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Recent Progress and Integrated Modelling

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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

A-1) Related issues to plasma wall interaction in fusion devices

(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

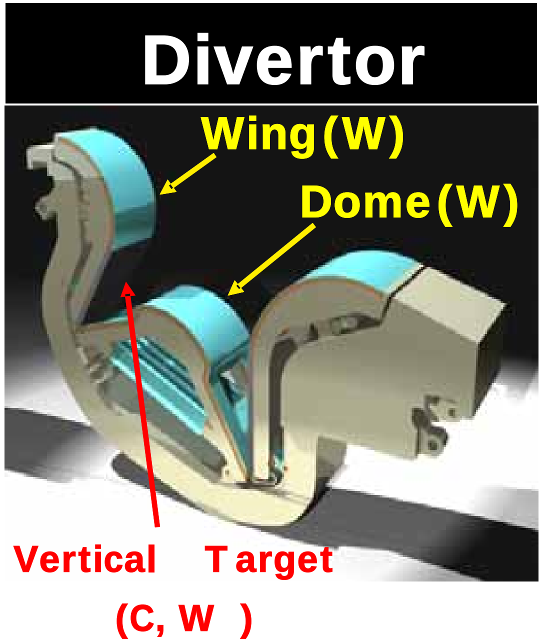
(3) Redeposition of eroded particles

Tritium retention in redeposited layers

Erosion, transport and redeposition of impurities is a crucial issue in fusion devices !

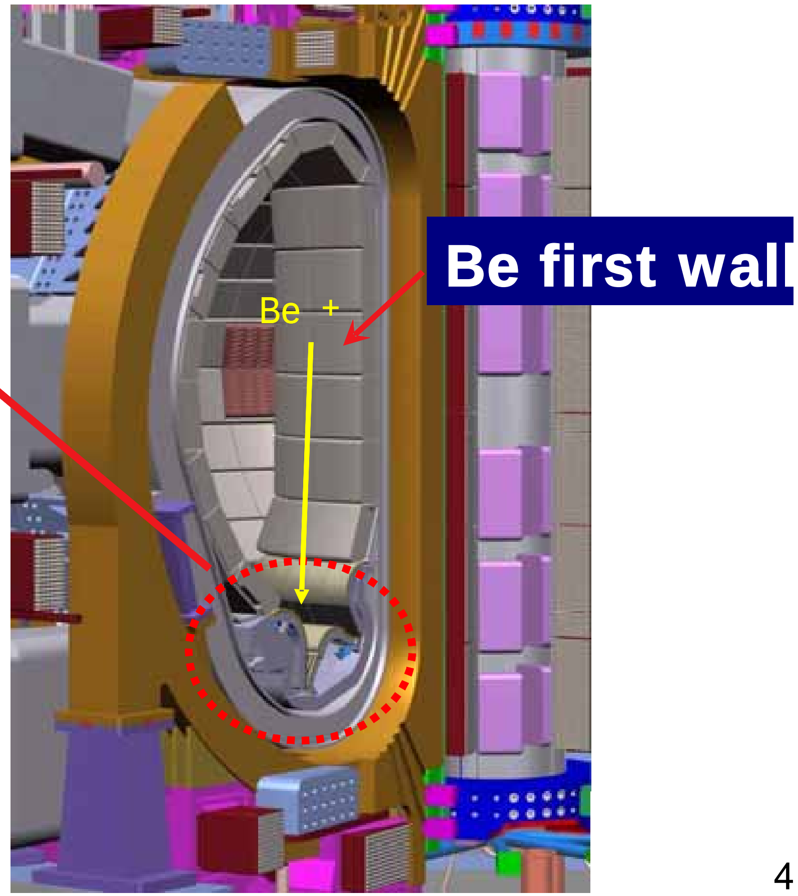
A-1) Related issues to plasma wall interaction in fusion devices

Global and Local PWIs related to Tritium Retention



Mutual contamination between C and W

Be deposition on C and W



Global transport of impurities

Codeposition with C and Be

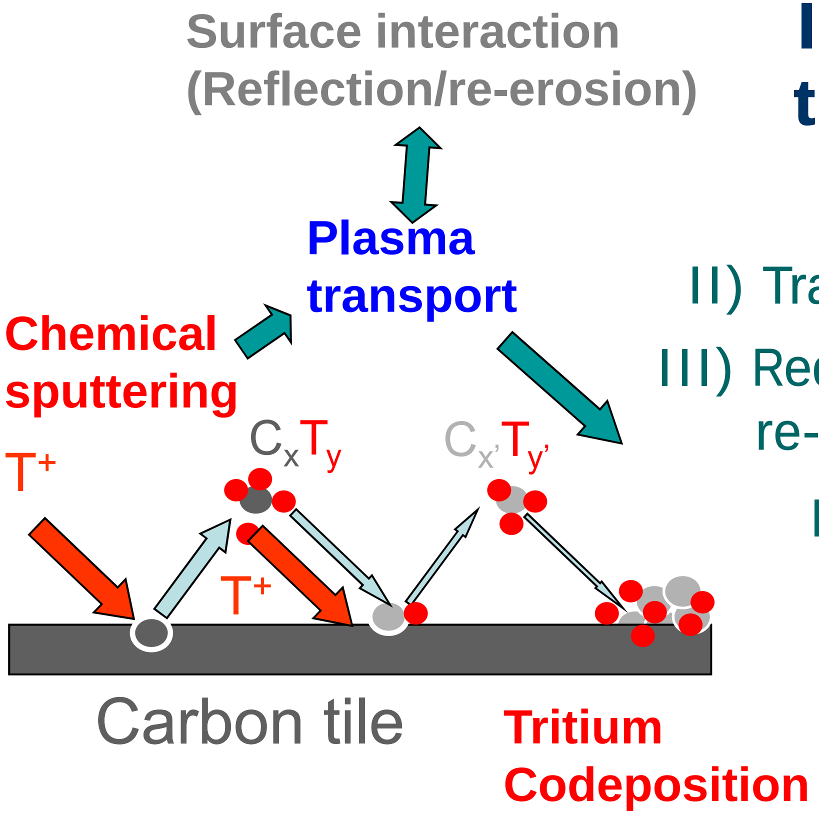
Local collision and thermal processes:

