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

(I) Modelling basics of erosion and redeposition

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Outline of lecture

(A) INTRODUCTION

A-1) Related issues to plasma wall interaction in fusion devices
A-2) Erosion and redeposition on plasma facing walls

(B) BASIC PROCESSES

B-1) Projectile reflection and physical sputtering
B-2) Chemical sputtering and hydrocarbon emission
B-3) Impurity deposition and material mixing
B-4) Thermal diffusion of impurities in materials
B-5) Transport and redeposition of eroded impurities
(1) Erosion of wall elements

**Reduced life time of wall elements**

(2) Eroded impurities can penetrate into the plasma

**Dilution and radiation cooling of core plasma**

(3) Redeposition of eroded particles

**Tritium retention in redeposited layers**

Erosion, transport and redeposition of impurities is a crucial issue in fusion devices!
Global and Local PWIs related to Tritium

Global transport of impurities
Codeposition with C and Be

Local collision and thermal processes:
Implantation, diffusion, trapping/detrapping and surface recombination

Global and Local PWIs related to Tritium
A-2) Erosion and redeposition on plasma facing walls

**Carbon based materials for PFW**

Key issues:
Physical/Chemical sputtering & Tritium incorporation

Impurity transport codes require to treat self-consistently:

I) Physical and chemical erosion of surface

II) Transport of released impurities above surface

III) Redeposition of returning impurities and re-erosion of redeposited impurities on surface

IV) Resultant material mixing below surface
A-2) Erosion and redeposition on plasma facing walls


Models and assumptions

Erosion
- Physical sputtering
  - Yield
  - Energy
  - Angle
  - TRIM database
  - Thompson Cosine

Chemical erosion
- Yield
- Energy
- Angle
- Roth formula or Input
- Thermal
- Isotropic or cosine

Transport
- Ionization (atoms)
- ADAS database
- Ionization/dissociation (molecules)
  - Janev/Reiter data set for methane, ethane and propane families

Redeposition
- Reflection/Sticking (atoms)
  - TRIM database
- Reflection/Sticking (molecules)
  - Input

Material mixing

Coupling codes

- Static/dynamic BCA codes
- Magnetic, sheath, friction, thermal, cross-field diffusion, elastic collisions, Radial electric field
- Molecular Dynamics codes or Database by MD
- Dynamic BCA codes
B-1) Projectile reflection and physical sputtering

**Binary Collision Approximation (BCA)**

**Vacuum**

**Sputtered atom**

\[ \Delta E_{el}(\theta_1) - E_{sb} \]

**Solid**

**Recoiled atom**

\[ \Delta E_{el}(\theta_2) \]

**Projectile ion**

\[ E_0 \]

\[ L_1 = -\ln \lambda(E_0) \]

\[ E_1 = E_0 - \Delta E_{inel}(L_1) - \Delta E_{el}(\theta_1) \]

\[ L_2 = -\ln \lambda(E_1) \]

\[ E_2 = E_1 - \Delta E_{inel}(L_2) - \Delta E_{el}(\theta_2) \]

**Analytic formula for scattering angle:**

\[ \cos \frac{\theta}{2} = \frac{b + \rho + \Delta}{\xi_c + \rho} \]

**Stopping power:**

\[ (dE / dx)_{nonlocal} = 1.212 \frac{Z_a^{7/6} Z_b}{\left(Z_a^{2/3} + Z_b^{2/3}\right)^{3/2}} \sqrt{E} \quad [eV \cdot A^2] \]

**Energy of sputtered atoms:**

\[ E = E' - E_{sb} \]

**Emission angle of Sputtered atoms:**

\[ \cos \beta = \sqrt{\frac{E' \cos^2 \beta' - E_s}{E' - E_s}} \]

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Joint ICTP-IAEA Workshop on Fusion Plasma Modelling Using Atomic and Molecular Data, Trieste, Italy, 23-27 January 2012
B-2) Chemical sputtering and hydrocarbon emission

Hydrogen ion penetrates into carbon and forms hydrocarbon after thermalization, which diffuses to surface and desorbs.

Formalization by J. Roth [JNM266-269(1999)51]:

\[
Y_{\text{chem}}(E,T,\phi) = \frac{Y_{\text{low}}(E,T)}{1 + \left(\frac{\phi}{6 \times 10^{21}}\right)^{0.54}}
\]

\[
Y_{\text{low}} = Y_{\text{therm}}(1 + D Y_{\text{dam}}) + Y_{\text{surf}}
\]

- \(Y_{\text{therm}}\): chemical erosion by thermalized ions
- \(Y_{\text{dam}}\): enhancement of thermal erosion by radiation damage
- \(Y_{\text{surf}}\): ion induced desorption of hydrocarbon radicals

Sputtering yield strongly depends on surface temperature (\(T\)) and energy (\(E\)) and ion flux (\(\phi\)) of bombarding ions.
Differential Fluence: \( \Delta \Phi = \Phi / N_H \) (\( \Phi \): Total fluence, \( N_H \): Number of pseudo ions)

