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Modelling Basics of Erosion and Redeposition

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Modelling Erosion and Redeposition on Plasma Facing Walls: Basics and Recent progress

(II) Recent progress and integrated modelling

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Outline of Lecture

(A) INTEGRATED MODELLING OF EROSION/DEPOSITION A-1) Local deposition of impurities on plasma facing materials

(B) MODELLING USING PLASMA AND MATERIAL CODES

- B-1) Particle-in-Cell simulation of plasma sheath B-1-1) Carbon deposition in the gaps of castellated tiles
- B-2) Molecular dynamics simulation of plasma wall interaction
 B-2-1) Reflection/sticking coefficient of deposited materials
 B-2-2) Re-erosion of deposited impurities on plasma facing walls

(C) TRITIUM RETENTION IN ITER WALL MATERIALS

- C-1) Long-distance transport of carbon and beryllium in plasmas
- C-2) Local tritium retention in tungsten divertor targets

Dynamic plasma wall interaction code, EDDY

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 CH₄ 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 (*MD simulation*) *particle species-, impact energy- and material-dependent.*
- (9) Re-erosion of deposited and mixed materials (IMD simulation)

A-1) Local deposition of impurities on plasma facing materials

¹³CH₄ injection experiments at TEXTOR



roof-like test limiter exposed to SOL plasma of TEXTOR A.Kreter et al.; J.Nucl.Mater. 363-365(2007)179.

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

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

Radial decay of the plasma parameter: $I_{Te}{=}I_{Ti}{=}40$ mm, and $I_{ne}{=}22$ mm

 $^{13}\mathrm{CH}_4$ was injected into the plasma through a hole in the limiter surface.

¹²C concentration of the background plasma was taken to be 3%. (Assumption)

Most unexpected observation was the very low local deposition of 13 C on the limiter surface (~0.2%).

A-1) Local deposition of impurities on plasma facing materials

2D patterns of ¹³C deposition



Standard condition:S=0.5 and Y_{chem}=3%Calculated:~50% depsoition efficiency, and
a factor of 100 larger than in experimentS=0.5, but enhanced erosion of redeposited
carbon atoms, Y_{enh}=30%Calculated:33% ¹³C depsoition

Still too large ¹³C depsoition and patterns still too much peaked

S=0 (or small) &

Enhanced erosion

K.Ohya & A.Kirschner; Phys.Scr.T138(2009)014010.

A-1) Local deposition of impurities on plasma facing materials

Deposition efficiency strongly changes with injection time.



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

Sticking probability	S=0.5	S=0.1	S=0.05	S=0.01	S=0
¹³ C deposition efficiency (%)					
EDDY	33.0	5.1	2.2	0.5*	0.1*
ERO	32.0	5.0	2.0	0.5	~0.1

*averaged between 5.29 s and 5.88 s

K.Ohya & A.Kirschner; Phys.Scr.T138(2009)014010.

B-1) Particle-in-Cell simulation of plasma sheath



PIC code solves the equations of motion and Poisson's equation self-consistently.
 The plasma particles with Maxwellian velocity distribution are generated at the edge region.
 The sheath potential vary with the charging of the wall.

B-1) Particle-in-Cell simulation of plasma sheath



Potential Profiles with Oblique Magnetic Field

- The magnetic presheath is formed due to the polarization between ions and electrons.
- When the magnetic field is almost parallel to the surface, the width of MP increases.
- The heavier hydrogen isotopes have larger Larmor radius, the width of MP increases.



With an oblique magnetic field, some of SEs are reabsorbed at the wall within a gyrocircle, the net SE yield decreases. Mizoshita et al. (1995), Inai el al. (2009)

Potential drop of the sheath is independent of the magnetic angle, but SE emission from W causes a decrease 8 in the potential drop.

B-1) Particle-in-Cell simulation of plasma sheath

Energy and angular distributions of ions incident on walls



The impact energy does not depend on angle of magnetic field because potential drop is same.
 The energy distribution of heavier hydrogen isotopes is shifted to higher energy.

The most probably angle is smaller than the angle of the magnetic field except for the case of the nearly normal magnetic field to the surface.

