

Cluster dynamics modeling of accumulation and diffusion of He in neutron irradiated W

Y.G. Li & W.H. Zhou & Z. Zeng

*Institute of Solid State Physics
Chinese Academy of Sciences*

2010-10-18

Contents

- Background
- Cluster dynamics model
- Results and discussions
- Conclusions

Background

● Radiation conditions:

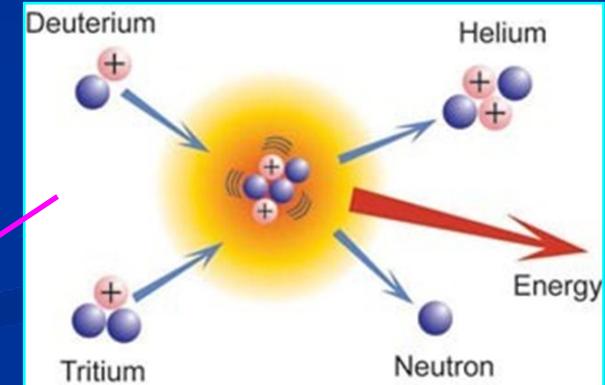
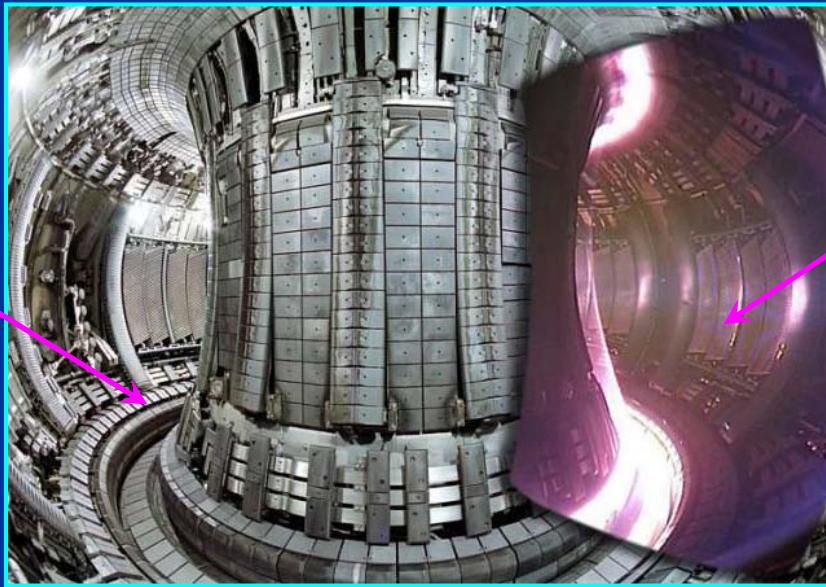
- Fission type reactor
- Nuclear fusion devices (e.g. ITER): Plasma-facing materials (PFMs)
- Spallation neutron source

<http://www.iter.org>

Federici et al., Nucl. Fusion 290-293 (2001) 260.

PFMS:

B,C, W ...



Heavy bombardment from the plasma: particles such as hydrogen isotope and He ions with the energies ranging from 10 eV to several keV as well as energetic neutrons and high heat loads generated by $D-T$ fusion reaction.

The peak particle flux (ITER):