Implantation, diffusion, trapping/detrapping and surface recombination

A-2) Erosion and redeposition on plasma facing walls

Carbon based materials for PFW

Key issues:
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

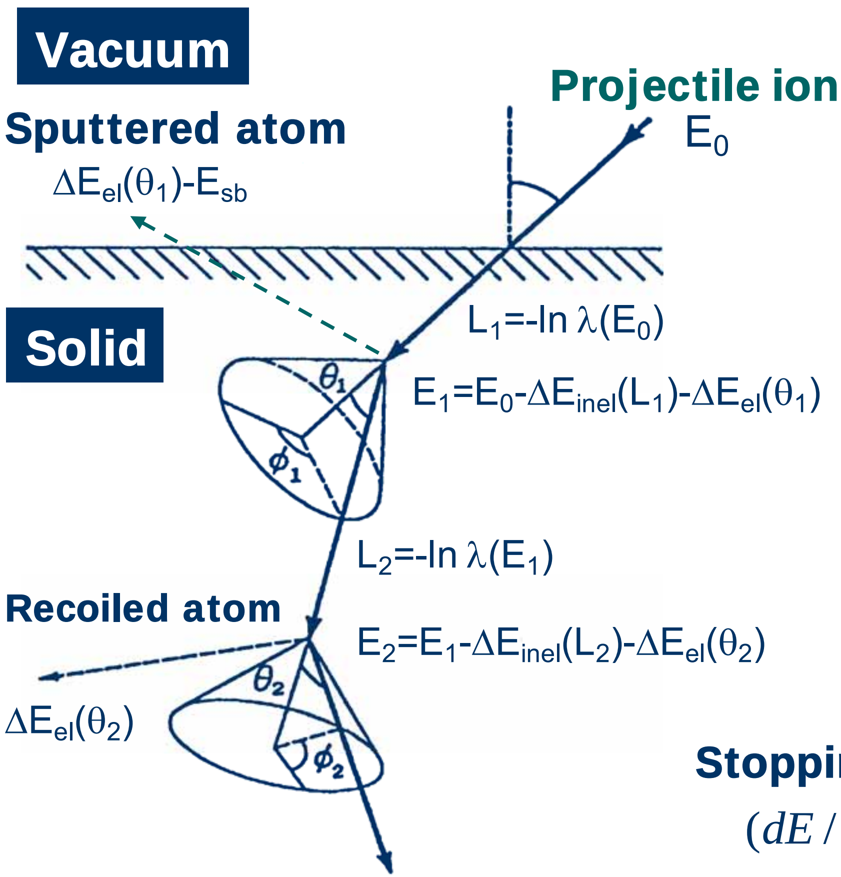
K.Ohya, A.Kirschner,
Phys.Scripta T138(2009)014010

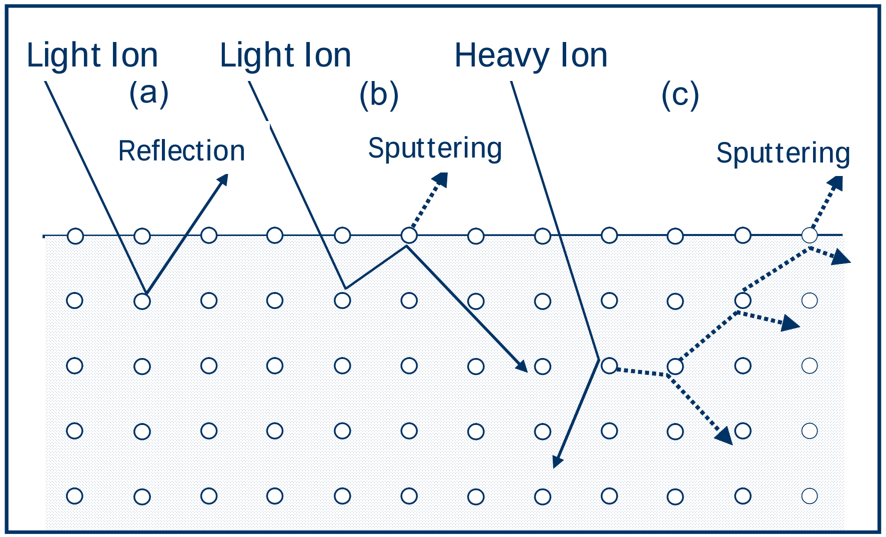
		Models and assumptions	***Coupling codes***
Erosion	**Physical sputtering**	Yield: **TRIM database** Energy: Thompson Angle: Cosine	**Static/dynamic BCA codes**
	Chemical erosion	Yield: Roth formula or Input Energy: Thermal Angle: Isotropic or cosine	
Transport	**Ionization (atoms)**	**ADAS database**	
	Ionization/dissociation (molecules)	**Janev/Reiter data set for methane, ethane and propane families**	
	Forces driven ionized particle	Magnetic, sheath, friction, thermal, cross-field diffusion, elastic collisions, Radial electric field	
Redeposition	**Reflection/Sticking (atoms)**	**TRIM database**	**Static/dynamic BCA codes**
	Reflection/Sticking(molecules)	Input	**Molecular Dynamics codes or Database by MD**
Material mixing			**Dynamic BCA codes**

B-1) Projectile reflection and physical sputtering

Binary Collision Approximation (BCA)

J.Biersack, H.G.Haggmark, Nucl.Instr.Methods 174(1980)257.





Analytic formula for scattering angle：

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

Stopping power:

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

Energy of sputtered atoms:

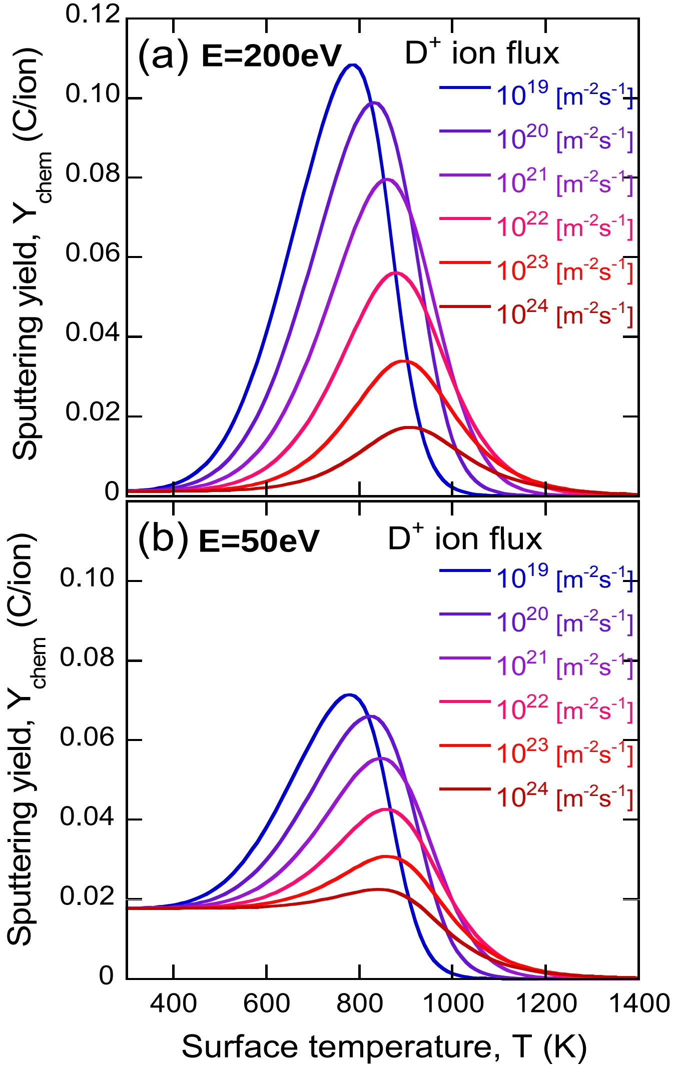
$$E = E' - E_{sb}$$

Emission angle of Sputtered atoms：

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

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] :

