Simulation Studies on Re-emission and Thermal Desorption of Deuterium from a Tungsten Material

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1) Abstract

The hydrogen retention and recycling properties of first wall materials are important factors controlling the particle balance. We have tried to follow Garcia-Rosales's experiment [1] on fluxes on re-emission and desorption of deuterium from a tungsten material using the ACAT-DIFFUSE code[2].

[1] C. Garcia-Rosales et al., J. Nucl. Mater. **233-237** (1996) 803

[2] Y. Yamamura, Nucl. Instr. Meth. **B28** (1987) 17

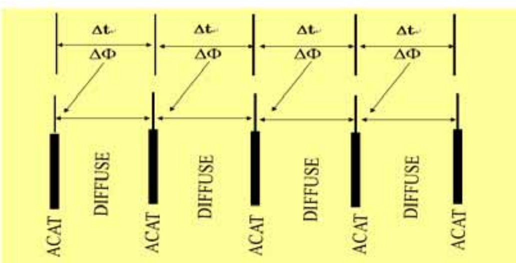
2) ACAT-DIFFUSE model

Logical representation

ACAT-DIFFUSE = [(ACAT)+(DIFFUSE)]^n

($n = \Phi/\Delta\Phi$, Φ: Total fluence [ions/cm^2])

ACAT-DIFFUSE model



$\Delta t = \Delta\Phi/J$ (J:flux [ions/cm^2/s])

2-1) ACAT Routine

- Monte Carlo method
- Binary collision approximation
- Amorphous target
- Unit cell

2-2) DIFFUSE Routine

$$\frac{\partial c_j(x,t)}{\partial t} = \nabla\left[D_j(x,t)\nabla c_j(x,t)\right] + G_j(x,t_0) - \sum_{i=1}^{2}\frac{\partial c^i_{Tj}(x,t)}{\partial t}$$

j : j-atom of a multi-component material, $c_j(x,t)$: concentration of j- atom (cm^{-3}), D_j : diffusion coefficient of j-atom (cm^2/s), c^i_{Tj} : concentration of j-atom in i-defect (cm^{-3}). $G_j(x,t_0)$: source term .

$$\frac{\partial c^i_{Tj}(x,t)}{\partial t} = \frac{D_j(x,t)c_j(x,t)C^i_{Te}(x,t)}{\lambda^2} - c^i_{Tj}(x,t)\nu_0\exp(-E^i_T/kT)$$

λ : the jump distance (cm), ν_0 : the detraping attempt frequency (s^{-1}), E^i_T : the detrapping energy of i-atom (eV).

$$C^i_{Te}(x,t) = C^i_{Te}(x,t_0) - \sum_j f^i_j c^i_{Tj}(x,t)$$

f^i_j : the saturation of the i-defect due to j-atom.

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

K_r : recombination coefficient (cm^4/s), D_j : diffusion coefficient (cm^2/s), $c_j(x=0)$: surface density of deuterium (cm^{-3}).

$$K_r = \frac{K_0}{\sqrt{T}}\exp\left[-E_r/kT\right]$$

K_0 : preexponential factor (cm・K$^{1/2}$/s), E_r : activation energy for recombination (eV), T : Temperature (K).

4) Results

Fig.1 : TDS Simulation

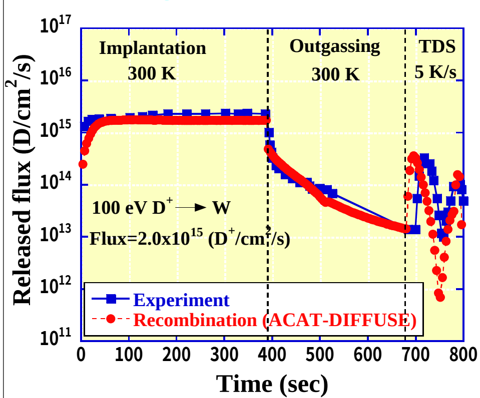


Fig.2 : Flux under the implantation

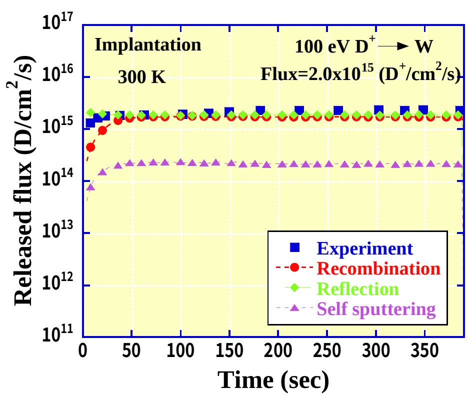


Fig.3 : Depth profile of D in C

(W.R.Wampler et al., JNM **103&104** (1981) 509)

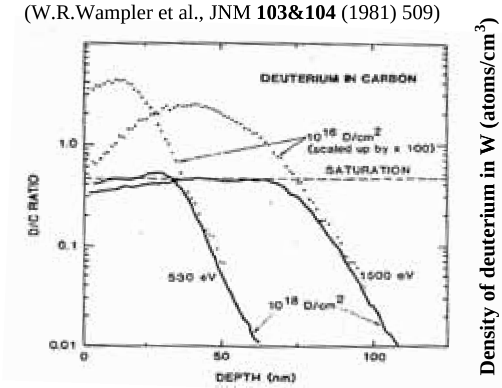


Fig.4 : Depth profile of D in W

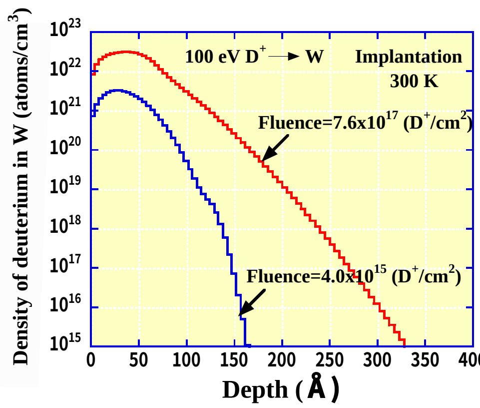


Fig. 5 : Mobile and trapped particles

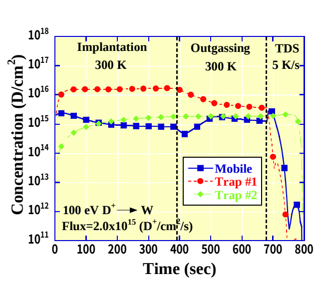
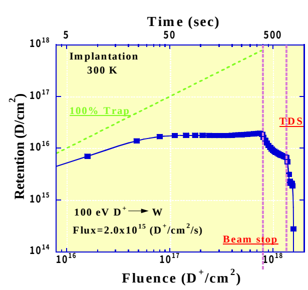


Fig.6 : Retention of D in W



Parameters for the simulations

Parameters	Values
Diffusion	
D_0	1.0×10^{-8} cm^2/s
E_D	0.39 eV
Recombination	
K_0	7.7×10^{-3} cm・K$^{1/2}$/s
E_r	-0.59 eV
Trap #1	
$E_{T,1}$	0.85 eV
$c_{T,1}$	0.05 traps/W
Trap #2	
$E_{T,2}$	2.2 eV
$c_{T,2}$	0.003 traps/W

5) Summary

- The ACAT-DIFFUSE code can predict the trend of the TDS experiment.
- In graphite almost all deuterium atoms are trapped in the implantation zone and don't diffuse, whereas in tungsten they distribute in a large zone larger than the implantation zone.