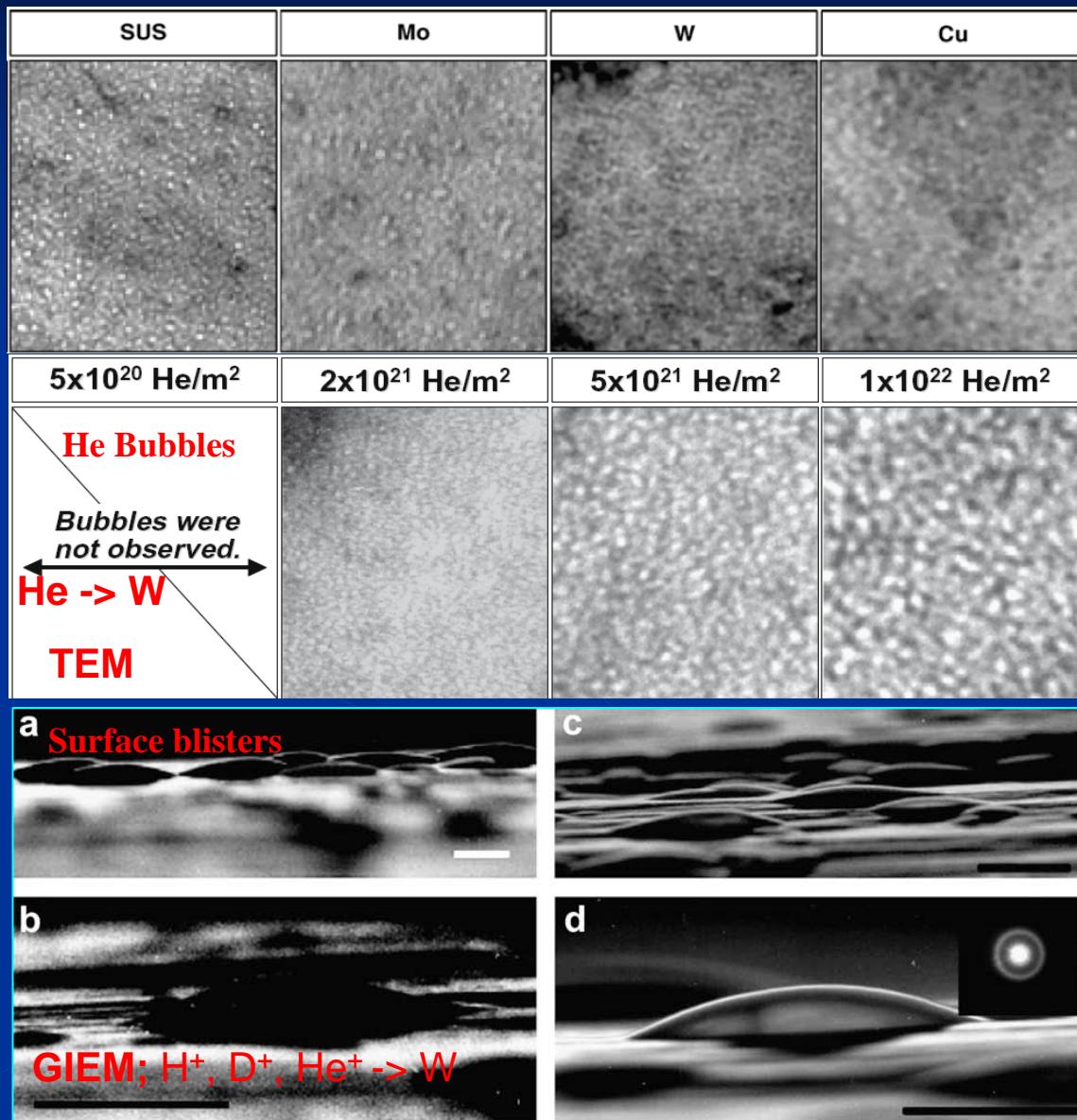
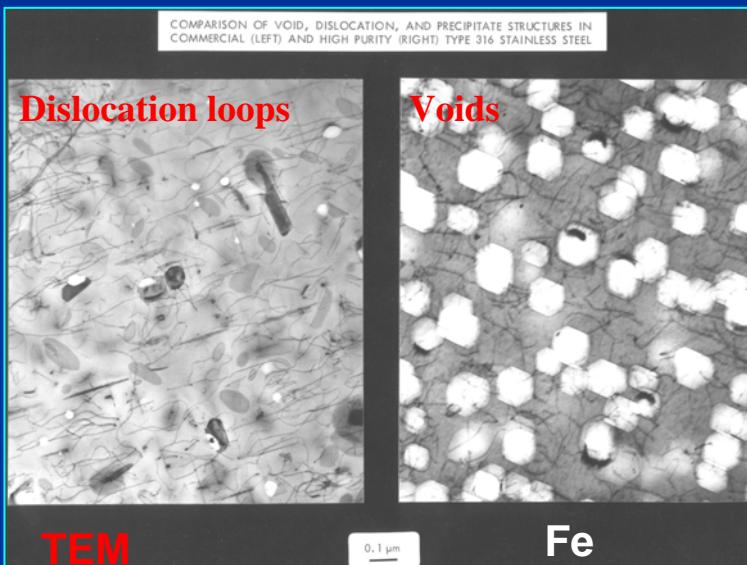
- $\sim 10^{21} m^{-2}s^{-1}$ with the expected average energy \sim several keV at the first wall;
- $\sim 10^{24} m^{-2}s^{-1}$ with the average energy of 0.5 keV at the divertor.

● Radiation damages

Experiments for
reactor relevant
plasma conditions

Tokitani et al., J. Nucl. Mater. 386-388 (2009) 173.

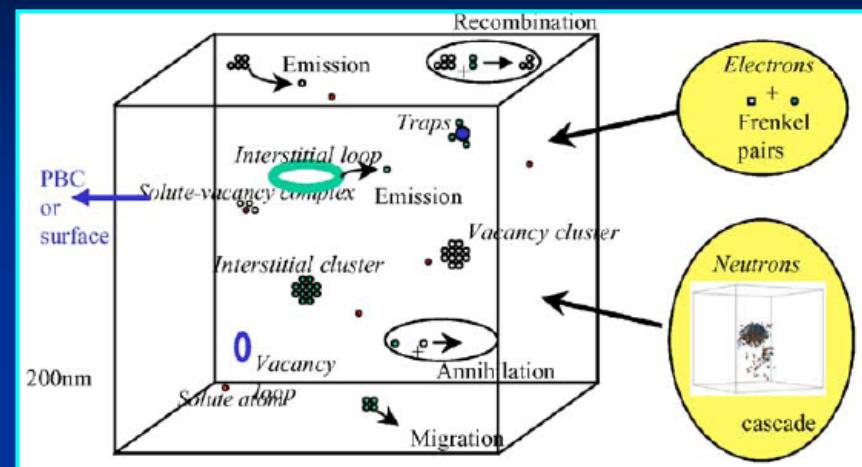
Naruaki Enomoto et al., J. Nucl. Mater. 385 (2009) 606.



● Rate Theory model Simulation study of Defects Reaction Dynamics

- Defects Reaction Dynamics
- Mean Field Rate Theory

Turkin et al.; J. Nucl. Matter. 358 (2006) 10.