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

$$Y_{low} = Y_{therm}(1+DY_{dam}) + Y_{surf}$$

Y_{therm}: chemical erosion by thermalized ions

Y_{dam}: enhancement of thermal erosion by radiation damage

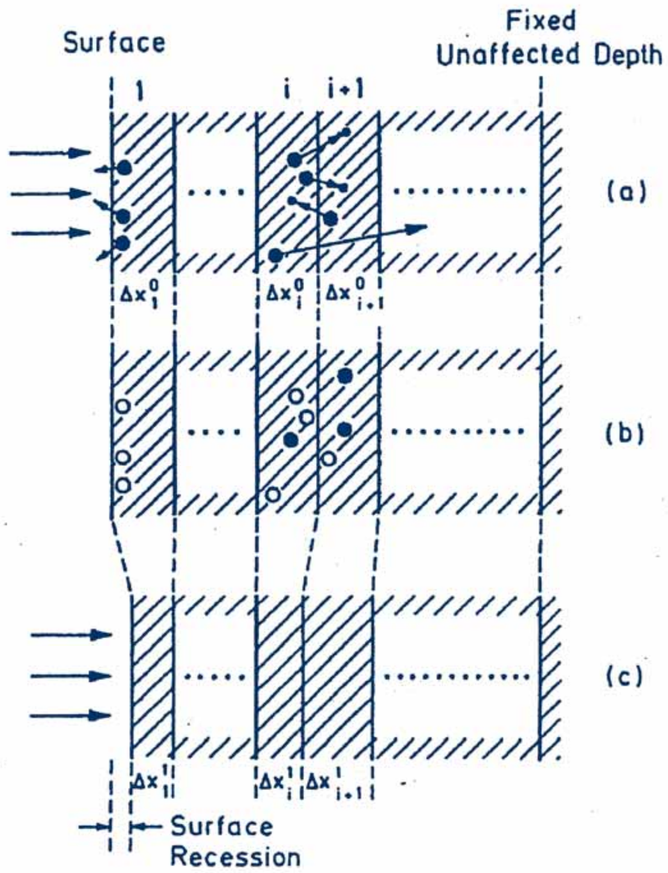
Y_{surf}: ion induced desorption of hydrocarbon radicals

Sputtering yield strongly depends on surface temperature (**T**) and energy (**E**) and ion flux (ϕ) of bombarding ions

B-3) Impurity deposition and material mixing

Differential Fluence: $\Delta\Phi = \Phi / N_H$ (Φ: Total fluence, N_H : Number of pseudo ions)

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



W.Moller et al.;
Comput.Phys. Commun. 51(1988)355.

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 :

$$A_{ij} = q_j n_i \Delta x_i + \Delta N_{ij} \Delta\Phi$$

(ΔN_{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 1th atom in i-th layer : $A_{i1}^{\max} = [q_1^{\max} / (1 - q_1^{\max})] \sum_{j=2}^{N_c} A_{ij}$

Reemission $\Delta A_{i1}^{reem} = A_{i1} - A_{i1}^{\max}$

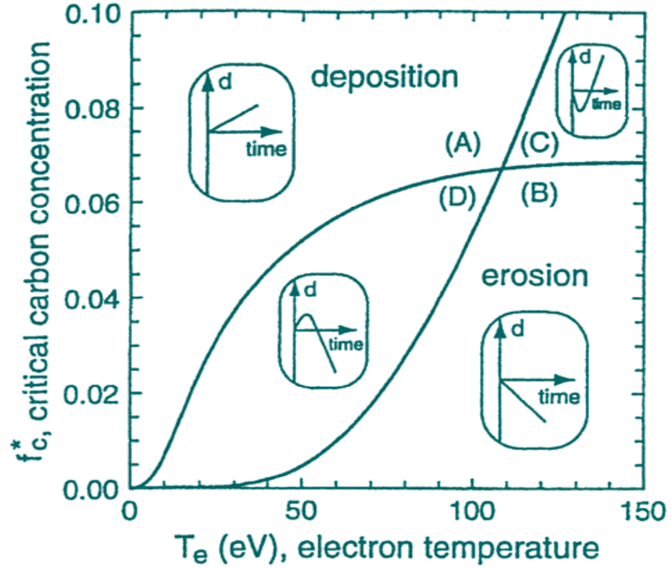
Saturation $A_{i1} = A_{i1}^{\max}$

} $A_{i1} > A_{i1}^{\max}$

B-3) Impurity deposition and material mixing

Dynamic erosion/deposition due to W-C mixing

$D^{+}+C^{3+}\rightarrow W$



D.Naujoks, W.Eckstein,
J.Nucl.Mater. 230 (1996) 93.

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

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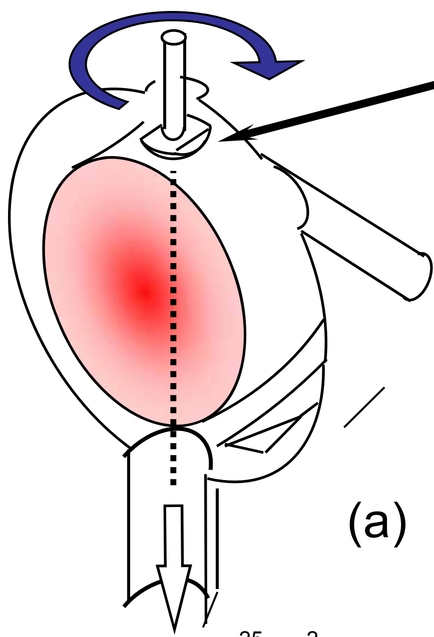
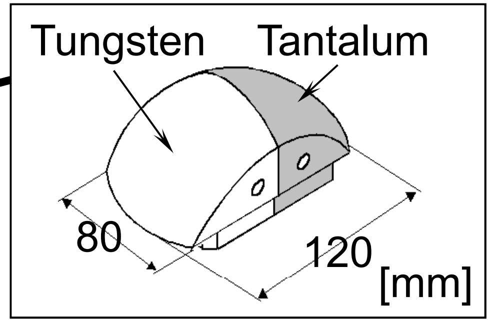
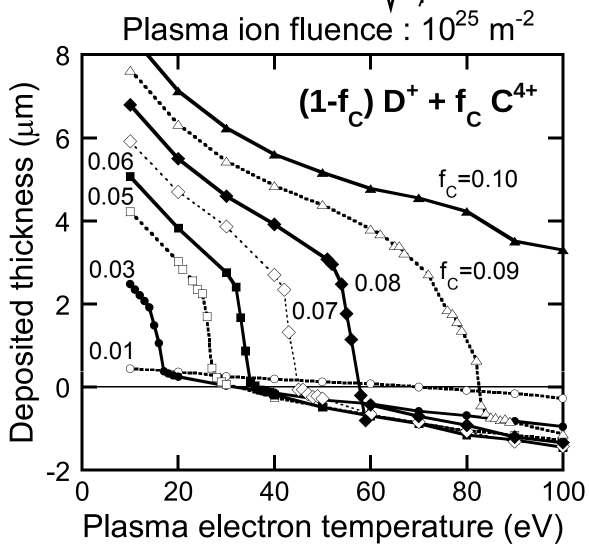
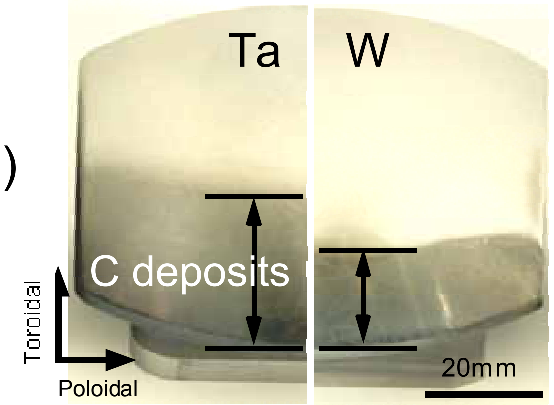