The energy and angular distributions affect

the sputtering and the reflection from the wall

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B-1-1) Carbon deposition in the gaps of castellated tiles



Plasma density an potential are strongly asymmetric between poroidal and toroidal gaps.
 Plasma distribution around the gaps, in particular, toroidal gap, depends on the magnetic field angle.
 K.Ohya; JNM415(2011)S10.

B-1-1) Carbon deposition in the gaps of castellated tiles



H ion with gyro radius of 0.1mm cannot penetrate into a narrow gap of 0.2mm.

When the gap width is 0.5mm, H ion cannot deeply penetrate due to E x B drift. 11

B-1-1) Carbon deposition in the gaps of castellated tiles

Penetration depth of hydrocarbons in the toroidal gap



- When the gap width is 0.5 mm or more, the redeposition can be found at the bottom of the gap.
- Very narrow gap (<0.2 mm) causes the redeposition is localized at the gap edge.

B-1-1) Carbon deposition in the gaps of castellated tiles





Species dependence



Using sticking coefficient calculated by MD, low energy hydrocarbons are reflected repeatedly.

The neutral species are liberated from a magnetic constrain, they are redeposited deeply.

Since the ionized particles are confined by the magnetic field and have high sticking coefficient due to sheath acceleration, they are redeposited in the gap edge.

B-1-1) Carbon deposition in the gaps of castellated tiles



B-2) Molecular Dynamics simulation of plasma wall interaction

Integrating equation of motions of constituent atoms : Small cell containing $\Delta t^2 \mathbf{F}(t)$: $10^3 - 10^7$ atoms

Verlet algorithm: $\mathbf{r}_{j}(t + \Delta t) = \mathbf{r}_{j}(t) + \Delta t \dot{\mathbf{r}}_{j}(t) + \frac{\Delta t^{2} \mathbf{F}_{j}(t)}{2m}$ $\dot{\mathbf{r}}_{k}(t + \Delta t) = \dot{\mathbf{r}}_{k}(t) + \frac{\Delta t}{2m} \{\mathbf{F}_{k}(t + \Delta t) + \mathbf{F}_{k}(t)\}$

The force on each atom calculated from the analytical derivation of appropriate interaction potential form.

 $V = \sum_{i>j} f_{ij}^{c}(r_{ij}) \left[V_{ij}^{R}(r_{ij}) - \frac{b_{ij} + b_{ji}}{2} V_{ij}^{A}(r_{ij}) \right]$: **Empirical bond order potential** Repulsive term: $V^{R}(r) = \frac{D_{0}}{S-1} \exp\left(-\beta\sqrt{2S}(r-r_{0})\right)$ Attractive term: $V^{A}(r) = \frac{SD_{0}}{S-1} \exp\left(-\beta\sqrt{2/S}(r-r_{0})\right)$ Attractive term: $V^{A}(r) = \frac{SD_{0}}{S-1} \exp\left(-\beta\sqrt{2/S}(r-r_{0})\right)$ Cutoff-function: $f^{c}(r) = \begin{cases} 1, & r \le R-D, \\ \frac{1}{2} - \frac{1}{2} \sin\left(\frac{\pi}{2}(r-R)/D\right), & |R-r| \le D, \\ 0, & r \ge R+D \end{cases}$ Angular function: $g(\theta) = \gamma \left(1 + \frac{c^{2}}{d^{2}} - \frac{c^{2}}{d^{2} + (h + \cos \theta)^{2}}\right)$

Fusion-related parameter sets for

C-C, C-H : Brenner (1990, 1992), REBO (2002) and AIREBO (2000) W-W, W-C, W-H : Juslin et al. (2005) Be-Be, Be-C, Be-H, Be-W : Bjorkas et al. (2009, 2010)

B-2) Molecular Dynamics simulation of plasma wall interaction

Coupling to an external bath (Langevin equation)

HJC.Brendsen et al.: JCP81(1984)3684.

: Excess heat dissipation in collisions with energetic atom.

$$\lambda = \sqrt{1 + \frac{\Delta t}{\tau_T} \left(\frac{T_0}{T} - 1\right)}$$

- Δt : time step, τ_T : time constant
- T: temperature of the system, T_0 : fixed reference temperature

It represents a proportional scaling of the velocities per time step.