- **He atoms:**
deeply trapped by lattice defects (e.g. vacancies & He-vacancy complexes)
- **W based materials:** (potential candidates for the divertor armor tiles in ITER)
excellent thermal properties; low solubility for hydrogen; low sputtering yield.

Cluster dynamics model: to study the accumulation and diffusion processes of helium in tungsten under synergistic effects of helium implantation and neutron irradiation.

Cluster dynamics model

● TRIM+Rate Theory

- Only I, I_2, V, He are mobile;
- The evolutions of mobile defects: a set of **one-dimensional spatial diffusion-reaction equations**;

The evolutions of immobile clusters: follow a Markovian chain process, the **master equations**:

$$\frac{\partial C_\theta}{\partial t} = G_\theta + D_\theta \nabla^2 C_\theta + \sum_{\theta'} \left(w(\theta', \theta) C_{\theta'} - w(\theta, \theta') C_\theta \right) - L_\theta$$

- **Rate coefficients** can be determined by the parameters such as structure factors, migration energy, binding energy, formation energy, etc.
- The **initial distributions of point defects** (the damages (dpa) and accumulations of He atoms (apa) in W) are estimated by **TRIM-code**.

● Rate theory/cluster dynamics model:

Reaction types	Rate coefficients
$I + V \rightleftharpoons 0;$	$k_{I+V}^+, G_{I/V}$
$I + I_n \rightleftharpoons I_{n+1};$	$\alpha_n^+, \alpha_{n+1}^-$
$I + V_n \rightarrow V_{n-1};$	$k_{V_n+I}^+$
$I + He_n \rightarrow He_n I;$	$k_{He_n+I}^+$
$I + He_m V_n \rightarrow He_m V_{n-1};$	$k_{He_m V_n+I}^+$
$I_2 + I_n \rightleftharpoons I_{n+2};$	β_n^+, β_{n+2}^-
$I_2 + V_n \rightarrow V_{n-2};$	$k_{V_n+I_2}^+$
$I_2 + He_m V_n \rightarrow He_m V_{n-2};$	$k_{He_m V_n+I_2}^+$
$V + I_n \rightleftharpoons I_{n-1};$	$k_{I_n+V}^+, k_{I_{n-1}-V}^-$
$V + V_n \rightleftharpoons V_{n+1};$	$\gamma_n^+, \gamma_{n+1}^-$
$V + He_n \rightleftharpoons He_n V;$	$k_{He_n+V}^+, k_{He_n V}^-$
$V + He_n I \rightarrow He_n;$	$k_{He_n I+V}^+$
$V + He_m V_n \rightleftharpoons He_m V_{n+1};$	$\omega_n^+, \omega_{n+1}^-$
$He + V_n \rightleftharpoons He V_n;$	$k_{V_n+He}^+, k_{He V_n}^-$
$He + He_n \rightleftharpoons He_{n+1};$	η_n^+, η_{n+1}^-
$He + He_n I \rightleftharpoons He_{n+1} I;$	$\mu I_n^+, \mu I_{n+1}^-$
$He + He_m V_n \rightleftharpoons He_{m+1} V_n;$	$\mu V_{mn}^+, \mu V_{(m+1)n}^-$

TRIM+Rate Theory

Ghoniem et al., J. Nucl. Mater. **92** (1980) 121.

Duparc et al., J. Nucl. Mater. **302** (2002) 143.

Surh et al., J. Nucl. Mater. **325** (2004) 44.

Christien et al., J. Nucl. Mater. **346** (2005) 272.

Ortiz et al., Phys. Rev. B **75** (2007) 100102.

Xu et al., J. Nucl. Mater. **367-370** (2007) 806.

Gokhman et al., Radiation Effects & defects in Solids **165** (2010) 216.