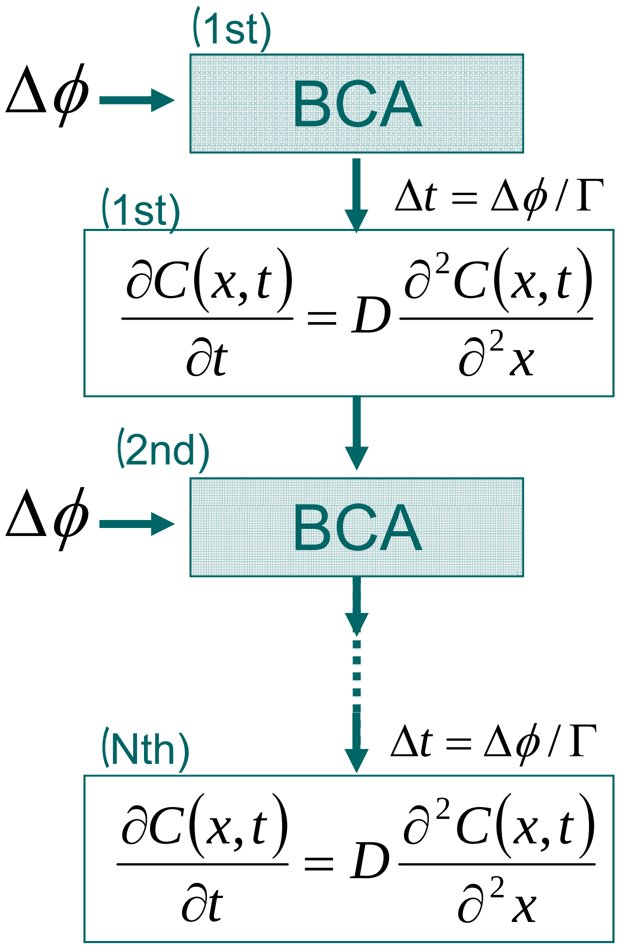
(a)



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

K.Ohya, T.Tanabe, M.Rubel et al.,
J.Nucl.Mater. 329-333 (2004) 732.

B-4) Thermal diffusion of impurities in materials



★ Impurity Deposition and Collisional Mixing

★ Thermal Diffusion of Deposited Impurities

Diffusion Coefficient $D = D_0 \exp(-Q_D / kT)$

D_0 : Material Constant (cm^2s^{-1})

Q_D : Activation Energy (eV)

T : Material Temperature (K)

Γ : Incident Ion Flux ($cm^{-2}s^{-1}$)

ϕ : Total Ion Fluence (cm^{-2})

t : $(= \phi / \Gamma)$ Irradiation Time (s)

N : Number of Pseudo Ions

$\Delta\phi$: $(= \phi / N)$ Differential Ion Flux (cm^{-2})

Δt : $(= t / N)$ Differential Irradiation time (s)

W.Eckstein et al.;
Nucl.Instr.Meth.B 153(1999)415.

B-4) Thermal diffusion of impurities in materials

Coupling of BCA code with diffusion codes

K.L.Wilson, M.I.Baskes, J. Nucl.Mater. 76-77(1978)291.

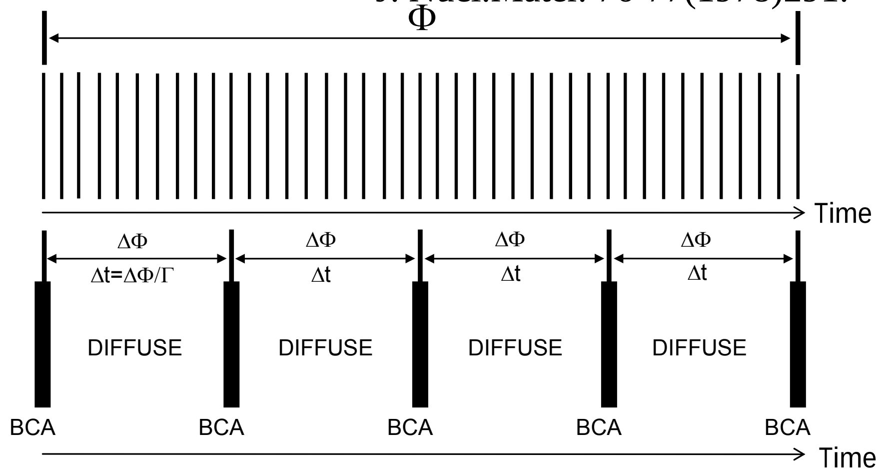
Fick's law with source and trapping terms

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

$C_j(x,t)$: j th solute concentration, D_j : Diffusion coefficient for j th solute

$G_j(x,t_0)$: source term (range profile)

$c_{Tj}^i(x,t)$: concentration of j th solute trapped I th trapping site



Rate equation for trapping and detrapping

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

$$C_{Te}^i(x,t) = C_{Te}^i(x,t_0) - \sum_j f_j^i c_{Tj}^i(x,t)$$

λ : jump distance,

ν_0 : detrapping attempt frequency

f_j^i : the inverse trap saturability of j th solute fot the I th trapping site

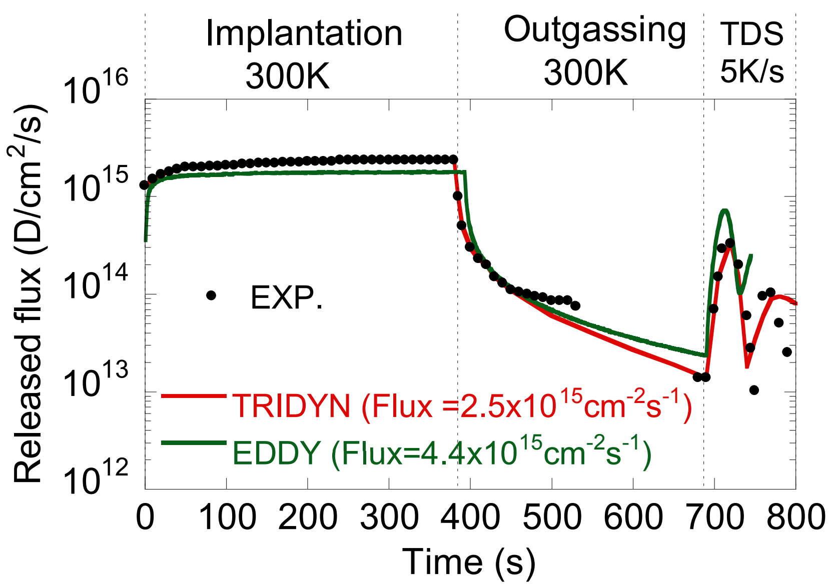
E_T^i : detrapping energy of I th trap

Boundary condition

e.g., recombination limited

$$\frac{\partial c_j}{\partial x} = \frac{K_r}{D_j} c_j^2(x=0) \quad \left[J = K_r c_j^2(x=0)\right]$$