Surface Thickness: \( d = \sum_{i=1}^{N} \Delta x_i \) (\( N \): Number of layers, \( \Delta x_i \): \( i \)-th Layer thickness)

**Collision process of a pseudo Ion:**

Reflection, Implantation, Physical Sputtering

**After simulation of collision process:**

- Areal density of \( j \)-th atom in \( i \)-th layer:
  \[
  A_{ij} = q_j n_i \Delta x_i + \Delta N_{ij} \Delta \Phi
  \]
  (\( \Delta N_{ij} \): Change in number of \( j \)-th atom in \( i \)-th layer)

- \( i \)-th layer thickness:
  \[
  \Delta x_i = \sum_{j=1}^{N_c} A_{ij} n_{0,j}^{-1}
  \]
  (\( n_{0,j} \): \( j \)-th atom density)

- \( j \)-th atom constituent in \( i \)-th layer:
  \[
  q_{ij} = A_{ij} / \sum_{k=1}^{N_c} A_{ik}
  \]

- Maximum areal density of 1st atom in \( i \)-th layer:
  \[
  A_{i1}^{\text{max}} = \left[ q_{11}^{\text{max}} / \left( 1 - q_{11}^{\text{max}} \right) \right] \sum_{j=2}^{N_c} A_{ij}
  \]

- Reemission:
  \[
  \Delta A_{i1}^{\text{reem}} = A_{i1} - A_{i1}^{\text{max}}
  \]

- Saturation:
  \[
  A_{i1} = A_{i1}^{\text{max}}
  \]

\[ A_{i1} > A_{i1}^{\text{max}} \]
Dynamic erosion/deposition due to W-C mixing


Depending on C concentration and temperature of plasmas, transition between erosion and deposition occurs at W surface during plasma exposure.

Dynamic BCA codes reproduce a sharp boundary between erosion and C deposition area observed on high-Z material surfaces.

B-4) Thermal diffusion of impurities in materials

★ Impurity Deposition and Collisional Mixing

★ Thermal Diffusion of Deposited Impurities

\[ \frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial^2 x} \]

Diffusion Coefficient

\[ D = D_0 \exp\left(\frac{-Q_D}{kT}\right) \]

- \( D_0 \): Material Constant (cm²s⁻¹)
- \( Q_D \): Activation Energy (eV)
- \( T \): Material Temperature (K)

\[ \Gamma \]: Incident Ion Flux (cm²s⁻¹)
\[ \phi \]: Total Ion Fluence (cm²)
\[ t \]: \( (\phi / \Gamma) \) Irradiation Time (s)

\[ N \]: Number of Pseudo Ions
\[ \Delta \phi \]: \( (\phi / N) \) Differential Ion Flux (cm²)
\[ \Delta t \]: \( (t / N) \) Differential Irradiation time (s)

B-4) Thermal diffusion of impurities in materials

**Coupling of BCA code with diffusion codes**

**Fick’s law with source and trapping terms**

\[ \frac{\partial c_j(x,t)}{\partial t} = \nabla [D_j \nabla c_j(x,t)] + G_j(x,t_0) - \sum_{i=1}^{n} \frac{\partial c_{Tj}^i(x,t)}{\partial t} \]

- \( c_j(x,t) \) : jth solute concentration,
- \( D_j \) : Diffusion coefficient for jth solute
- \( G_j(x,t_0) \) : source term (range profile)
- \( c_{Tj}^i(x,t) \) : concentration of jth solute trapped Ith trapping site

**Rate equation for trapping and detrapping**

\[ \frac{\partial c_{Tj}^i(x,t)}{\partial t} = \frac{D_j c_j(x,t) C_{Te}^i(x,t)}{\lambda^2} - c_{Tj}^i(x,t) \nu_0 \exp(-E_T^i / kT) \]

- \( \lambda \) : jump distance,
- \( \nu_0 \) : detrapping attempt frequency
- \( f_j^i \) : the inverse trap saturability of jth solute for the Ith trapping site
- \( E_T^i \) : detrapping energy of Ith trap

**Boundary condition**

e.g., recombination limited

\[ \frac{\partial c_j}{\partial x} = \frac{K_r}{D_j} c_j^2(x = 0) \]

- \( K_r \) : recombination coefficient

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**Parameters**

<table>
<thead>
<tr>
<th>Diffusion</th>
<th>Values</th>
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<tr>
<td>( D_0 ) (cm(^2)/s)</td>
<td>( 3.5 \times 10^{-7} )</td>
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<tr>
<td>( E_D ) (eV)</td>
<td>0.39</td>
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<th>Recombination</th>
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<tr>
<td>( K_0 ) (cm(^4)K(^{-1/2})/s)</td>
<td>( 1.2 \times 10^{25} )</td>
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<tr>
<td>( E_R ) (eV)</td>
<td>-0.59</td>
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<th>Trap #1</th>
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<td>( E_{T,1} ) (eV)</td>
<td>0.85</td>
</tr>
<tr>
<td>( C_{T,1} ) (Traps/W)</td>
<td>0.01</td>
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<tr>
<th>Trap #2</th>
<th></th>
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<tbody>
<tr>
<td>( E_{T,2} ) (eV)</td>
<td>1.4</td>
</tr>
<tr>
<td>( C_{T,2} ) (Traps/W)</td>
<td>0.01</td>
</tr>
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</table>
Monte Carlo Modeling of Impurity Transport

The released $C_xH_y$ molecule successively collides with plasma electrons and ions.