The Master Equations

$$\begin{aligned}
& \mathbf{I}, \mathbf{I}_2, \mathbf{V}, \mathbf{X}, \mathbf{I}_n, \mathbf{V}_n, \mathbf{He}_n, \mathbf{He}_n \mathbf{I}, \mathbf{He}_m \mathbf{V}_n \\
\frac{\partial C_I}{\partial t} = & G_I + D_I \nabla^2 C_I - k_{I+V}^+ (C_I C_V - C_I^{eq} C_V^{eq}) - 2(\alpha_1^+ C_I^2 - \alpha_2^- C_{I_2}) + k_{V+I_2}^+ C_V C_{I_2} - \sum_{n=2}^{N_V} k_{V_n+I}^+ C_I C_{V_n} \\
& - \sum_{n \geq 2} (\alpha_n^+ C_I C_{I_n} - \alpha_{n+1}^- C_{I_{n+1}}) - \sum_{n=1}^{N_X} k_{X_n+I}^+ C_I C_{X_n} - \sum_{n=1}^{N_V} \sum_{m=1}^{M_X} k_{X_m V_n+I}^+ C_I C_{X_m V_n} - L_I \\
\frac{\partial C_{I_2}}{\partial t} = & \dots, \frac{\partial C_V}{\partial t} = \dots \\
\frac{\partial C_X}{\partial t} = & G_X + D_X \nabla^2 C_X - 2(\eta_1^+ C_X^2 - \eta_2^- C_{X_2}) - \sum_{n=1}^{N_V} (k_{V_n+X}^+ C_X C_{V_n} - k_{X_n V}^- C_{X_n V}) \\
& - \sum_{n=2}^{N_X} (\eta_n^+ C_X C_{X_n} - \eta_{n+1}^- C_{X_{n+1}}) - \sum_{n=1}^{N_X} (\mu I_n^+ C_X C_{X_n I} - \mu I_{n+1}^- C_{X_{n+1} I}) \\
& - \sum_{n=1}^{N_V} \sum_{m=1}^{M_X} (\mu V_{mn}^+ C_X C_{X_m V_n} - \mu V_{(m+1)n}^- C_{X_{m+1} V_n}) - L_X \\
\frac{\partial C_{I_n}}{\partial t} \Big|_{n \geq 3} = & -(\alpha_n^+ C_I C_{I_n} - \alpha_{n+1}^- C_{I_{n+1}}) + (\alpha_{n-1}^+ C_I C_{I_{n-1}} - \alpha_n^- C_{I_n}) - (\beta_n^+ C_{I_2} C_{I_n} - \beta_{n+2}^- C_{I_{n+2}}) \\
& + (\beta_{n-2}^+ C_{I_2} C_{I_{n-2}} - \beta_n^- C_{I_n}) - (k_{I_n+V}^+ C_V C_{I_n} - k_{I_{n-1}-V}^- C_{I_{n-1}}) + (k_{I_{n+1}+V}^+ C_V C_{I_{n+1}} - k_{I_n-V}^- C_{I_n}) \\
\frac{\partial C_{X_n}}{\partial t} \Big|_{2 \leq n \leq N_X} = & -k_{X_n+I}^+ C_I C_{X_n} - (k_{X_n+V}^+ C_V C_{X_n} - k_{X_n V}^- C_{X_n V}) + k_{X_n I+V}^+ C_V C_{X_n I} \\
& - (\eta_n^+ C_X C_{X_n} - \eta_{n+1}^- C_{X_{n+1}}) + (\eta_{n-1}^+ C_X C_{X_{n-1}} - \eta_n^- C_{X_n}) \\
\frac{\partial C_{V_n}}{\partial t} \Big|_{2 \leq n \leq N_V} = & \dots, \frac{\partial C_{X_n I}}{\partial t} \Big|_{1 \leq n \leq N_X} = \dots, \frac{\partial C_{X_m V}}{\partial t} \Big|_{1 \leq m \leq M_X} = \dots \\
\frac{\partial C_{X_m V_n}}{\partial t} \Big|_{2 \leq n \leq N_V, 1 \leq m \leq M_X} = & -(k_{X_m V_n+I}^+ C_I C_{X_m V_n} - k_{X_m V_{n+1}+I}^+ C_I C_{X_m V_{n+1}}) - k_{X_m V_n+I_2}^+ C_{I_2} C_{X_m V_n} \\
& - (\omega_n^+ C_V C_{X_m V_n} - \omega_{n+1}^- C_{X_m V_{n+1}}) + (\omega_{n-1}^+ C_V C_{X_m V_{n-1}} - \omega_n^- C_{X_m V_n}) \\
& - (\mu V_{mn}^+ C_X C_{X_m V_n} - \mu V_{(m+1)n}^- C_{X_{m+1} V_n}) + (\mu V_{(m-1)n}^+ C_X C_{X_{m-1} V_n} - \mu V_{mn}^- C_{X_m V_n})
\end{aligned}$$