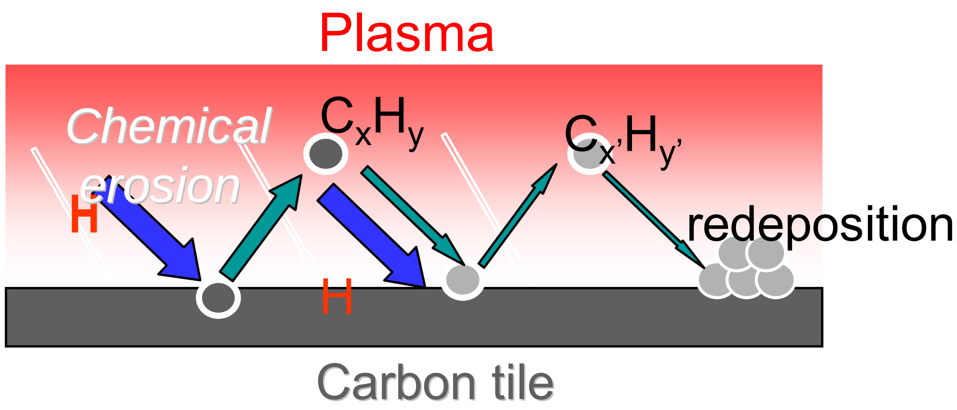
K_r : recombination coefficient

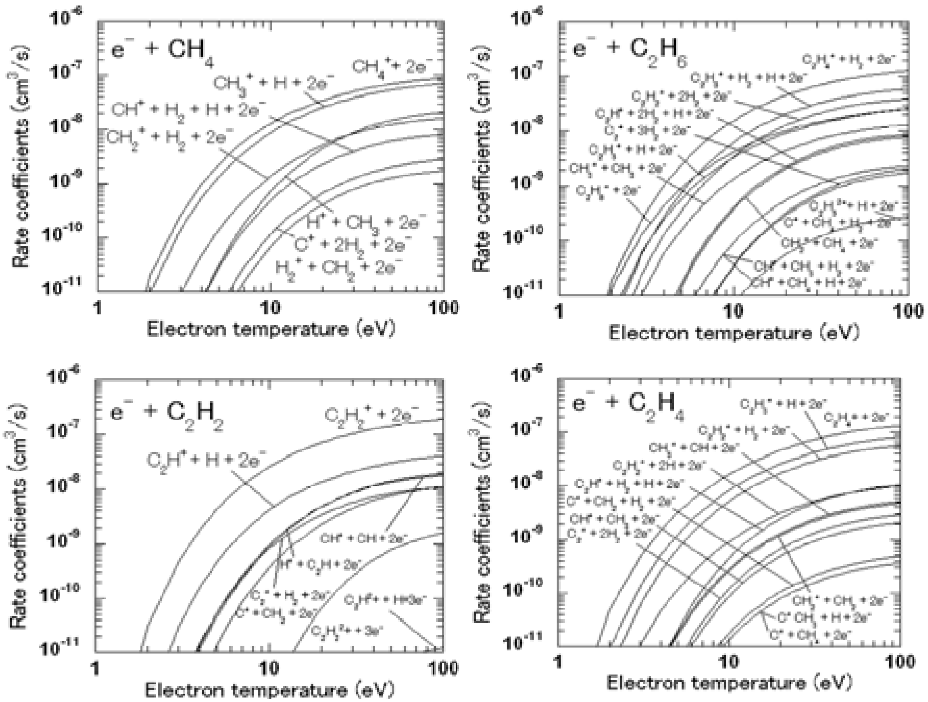


Parameters	Values
Diffusion	
D_0(cm²/s)	3.5x10^-7
E_D (eV)	0.39
Recombination	
K_0 (cm^{4}K$^{1/2}$/s)	1.2x10^25
E_r (eV)	-0.59
Trap #1	
$E_{T,1}$ (eV)	0.85
$C_{T,1}$(Traps/W)	0.01
Trap #2	
$E_{T,2}$ (eV)	1.4
$C_{T,2}$(Traps/W)	0.01

B-5) Transport and redeposition of eroded impurities

Monte Carlo Modeling of Impurity Transport





- <u>The released C_xH_y molecule successively collides with plasma electrons and ions.</u>

More than 700 reactions are included.

(R.K.Janev, D.Reiter, Rep.FZ-Juelich, Jul-3966(2002); Jul-4005 (2003))

- <u>The elastic collisions with the **residual neutral hydrogen atoms**</u>

B-5) Transport and redeposition of eroded impurities

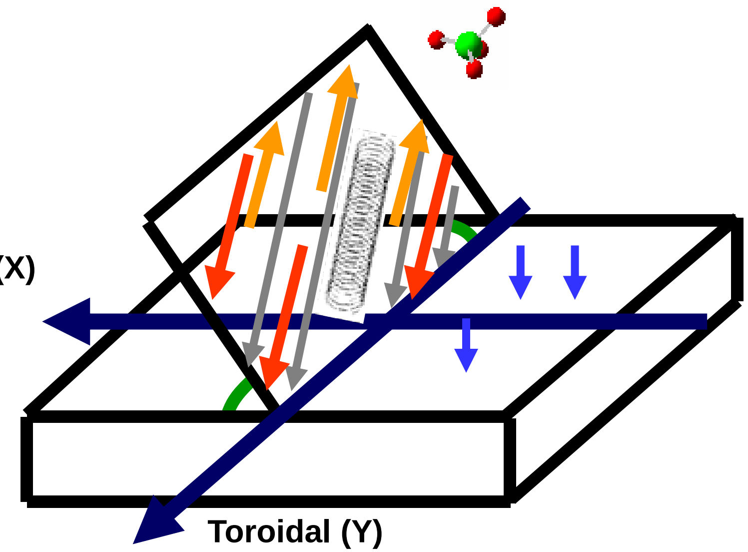
The model includes

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

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

: P.C.Stangeby, *The Plasma Boundary of Magnetic Fusion Devices* (IOP, Bristol, 2000) p.296.

Poloidal(X)



- Debye sheath and magnetic pre-sheath potential

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

ϕ_0 : sheath potential

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

: J.N.Brooks, Phys. Fluids B2(1990)1858.

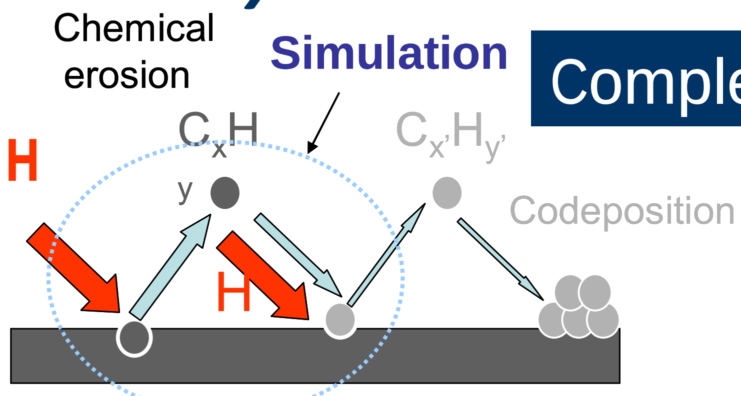
- Cross-field diffusion

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

: K. Shimizu, T. Takizuka purakakugakkaishi 71 (1995) 1135.