Periodic boundary condition

: Topmost atoms are free, but bottommost atoms are fixed.

The simulation cell is replicated throughout the space to form an infinite lattice.

If an atom leaves the simulation cell, one of its images will enter through the opposite face.

Simulation cell:should | be large

More realistic, but time-consuming.



B-2) Molecular Dynamics simulation of plasma wall interaction



B-2) Molecular Dynamics Simulation of plasma wall interaction



@ Changes in C and W sputtering yields are in good agreement with those between MD and dynamic MC code, EDDY.

@ For C reflection coefficients, it is different from each other at low energy.

B-2-1) Reflection/sticking coefficient of deposited materials

Preparation of Realistic PFW Surfaces



- The W surface is bombarded with C atoms at the temperature of 10eV and 100eV.
- At low plasma temperature, the W is covered by deposited C and at higher temperature W-C mixed layer is formed.
- The **a-C:H layer** with different H/C is formed when a-C is bombarded with H atom.

B-2-1) Reflection/sticking coefficient of deposited materials



Most of incident methane reflect at thermal energy and break up at higher energy (>10eV).
 Increase of hydrogen in amorphous carbon increases the reflection coefficients. 20
 The W surface increases the reflection coefficients and there reflected much more C atoms.

B-2-1) Reflection/sticking coefficient of deposited materials

Incident species dependence of reflection coefficient



B-2-2) Re-erosion of deposited impurities on plasma facing walls

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 $\sim 0.1\%$ in the plasma.



Mitigation of chemical carbon erosion by Be deposition

Plasma divertor simulator PISCES-B

B-2-2) Re-erosion of deposited impurities on plasma facing walls Deposition of Beryllium 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 %.

B-2-2) Re-erosion of deposited impurities on plasma facing walls



Interaction depth in C and Be deposition

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 $0^{\circ} - 180^{\circ}$.

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.

B-2-2) Re-erosion of deposited impurities on plasma facing walls



Hydrogenated carbon

At <u>300 K</u>, 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_v emission is strongly enhanced.

At <u>800 K</u>, 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.

At <u>1200 K</u>, the numbers of emitted C and CD_y increase monotonously with increasing D energy.



B-2-2) Re-erosion of deposited impurities on plasma facing walls

Hydrogenated C with beryllium deposition



Decrease in the emission yield is much faster than an increase in Be coverage on the surface.

This result shows <u>a good correlation with the mitigation</u> 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].

[8] R.P.Doerner et al., Phys.Scr. T128(2007)115.

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

[9] D.Nishijima et al., J.Nucl.Mater. 363-365(2007)1261.

The reduction rate changes in the different manner from the experiments with increasing surface temperature. <u>The calculation indicates a maximum reduction rate at</u> <u>~800 K where the CD_v emission yield peaks.</u>

C-1) Long-distance transport of carbon and beryllium in plasmas



C-1) Long-distance transport of carbon and beryllium in plasmas

Model geometry of edge plasma and walls



Plasma parameters in an ITER edge plasma with D and impurities (C and He) are taken from a B2/Eirene calculation [1].

[1] G.Federici et al., J.Nucl.Mater.290-293(2001)260. Aside from sputtering by plasma ions, sputtering by charge exchange (CX) neutrals is taken into account at the first wall.

Physical sputtering yield of C target in the divertor and Be first wall is calculated by using EDDY [2].

[2] K.Ohya, Phys.Scr. T124 (2006)70. Due to high threshold energy for physical sputtering by D ions, sputtering of W baffle and dome is not taken into account.

Chemical sputtering of C target is calculated using Roth formulae [3]. Only CD_4 molecules are released from the target.

[3] J.Roth et al., J.Nucl.Mater. 266-269(1999)1/337-339(2005)970.

C-1) Long-distance transport of carbon and beryllium in plasmas



Poloidal distributions of the flux of CX neutrals and of their mean energy along the grid edge are taken from ref. [5].

[5] R.Behrisch et al., J.Nucl.Mater. 313-316(2003)338.