● Parameters

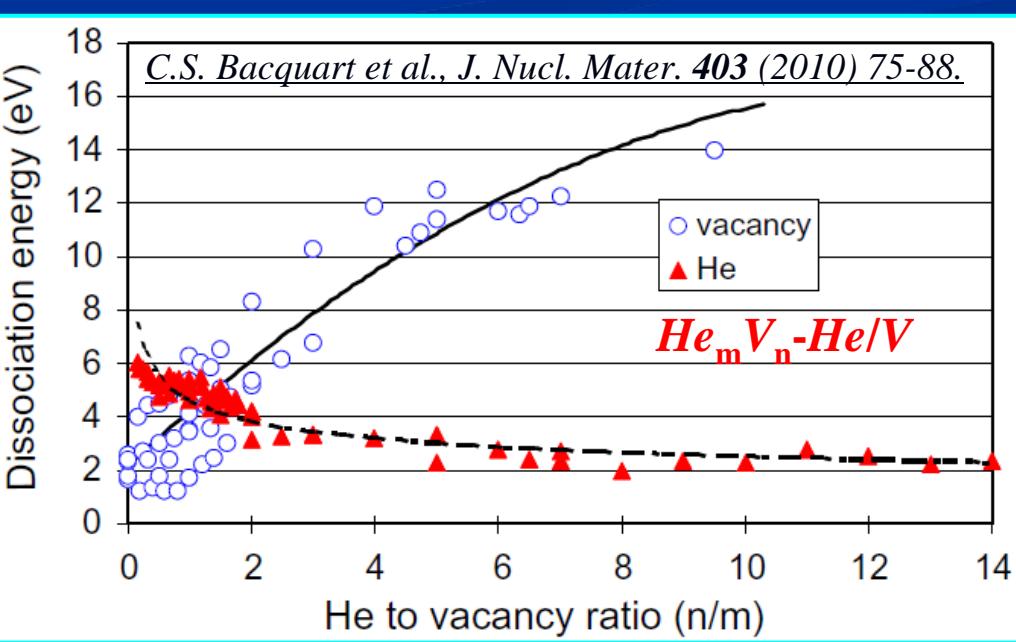
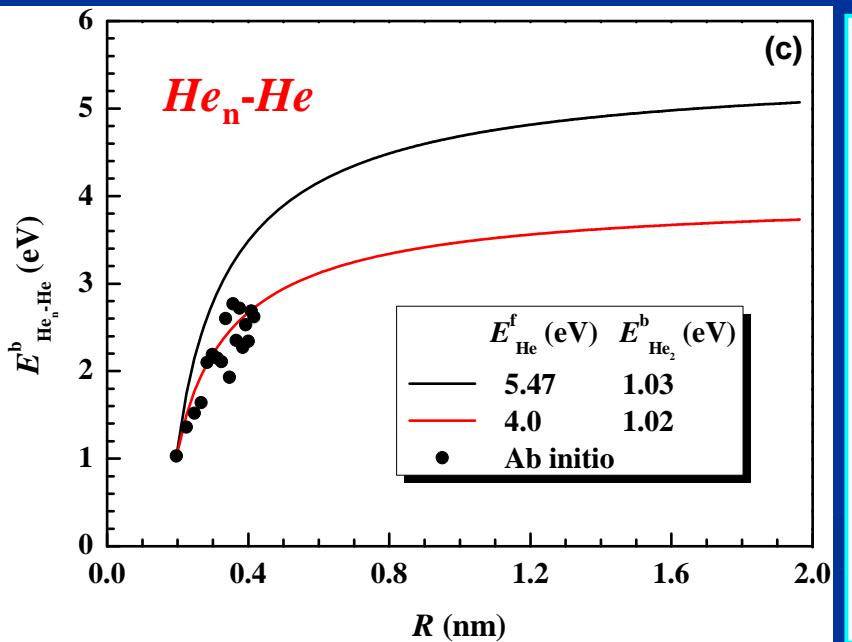
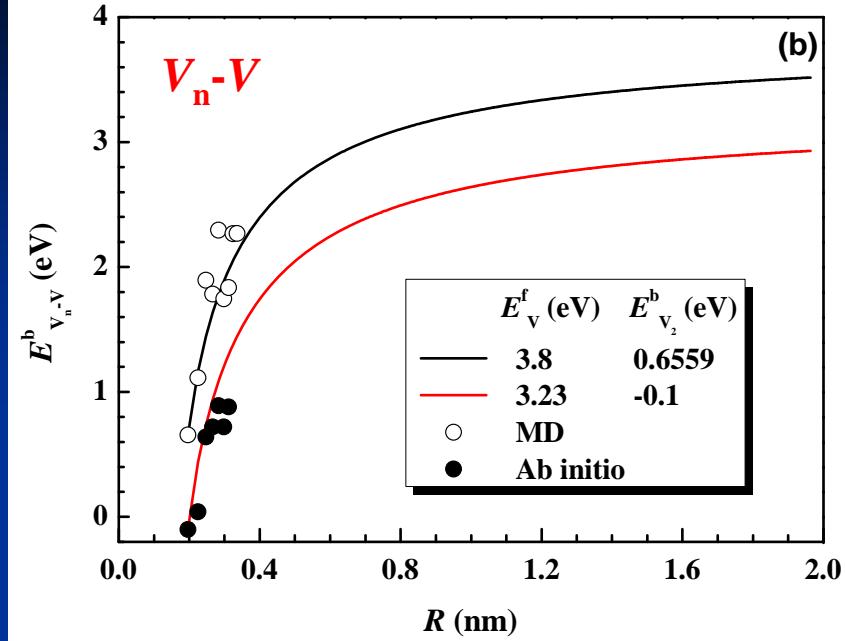
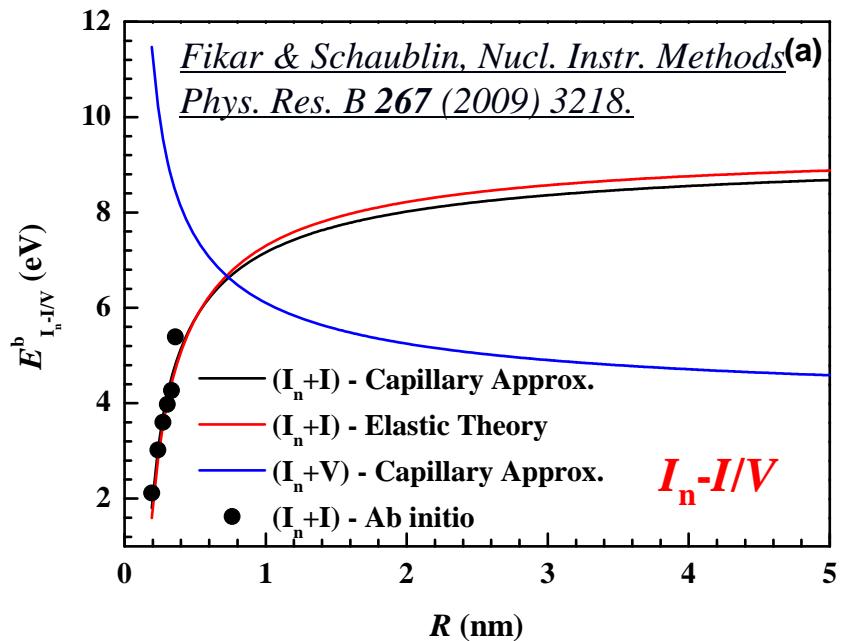
He atoms and neutrons
irradiated on W