B-5) Transport and redeposition of eroded impurities

Hydrocarbon Redeposition on PFW Surfaces



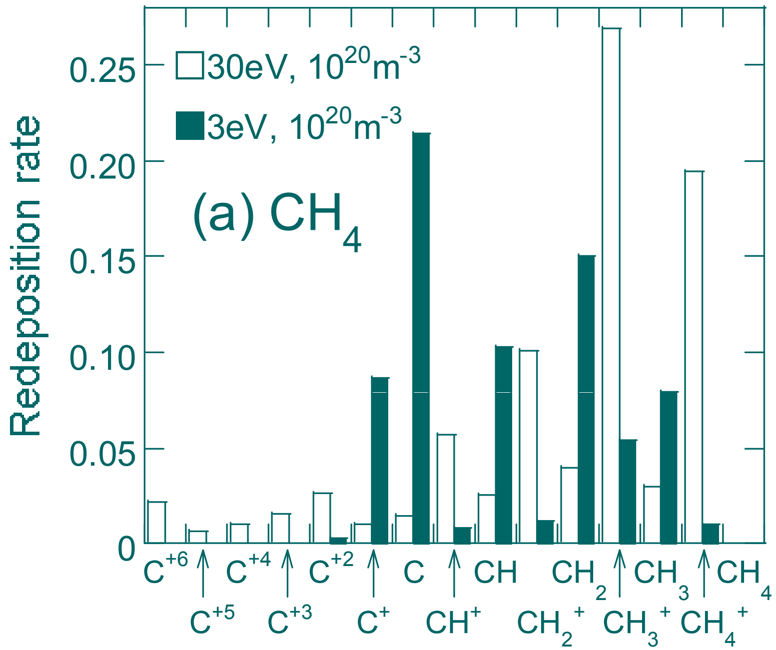
Carbon tile

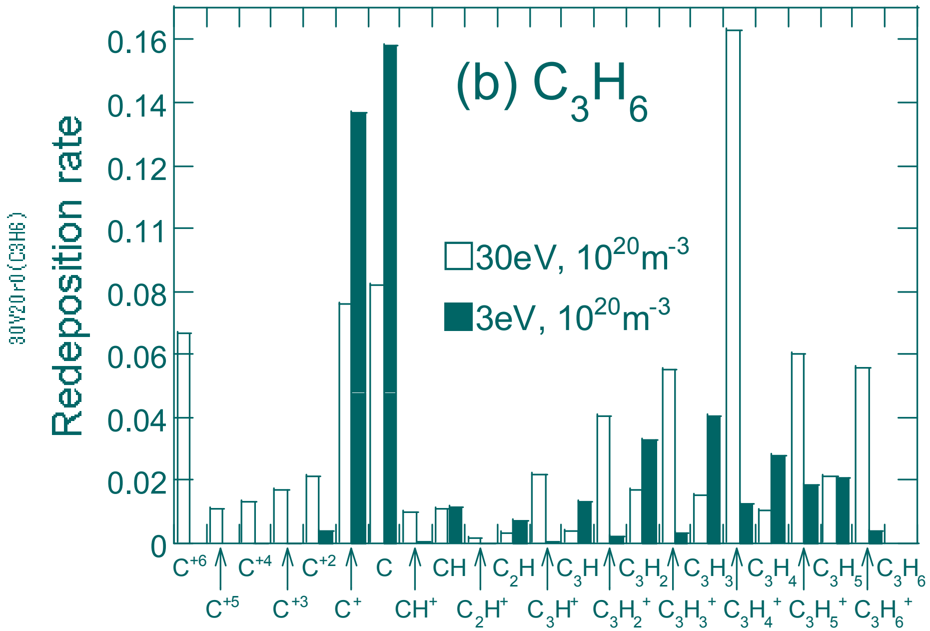
Complex distribution of redeposition species

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

⇒**Strong influence of atomic and molecular processes**

K.Ohya et al.; FED81(2006)205.





B-5) Transport and redeposition of eroded impurities

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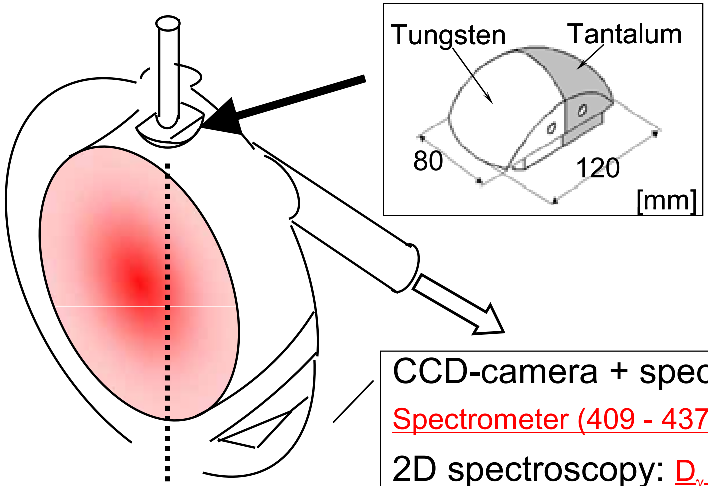


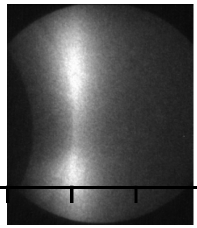
Inverse photon efficiency, D/XB, defined as
(the number of the launching hydrocarbons)
/(the number of photon emission events)

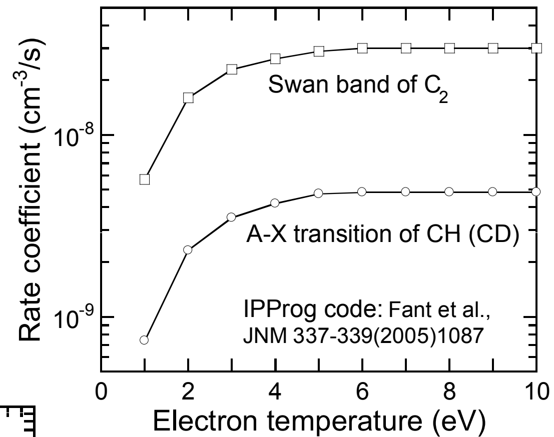
Correlation of CH (C_2) radiations with chemically sputtered CH_4 (C_2H_4, C_2H_6) are important, depending on plasma parameters and hydrocarbon species.

CCD-camera + spectrometer

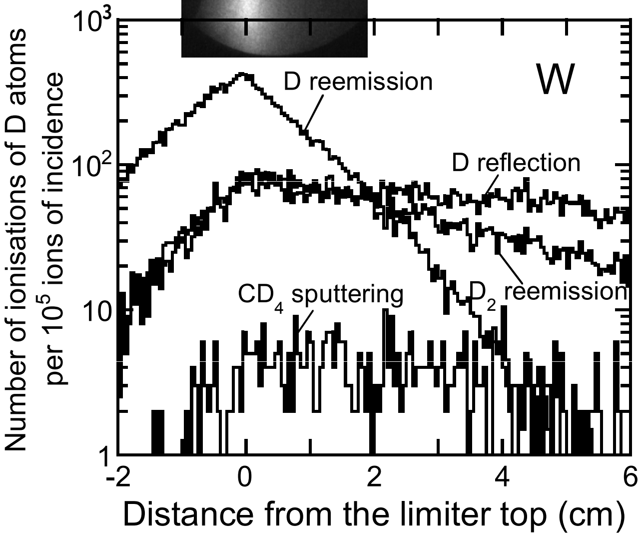
Spectrometer (409 - 437nm)

