Molecular Dynamics Study of Hydrogen and Hydrocarbon Interaction of Carbon and Beryllium deposits

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(1) Introduction

(2) Modeling Long-Distance Transport of Carbon and Beryllium in an ITER edge Plasma

(3) Modeling Tritium Retention in Tungsten Divertor Targets of ITER

(4) Molecular Dynamics Study of Hydrogen and Hydrocarbon Interaction of Carbon and Beryllium Deposits
Plasma ion bombardment of Material Surfaces
(1) Simultaneous bombardment with hydrogen and impurity ions; $H^+ + C^{q+} + Be^{q+} + W^{q+}$
(2) Maxwellian velocity distribution and sheath acceleration
   *(PIC simulation of plasma density and potential)*

Dynamic Erosion and Deposition Processes
(3) **Physical** sputter erosion and plasma impurities deposition *(dynamic BCA)*
(4) **Chemical** sputter erosion due to hydrocarbons formation *(Roth formulae)*
(5) Collisional mixing and thermal diffusion *materials mixing*

Impurity Transport in Plasma above Surfaces
(6) Multiple ionizations and dissociations of sputtered and reflected impurities, including $CH_4$ and higher hydrocarbons
   *a set of rate coefficients from Janev/Reiter*
(7) Gyromotion of the ionized impurities, simultaneously receiving
   (a) collisional friction force,    (b) temperature gradient thermal force,
   (c) crossed field diffusion,      (d) sheath and presheath electric field, and
   (e) elastic collision with neutral hydrogen. *(Also, PIC simulation)*

Local Redeposition of Impurities on Surfaces
(8) Reflection or sticking of carbon and hydrocarbons *particle species-, impact energy- and material-dependent.*
(9) Re-erosion of deposited and mixed materials
Hydrocarbon Redeposition on PFW Surfaces

Complex distribution of redeposition species

- Ion species dominate at high temperature
- Neutral species dominate at low temperature

⇒ Strong influence of atomic and molecular processes

Full sticking (S=1) of carbon and hydrocarbons on a flat wall surface
**13CH₄ injection experiments at TEXTOR**

Impurity transport, erosion and deposition process in EDDY and ERO codes were compared to be benchmarked against the experiments.

**roof-like test limiter exposed to SOL plasma of TEXTOR**

Top of the limiter was positioned at LCFS, the radial position of which is \( r = 46 \) cm.

At LCFS, \( T_e = 54 \) eV, \( T_i = 1.5 T_e \) and \( n_e = 1.9 \times 10^{12} \) cm\(^{-3} \).

Radial decay of the plasma parameter:
\[ l_{Te} = l_{Ti} = 40 \text{ mm}, \text{ and } l_{ne} = 22 \text{ mm} \]

\( 13\text{CH}_4 \) was injected into the plasma through a hole in the limiter surface.

\( 12\text{C} \) concentration of the background plasma was taken to be 3%.

(Assumption)

Most unexpected observation was the very low local deposition of \( ^{13}\text{C} \) on the limiter surface (\( \sim 0.2\% \)).
Observed 2D patterns of $^{13}$C deposition

Kreter et al.

$^{13}$CH$_4$ Injection hole

Observed pattern

Standard condition: $S=0.5$ and $Y_{chem}=3\%$

For both EDDY and ERO:

$\sim50\%$ deposition efficiency

– a factor of 100 larger than in experiment

Very localized deposition pattern (too much peaked)

$S=0.5$, but enhanced erosion of redeposited carbon atoms, $Y_{enh}=30\%$

EDDY: 33% $^{13}$C deposition
ERO: 32% $^{13}$C deposition

Still too large $^{13}$C deposition and patterns still too much peaked

$S=0$ (or small) & Enhanced erosion
Deposition efficiency strongly changes with injection time.

With increasing injection time, deposition efficiency strongly decreases due to increasing re-erosion of the redeposited $^{13}$C.

With further increasing time, deposition efficiency approaches a steady state value due to smaller change in the $^{13}$C concentration.

Deposition efficiency in steady state is in fair agreement with the efficiency calculated by ERO-HMM, not only for $S=0$ but also for $S=0.01$-$0.5$.

**Sticking probability of hydrocarbons and re-erosion of redeposited carbon** are still unknown parameters, which determine erosion and deposition of plasma facing materials.

<table>
<thead>
<tr>
<th>Sticking probability</th>
<th>S=0.5</th>
<th>S=0.1</th>
<th>S=0.05</th>
<th>S=0.01</th>
<th>S=0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{13}$C deposition efficiency (%)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EDDY</td>
<td>33.0</td>
<td>5.1</td>
<td>2.2</td>
<td>0.5*</td>
<td>0.1*</td>
</tr>
<tr>
<td>ERO</td>
<td>32.0</td>
<td>5.0</td>
<td>2.0</td>
<td>0.5</td>
<td>~0.1</td>
</tr>
</tbody>
</table>

*averaged between 5.29 s and 5.88 s
Coupling to an external bath (Langevin equation)

Periodic boundary condition

Initial computational cell

**W**: 3.165 nm x 3.165 nm x 6.33 nm, 4000 atoms (bcc),
**Graphite**: 2.13 nm x 2.46 nm x 0.671 nm, 400 atoms (hexagonal).