Exp. / Ab initio / MD

Watanabe et al., Nucl. Instr. And Meth. In Phys. Res. B 255 (2007) 32.
Xu et al., J. Nucl. Mater. 367-370 (2007) 806.
Becquart et al., J. Nucl. Mater. 385 (2009) 223; 403 (2010) 75.
Fikar & Schaublin, Nucl. Instr. And Meth. In Phys. Res. B 267 (2009) 3218.
Ahlgren et al., J. Appl. Phys. 107 (2010) 033516.
Becquart & Domain, Nucl. Instr. And Meth. In Phys. Res. B 255 (2007) 23.
Federici et al., Nucl. Fusion 290-293 (2001) 260.
Olsson, Compu. Mater. Sci. 47 (2009) 135.
Carlsson, Solid State Phys. 43 (1990) 1.

	Symbol	Value
He beam intensity	I_{He}	$10^{18} - 10^{22} m^{-2} s^{-1}$
Temperature	T	$300K, 873K$
Point defect creation rate	$G_{I/V}$	$10^{-6} dpa s^{-1}$
Lattice parameter	a_0	3.1652 \AA
He radius	r_{He}	0.49 \AA
Burgers vector	b	2.74 \AA
Recombination radius	r_{IV}	4.65 \AA
Interstitial pre-exponential factor	D_{I_0}	$1.0e^{-8} m^2 s^{-1}$
Vacancy pre-exponential factor	D_{V_0}	$1.0e^{-4} m^2 s^{-1}$
He pre-exponential factor	D_{He_0}	$1.0e^{-8} m^2 s^{-1}$
Bias factor of interstitial loops	Z_I	1.0
Formation energy of SIA	E_I^f	9.466 eV
Formation energy of Vacancy	E_V^f	3.80 eV
Formation energy of He	E_{He}^f	4.0 eV
Migration energy of SIA	E_I^m	0.013 eV
Migration energy of Vacancy	E_V^m	1.66 eV
Migration energy of He	E_{He}^m	0.06 eV
Binding energy of I_2	$E_{I_2}^b$	2.12 eV
Binding energy of V_2	$E_{V_2}^b$	0.6559 eV
Binding energy of He_2	$E_{He_2}^b$	1.02 eV
Binding energy of $He - I$	E_{He-I}^b	0.94 eV

The binding energies of I_n - I/V , V_n - V , He_n - He and $He_m V_n$ - He/V :



● Numerical Method:

For larger dislocation loops ($x > N$):

The discrete Master equation $\xrightarrow{\text{Taylor series expansion (second-order terms)}}$ The continuous Fokker-Planck equation:

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x} \left(-F(x,t)C(x,t) + \frac{1}{2} \frac{\partial}{\partial x} D(x,t)C(x,t) \right), \quad x > N$$

where,

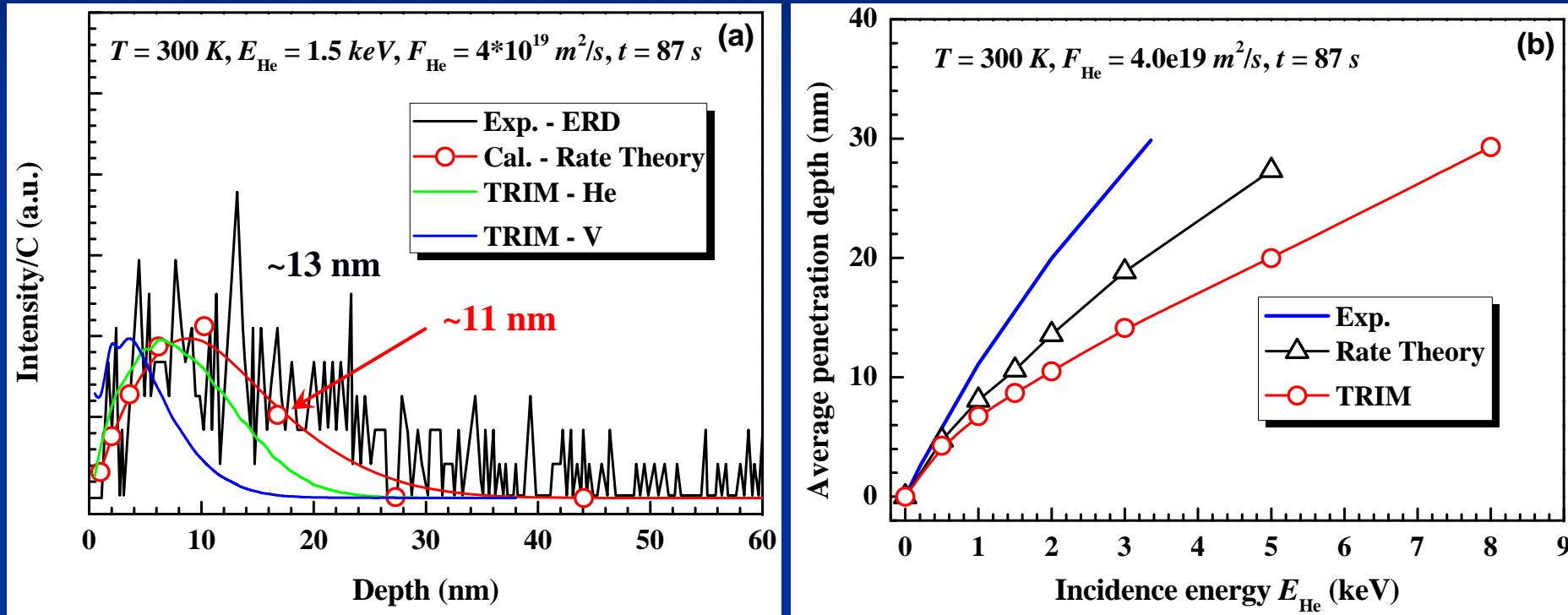
$$\begin{cases} F(x,t) = \kappa(x,t) - \lambda(x,t) \\ D(x,t) = \kappa(x,t) + \lambda(x,t) \end{cases} \quad \begin{cases} \kappa_I(x(n),t) \cong \gamma_n^+ C_I(t) + k_{I_n+V}^- \\ \lambda_I(x(n),t) \cong \gamma_n^- + k_{I_n+V}^+ C_V(t) \end{cases}$$