<u>Angular distribution of ions is influenced by gyro-</u> <u>motion of the ions;</u> most probable angles of the distribution are 12°~18°, which are much larger than the magnetic angles intersecting the wall.

Average angle of magnetic field lines intersecting the first wall equipped with blanket modules is chosen to $\frac{50}{2}$, which results in an incident angle of ~21° to the first wall.

<u>Ion flux at the first wall is assumed to decay</u>
 <u>exponentially from the grid edge to the wall.</u>
 The decay length is taken to be 1 cm, 3 cm and 10 cm.

C-1) Long-distance transport of carbon and beryllium in plasmas



Dominant erosion mechanism at the outer divertor target is physical sputtering. Asymmetric erosion between the inner and outer targets is observed, depending on the incident ion energy.

Erosion of the inner target is dominated by chemical sputtering, a maximum yield of which occurs at the strike point.

Erosion of the first wall is at least by factors of 10 – 100 smaller than that of the divertor targets. Localized gas puffing and recycling at the top of the first wall causes sputtering flux to be strongly decreased.

If decay length of ion flux between the grid edge and the first wall is taken to be 10 cm, the sputtering flux by ions is high enough to be comparable to the flux by CX neutrals. With decreasing length, the ion flux is strongly reduced, showing complicated profile closely related to the

local distance between the grid edge and the first wall.

C-1) Long-distance transport of carbon and beryllium in plasmas



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.

 CD_v is rather limited within the private flux region (PFR) of the divertor.

Be atoms are ionized and subsequently transported along the magnetic field lines for a long distance, therefore, they distribute over the whole area of the machine.

C-1) Long-distance transport of carbon and beryllium in plasmas

Net erosion and deposition profile on walls



<u>Physical and chemical sputtering yields of original</u> materials are used for the re-erosion yields for C (CD_y) and Be deposits.

Net erosion and deposition profiles of C, CD_y and Be, calculated as the flux difference between redeposition and re-erosion.

C deposits in the inner divertor are strongly reeroded except for the dome where sputtering is negligibly small.

Position near the strike point, as well as the dome, is a deposition zone whereas the position far from it is an erosion zone.

<u>Be deposits on the inner and outer targets are</u> <u>strongly re-eroded</u> due to low threshold energy for physical sputtering.

The top of the first wall and the inner dome are deposition zones.

C-1) Long-distance transport of carbon and beryllium in plasmas

Tritium codeposition profile on walls



Empirical formulae recently proposed by Doerner et al. [6] are used for atomic ratios of D to C and of D to Be. [6] R.P.Doerner et al., Nucl.Fusion 49(2009)035002. (The estimation of T retention, corresponding D data, are performed in this work.)

Using surface temperature and D energy on the inner and outer targets and the first wall, D/C and D/Be values are calculated as a function of the position.

Net redeposition flux profiles are multiplied with D/C and D/Be profiles to obtain T codeposition profile.

Finally, <u>assuming toroidal symmetry</u>, total retention rate can be estimated from the calculated T codeposition profile.

C-1) Long-distance transport of carbon and beryllium in plasmas

Tritium retention rate in C and Be deposits

Decay length ^{*1}	Divertor ^{*2}			First wall	Total
(cm)	Inner target	dome	Outer target		
(a) Carbon depos	ition				
	1.26 [mgT/s]	0.01 [mgT/s]	2.51 [mgT/s]	0.12 [mgT/s]	3.89 [mgT/s]
(b) Beryllium dep	osition				
1	0.06	0.03	0	0.48	0.58
3	0.06	0.04	0	0.60	0.70
10	0.03	0.14	0	1.48	1.65

Dominant T retention in C occurs at the inner and outer divertor target, whereas it occurs at the first wall. Retention rate in Be is strongly influenced by decay length of plasma parameters from the grid edge to the first wall.

Using a discharge duration of 400 s, the number of discharge after which an in-vessel T safety limit of <u>700 g is reached</u> are estimated from the sum of the T retention rate in C and Be deposits, if the retention rate in W is negligibly low.

It is predicted to be 295 - 395 discharges, depending on the decay length.