More than 700 reactions are included.


The elastic collisions with the residual neutral hydrogen atoms.
The model includes

- **Lorenz force**  \( F_z = q(v \times B) \)
- **friction force** and **temperature gradient thermal force**

\[
F_z = m_z \left( \frac{v_i - v_z}{\tau_s} + \alpha_e \frac{d(kT_e)}{ds} + \beta_i \frac{d(kT_i)}{ds} \right)
\]


- **Debye sheath and magnetic pre-sheath potential**

\[
\phi(z) = \phi_1 \exp\left(-\frac{z}{2\lambda_{Debye}}\right) + (\phi_0 - \phi_1)\exp\left(-\frac{z}{R_{gyro}}\right)
\]

\[
f_D = 1 - \phi(6\lambda_{Debye}) / \phi_0 \approx 0.25
\]


- **Cross-field diffusion**

\[
(\Delta x, \Delta y) = \sqrt{2D_\perp \Delta t} \bullet (r_{Gx}, r_{Gy}) \quad D_\perp = 1 \text{ [m}^2/\text{s]}
\]

: K. Shimizu, T. Takizuka  
*purakakugakkaishi* 71 (1995) 1135.
B-5) Transport and redeposition of eroded impurities

**Hydrocarbon Redeposition on PFW Surfaces**

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

⇒Strong influence of atomic and molecular processes

Inverse photon efficiency, \( D/XB \), defined as
\[
\frac{\text{the number of the launching hydrocarbons}}{\text{the number of photon emission events}}
\]

Correlation of \( \text{CH} \left( \text{C}_2 \right) \) radiations with chemically sputtered \( \text{CH}_4 \)
\( (\text{C}_2\text{H}_4, \text{C}_2\text{H}_6) \) are important, depending on plasma parameters and hydrocarbon species.

D/XB of \( \text{CH} \) and \( \text{C}_2 \) decreases with decreasing temperature up to 5 eV, and then increases with a further decrease of temperature.
B-5) Transport and redeposition of eroded impurities

TEXTOR tokamak

W-C twin test limiter in TEXTOR

Top surface = sphere (r=7cm)

WI light emission appears on C-side!


CII light distribution in near-surface plasma

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

"Suppression" of chemical sputtering due to W deposition
Many assumptions:
- 0.1% Be to outer, 1% Be to inner divertor
- plasma parameter from a plasma code, B2-Eirene
- zero sticking of CₓHᵧ (S = 0), Trim/MolDyn for atoms
- enhanced erosion of redeposited carbon
- Variable (T+D)/C and (T+D)/Be ratios for deposits,
  \[ D/C = 0.0204 \cdot 10^{-0.43} \cdot \exp(2268/T) \]
  \[ D/Be = 5.82 \cdot 10^{-5} \cdot E^{1.17} \cdot (D/Be)_{flux}^{-0.21} \exp(2273/T) \]
  and (T+D)/C = (T+D)/Be = 1 for remote deposits.
- Temperature distribution on target calculated,
summarizes of lecture

(I) “Erosion/deposition” on plasma facing walls in fusion devices is a critical issue related to
   (a) transport of impurities in plasma boundary,
   (b) lifetime of plasma-facing components and
   (c) tritium retention in plasma-facing components.

(II) Modelling codes of “erosion/deposition” require to treat self-consistently:
   (a) Physical and chemical erosion of surface,
   (b) Transport of released impurities above surface,
   (c) Redeposition of returning impurities and re-erosion of redeposited impurities on surface, and
   (d) Resultant material mixing below surface

(III) Models and assumptions in the codes have to be evaluated in cross-code and code-experiment benchmarking,
      whereas reliable database of physical parameters used in codes have to be prepared.
(VI) Integration of “erosion/deposition” codes with plasma and material codes is an urgent issue for understanding of plasma wall interactions in fusion devices in more realistic in-vessel geometry.
Integrated simulation for in-vessel retention of tritium

Research project:
Theory and code development for evaluation of tritium retention and exhaust in fusion reactor

TOPICS, TASK

Transport
Erosion
Re-erosion
Reflection
Re-deposition

Coupling with core plasma

Coupling with edge plasma

Coupling with impurity transport

Coupling with wall

MD simulation

SOLPS
IMPGYRO
IMPMC
EDDY
SOLDOR

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Integrated simulation for in-vessel retention of tritium