- Discrete Master equation / Continuous Fokker-Planck equation;
- The first-order boundary conditions in both surface and sufficient depth are used;
- Numerical Method: using of *lsoda* subroutine packages to solve the ODEs.

Turkin et al., J. Nucl. Matter. 358 (2006) 10.
Ghoniem et al., J. Nucl. Matter. 92 (1980) 121.

Results and discussions

- Compare with experiments: He in W



TRIM+RT

Trapping & Diffusion

● Two typical cases (ITER):

- Case 1: He, $1\text{keV}, 10^{18} \text{m}^{-2}\text{s}^{-1}$ → first wall;
- Case 2: He, $30\text{eV}, 10^{22} \text{m}^{-2}\text{s}^{-1}$ → divertor;
- $\sim 10^{-6} \text{ dpa/s}$, uniform damages by **neutron**.

He in W

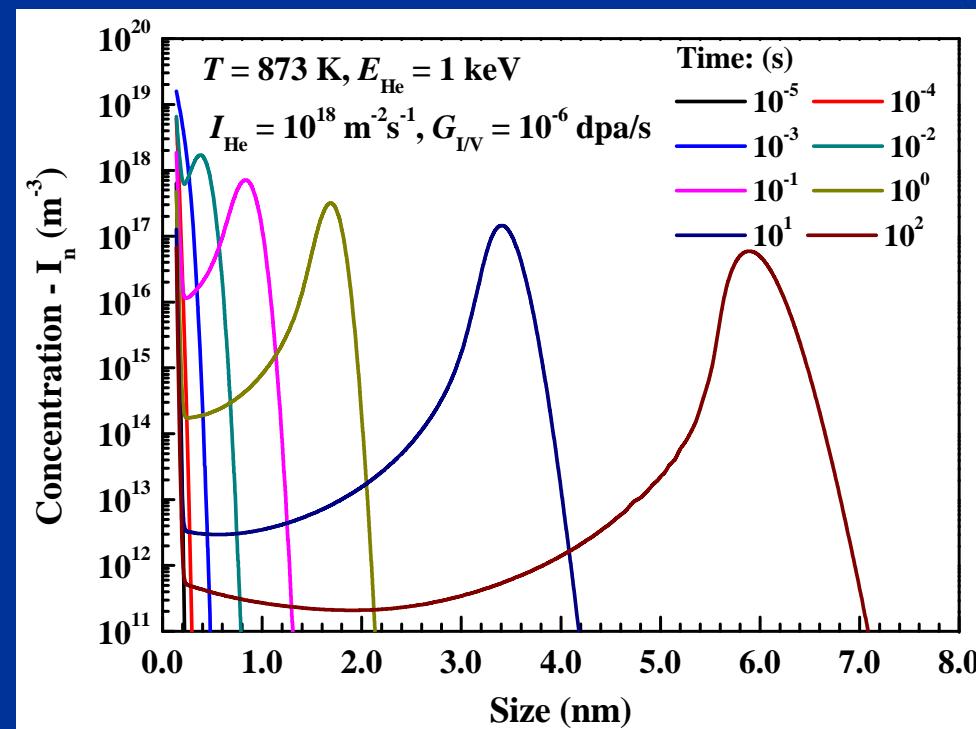
Xu et al., J. Nucl. Mater. 367-370 (2007) 806.