Local plasma wall interaction related to Tritium Retention



Local collision and thermal processes:

Implantation, diffusion, trapping/detrapping and surface recombination





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Parameter Fitting with a TDS experiment



Time evolution of the areal density of trapped D in W is shown along with that of the density retained as mobile atoms. In the experiment [1], a wrought W surface was irradiated by D_3^+ ions with an energy of 100 eV/D and ϵ flux of 2.5 × 10¹⁵ cm⁻²s⁻¹. [1] C.Garcia-Rosales et al., J.Nucl.Mater.233-237(1996)803.

(a) Dif	(a) Diffusion (b		o) Surface recombination		
$D_0 (cm^2 s^{-1})$	$E_{D}(eV)$	$E_r (eV)$	$K_r (cm^4 K^{1/2} s^{-1})$		
0.39	2.5×10^{-7}	-0.59	1.2×10^{-25}		
(c) Trapping					
$E_{T1} (eV)$	D _{trap1} /W	E _{T2} (eV)	D _{tarp2} /W		
0.85	0.001	1.5	0.001		

Density of mobile and trapped D atoms increases successively during implantation.

After implantation, a part of mobile D atoms are released due to surface recombination. Trapped D atoms are kept to be retained in the bulk.

At the early stage of the TDS phase, D atoms in the Trap 1 are released via mobile D atoms. At the delayed stage , D atoms in the deeper trap (Trap 2) are released. 37

Plasma Parameters used for calculation

Incident energy (T), angle (β) and flux (Γ) and target temperature (T_{tar}) as a function of the position on the inner and outer target.

The plasma parameters in front of the targets are taken from a B2-EIRENE calculation [2], as a function of the distance from the strike point. [2] G.Federici et al., J.Nucl.Mater.290-293(2001)260.

The surface temperature depending on the position on the target is taken from [3], where the temperature were calculated assuming CFC, not W, with the thickness of 10 mm. [3] G.Federici et al., Plasma Phys. Control.Fus.45(2003)1523.

Typical duration of a discharge in ITER is 400 s. The surface temperature at each position is kept constant after discharge as well as during it.

The trap concentration strongly depends on the material and additional traps may be produced in the near-surface region due to high D fluxes to the target, resulting in a depth-dependent concentration.

<u>At the position where the temperature is high</u>, the number of retained D atoms increases without any saturation. Most of D atoms are retained as mobile atoms. <u>At the low temperature position</u>, it tends to saturate where most of trap sites near the surface are occupied by implanted D atoms.

<u>After discharge (>400 s)</u>, most of D atoms are kept to be retained in the bulk, where they can diffuse deeper.

Time evolution of Tritium Retention in Targets

In case of the inner target, dominant retention mechanism is the trapping in the deep trap (Trap 2) during discharge and most of the T atoms are kept in the trap even after discharge.

Mobile T atoms dominate the T retention in the outer target due to its high temperature leading to detrapping from the trap and subsequent diffusion inside the bulk.

The T atoms are retained ten times more in the outer target than in the inner target during discharge, whereas sufficiently after discharge the T retention is reduced due to surface recombination of mobile atoms.

From the distribution of retained D atoms during and after discharge, the T retention in the inner and outer targets are estimated by taking the <u>atomic mass</u> <u>difference between D and T</u> into account, and <u>assuming toroidal symmetry</u>.

Tritium Retention in Divertor Targets

Trap concentration	Dive	Total			
T _{trap} /W	Inner target	Outer target			
(a) Just after discharge (400 s)					
0.01	10.8	47.3	58.0		
0.001	2.6	31.1	33.7		
0.0001	1.0	28.5	29.6		
(b) Subsequently after discharge (1000 s)					
0.01	8.5	23.4	31.90		
0.001	2.0	12.8	14.90		
0.0001	0.6	11.1	11.70		

Tritium retention (mgT) after a discharge (400 s) in tunsgten.

Finally, the number of discharges, after which an in-vessel T safety limit of 700 g is reached, is estimated from the sum of T retention of the inner and outer targets; T retention in other walls is not taken into account.

The number of discharges is of the range between 12000 and 24000, depending on the trap concentration from 0.01 to 0.0001. It is increased to the values between 22000 and 60000, if the T retention sufficiently after discharge (1000 s) is used.