Atomic trajectories are followed using a variable-time-step Verlet algorithm.

Temperature control in order to dissipate the excess heat between impacts.

**Interaction Potential for ternary system W-C-H**


**Force on each atom in a system is calculated from analytical derivation of interaction potentials.**
To prepare the fusion-relevant wall surface:

- Amorphized C layer on W
- Bombardment with 10 eV C atoms
- Bombardment with 100 eV C atoms
- Hydrogenated amorphous C
- W-C mixed layer

Preparation of PFWs using MD Simulation
**Noncumulative** bombardments with hydrocarbon molecules

CH\(_x\) (x=1-4) and C\(_2\)H\(_x\) (x=1-6) with random direction hit random position of the top surface. Incident angle is 45°.

Same initial surface was used for each incidence.

With increasing impact energy, emission of large molecules is suppressed.

Carbon atoms emitted from W surface are much more than for graphite surface.
Both amorphization of graphite and hydrogen uptake in the amorphized C reduce emission of small hydrocarbons and carbon. Mixing of W with C reduces emission of both CH$_4$ (<30 eV) and C (>30 eV).
Species dependence of reflection coefficient

![Reflection coefficient graphs for CH_y and C_2H_y](image)

**CH_y (y=0 - 4)**

**C_2H_y (y=0 - 6)**

Reflection coefficient takes all of emitted species into account.

Frequent dissociation due to impact on surface leads reflection process to be more complex for heavier hydrocarbons.

Heavy hydrocarbons are reflected more.

With *increasing impact energy*, reflection coefficient *decreases*.

*At energies of several tens of eV or more*, most of projectiles can stick.
Deposition in the gaps of castellated tiles

The calculated redeposition profiles reproduce the experimental profiles of C deposition.

The redeposition layer is re-eroded by the bombardment of background plasma, therefore, C deposition is reduced at the gap edge of plasma-open side.

The redeposition on plasma-open side is suppressed due to the tilt of top surface of the cell.
Plasma Surface Interactions in ITER

Divertor
- Wing (W)
- Dome (W)

Vertical Target
- (C)

Chemical erosion

C deposition (a-C:H)

Mutual contamination between C and W

Be deposition on C and W

Be first wall

Carbon tile

H

C_xH

C_xH_y

Codeposition
Erosion and deposition characteristics of W is clearly different from simple sputtering of W (EDDY calculation).

W deposition on the C side strongly decrease CII light intensity above the surface.

“Suppression” of chemical sputtering due to W deposition
Be coverage effect of plasma impurities on C has been recently demonstrated in the experiments. Be seeding on a plasma in contact with a C target decreases to negligible levels the chemical sputtering yield of carbon even at Be concentration of ~0.1% in the plasma.
Deposition of Be on hydrogenated carbon

Be atoms are deposited on a hydrogenated C layer by simultaneous bombardment with 10 eV Be and 1 eV D atoms. The Be deposition grows up with increasing number of incident Be atoms, where incident D atoms are codeposited as well. The percent coverage of Be is increased with increasing number of incidence, up to 92%.
Noncumulative bombardments with 1000 D atoms with energies of 1–100 eV are performed and the same initial surface is used for each simulation.

Incident atoms hit the top surface at random positions. Incident polar angle is 45°, whereas the azimuthal angle is randomly selected from 0° – 180°.

Target temperature is changed from 300 K to 1200 K.

Dominant interaction occurs within a hydrogenated C layer and Be deposition.

Interaction layer tends to move from the C layer to the Be deposition layer with increasing Be coverage and decreasing D impact energy.
At 300 K, dominant emission species are small molecules. Larger molecules (CD$_2$ and CD$_3$) are emitted with increasing D/(C+D) ratio.

C atoms are emitted through physical sputtering mechanism.

With increasing temperature, CD$_y$ emission is strongly enhanced.

At 800 K, a maximum value of the emission yield is observed in the energy range of eV, where CD$_y$'s are more emitted with decreasing D impact energy.

Clearly, D uptake in the C layer induces sputtering of C atoms at energies much less than the threshold energy for physical sputtering.

If there is no uptake of D in the layer (D/(C+D)=0), hydrocarbon emission is very rare and sputtering of C atoms shows a clear threshold for physical sputtering.

At 1200 K, the numbers of emitted C and CD$_y$ increase monotonously with increasing D energy.
This result shows a good correlation with the mitigation of chemical erosion (i.e., the decrease in CD band light emission) of a C target exposed to a Be-seeded plasma in PISCES-B experiments [8].

The reduction rate increases monotonically with decreasing D impact energy. This explain the ion energy dependence of decay time of chemical CD light emission observed [9].

The reduction rate changes in the different manner from the experiments with increasing surface temperature. The calculation indicates a maximum reduction rate at ~800 K where the $C_D$ emission yield peaks.

Decrease in the emission yield is much faster than an increase in Be coverage on the surface.
A part of C atoms is promptly ionized and redeposit in the vicinity of the birthplace. The other part is transported away from it and some of them distribute out of the divertor. \( \text{CD}_y \) is rather limited within the private flux region (PFR) of the divertor.

**Be used for the first wall is strongly eroded due to its low surface binding energy and a portion of eroded Be atoms migrates towards the divertor targets, although most of atoms redeposit on the other areas of the first wall.**