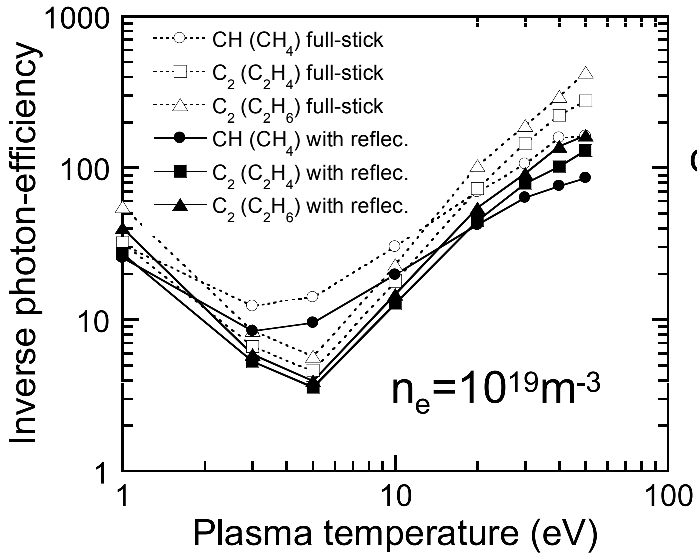
2D spectroscopy: D_γ (434nm)





K.Ohya et al.;
JNM313-316(2003)568.; JPFRS8(2009)1116.

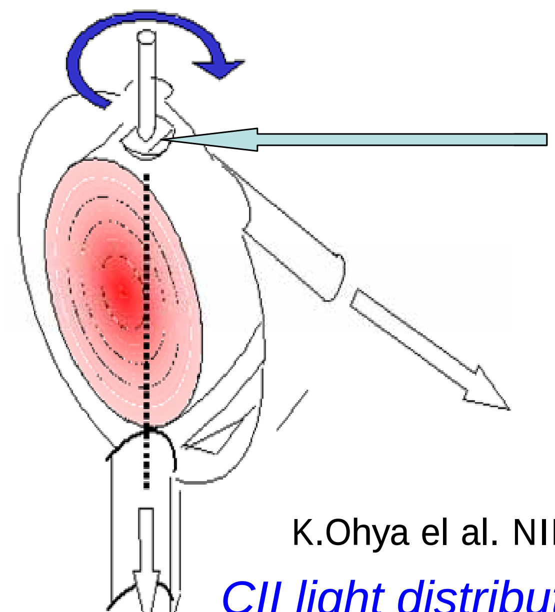


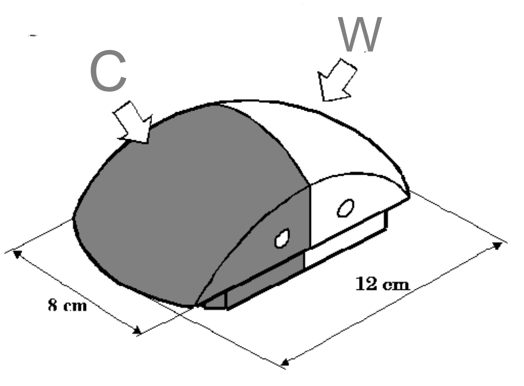


D/XB of CH and C_2 decreases with deceasing temperature up to 5 eV, and then increases with a further decrease of temperature.

B-5) Transport and redeposition of eroded impurities

TEXTOR tokamak

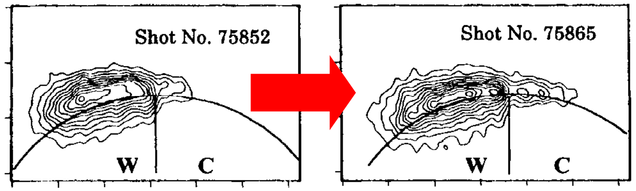




Top surface = sphere (r=7cm)

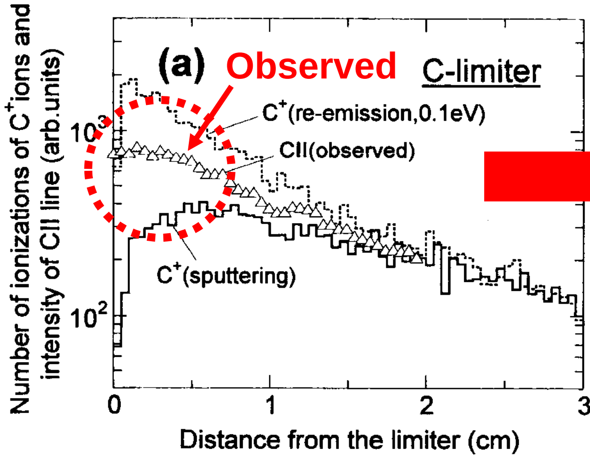
W-C twin test limiter in TEXTOR

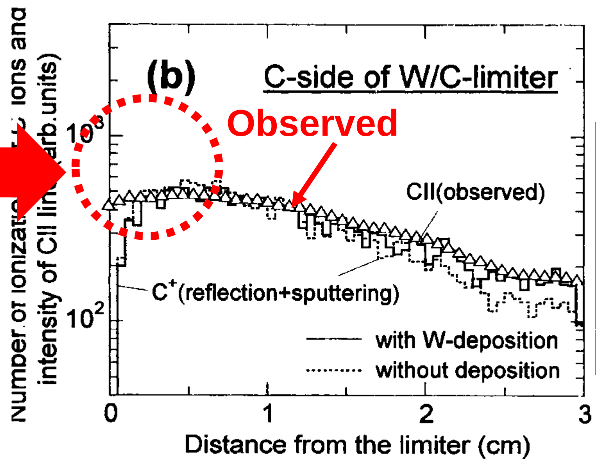
WI light emission appears on C-side !



K.Ohya el al. NIMB153(1999)354.

CII light distribution in near-surface plasma





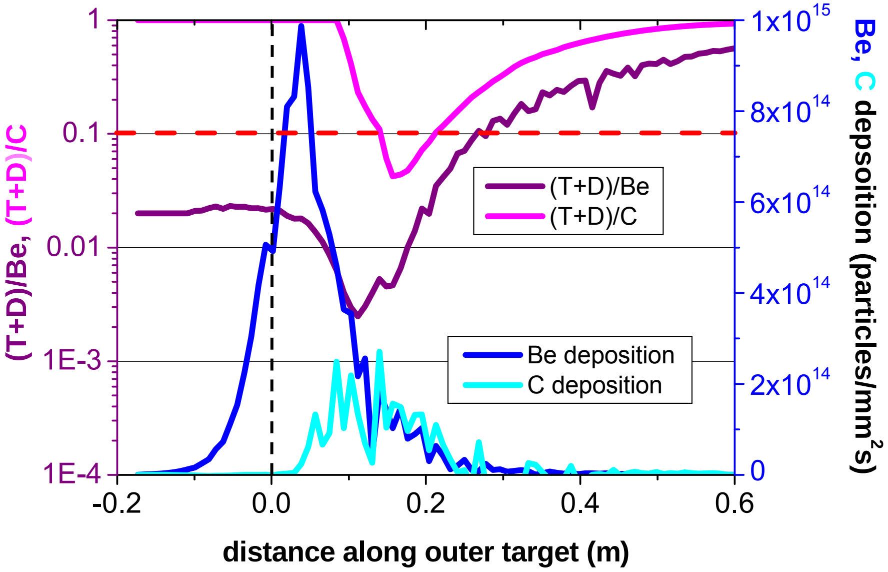
W deposition on the C side strongly decrease CII light intensity above the surface.

