5$ eV are enhanced from 0 % to 10 % [Fig. 3(b')]. On the other hand, at the low density, there is little influence of the charge transfer reactions [Figs. 3(a) and 3(a')]. Thus, at the high density plasma, the net erosion rates for CD$_4$ and C$_2$D$_4$ are expected to be suppressed by their strong local redeposition resulting from the charge transfer reactions.

For the normal ITER divertor plasma [4,15], the net erosion rates along the outer target plate for CD$_4$ and C$_2$D$_4$ are calculated assuming $Y_{CD4} = Y_{C2D4} = 1.0 \%$, as shown in Fig. 4. At locations of $z < -0.1$ m, i.e., at the private region and the strike point vicinity (where the density increases from $5 \times 10^{19}$ m$^{-3}$ to $2 \times 10^{21}$ m$^{-3}$ with increasing $z$, while the temperature keeps ~ 3 eV), the net erosion rate for C$_2$D$_4$ with e$^-$ is higher than that for CD$_4$ with e$^-$. This indicates that, for C$_2$D$_4$, the net erosion at these plasma regions would be more serious if $Y_{CD4} = Y_{C2D4}$. In contrast, at $z > -0.1$ m, i.e., at the SOL region (where the density decreases to $5 \times 10^{18}$ m$^{-3}$ with increasing $z$, while the temperature increases to 18
4. Conclusion

The simulated C\textsuperscript{1+} penetration at $n_{\text{LCFS}} = 10^{18}$ m\textsuperscript{-3} and $T_{\text{LCFS}} = 30$ eV reproduces the experimental one, which indicates that the contribution of CD\textsubscript{4} is stronger than that of C\textsubscript{2}D\textsubscript{4}. For C\textsuperscript{2+} and C\textsuperscript{3+}, however, the opposite result occurs near the target, which indicates the strong contribution of C\textsubscript{2}D\textsubscript{4}. For their penetrations, however, the contribution of CD\textsubscript{4} is essential. For a high density and low temperature plasma, there is a significant influence of the charge transfer reactions of C\textsubscript{x}D\textsubscript{y} with D\textsuperscript{+}, by which the penetrations are significantly suppressed. For the net erosion rate, there is also an influence of the charge transfer reactions: the net erosion rates for CD\textsubscript{4} and C\textsubscript{2}D\textsubscript{4} are suppressed by their local redeposition. Also, the net erosion rate for C\textsubscript{2}D\textsubscript{4} is higher than that for CD\textsubscript{4} if $Y_{\text{CD4}} = Y_{\text{C2D4}}$. However, if the temperature becomes high, the rate for C\textsubscript{2}D\textsubscript{4} is suppressed by its local redeposition, and approaches that for CD\textsubscript{4}.

References