"Suppression" of chemical sputtering due to W deposition

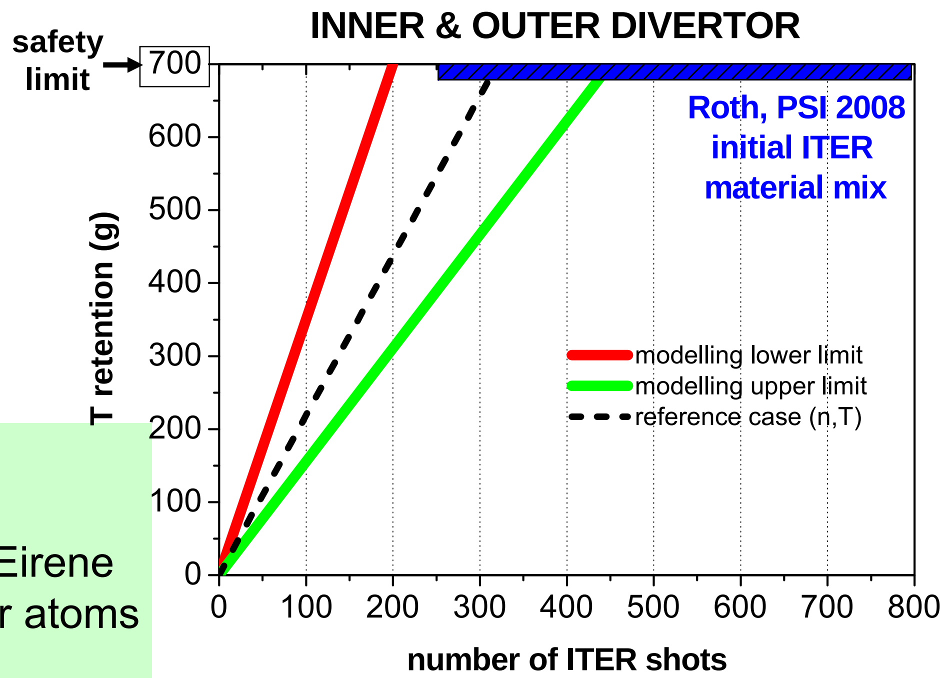
B-5) Transport and redeposition of eroded impurities

T and C profiles along ITER divertor target

A.Kirschner et al.;
Phys.Scr. T138(2009)014011.



Prediction of Long-term tritium retention rates



Many assumptions:

- 0.1% Be to outer, 1% Be to inner divertor
- plasma parameter from a plasma code, B2-Eirene
- zero sticking of C_xH_y (S = 0),Trim/MolDyn for atoms
- enhanced erosion of redeposited carbon
- Variable (T+D)/C and (T+D)/Be ratios for deposits,

  $D/C = 0.0204 \cdot E^{-0.43} \cdot \exp(2268/T)$

  $D/Be = 5.82 \cdot 10^{-5}\, E^{1.17}\, (D/Be)_{flux}^{-0.21} \exp(2273/T)$

  and (T+D)/C = (T+D)/Be = 1 for remote deposits.
- Temperature distribution on target calculated,

Summaries 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,

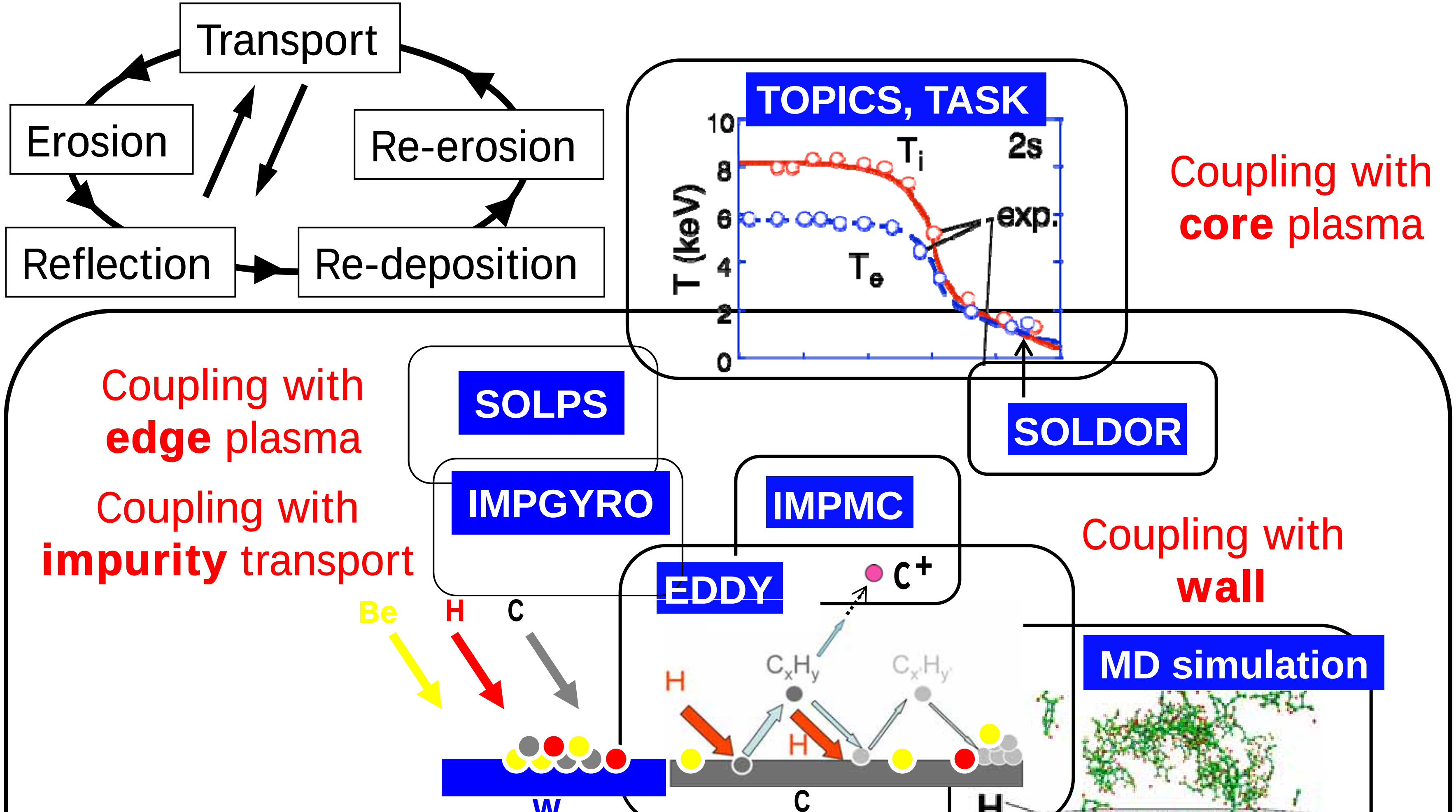
whereas reliable database of physical parameters used in codes have to be prepared.

Summaries of Lecture

(continued)

(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