Case 1: first wall

Interstitial loops

Migration energy of I :

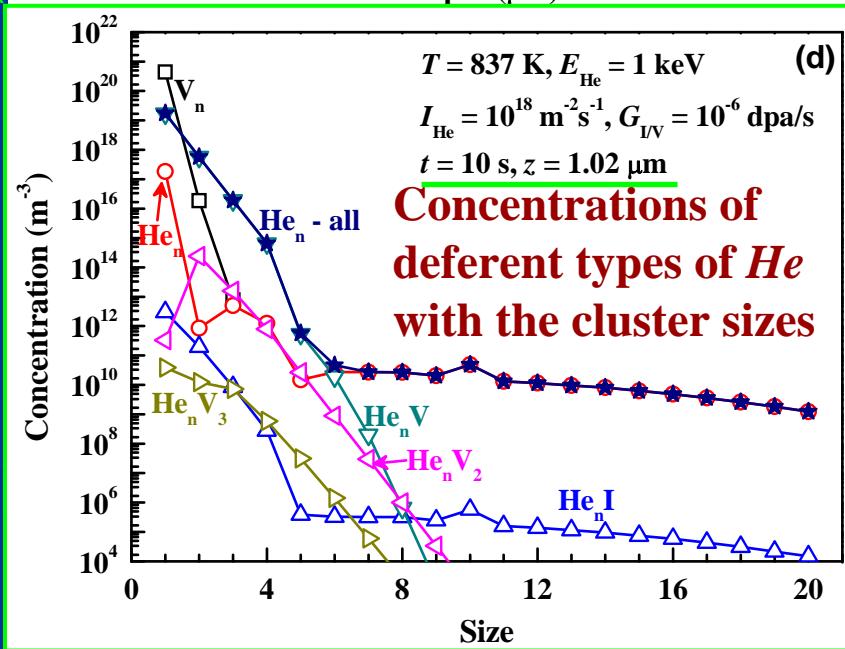
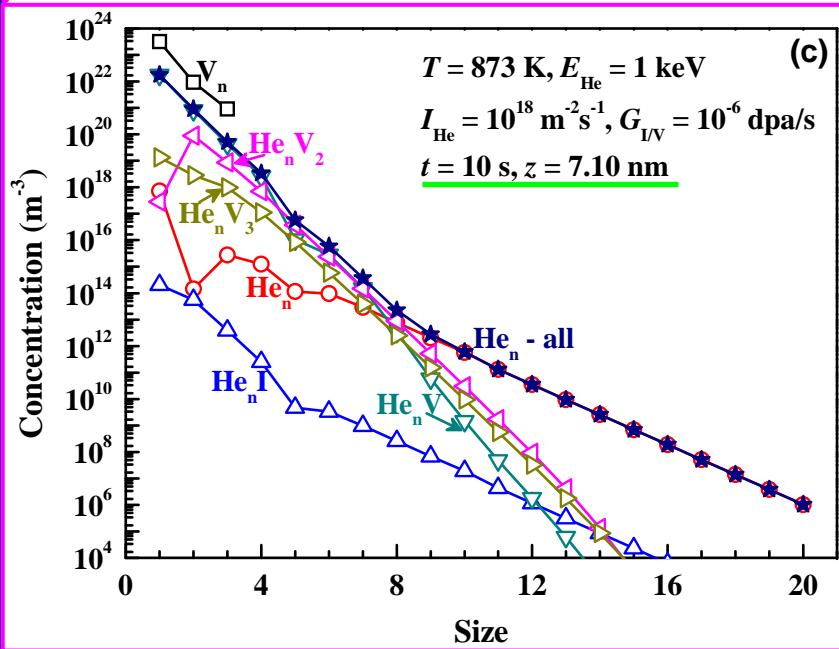
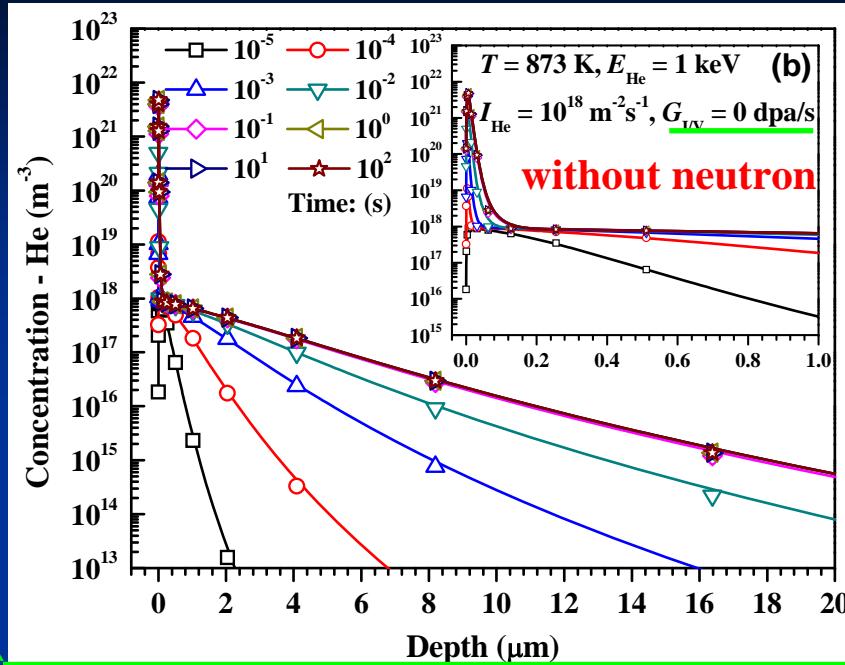
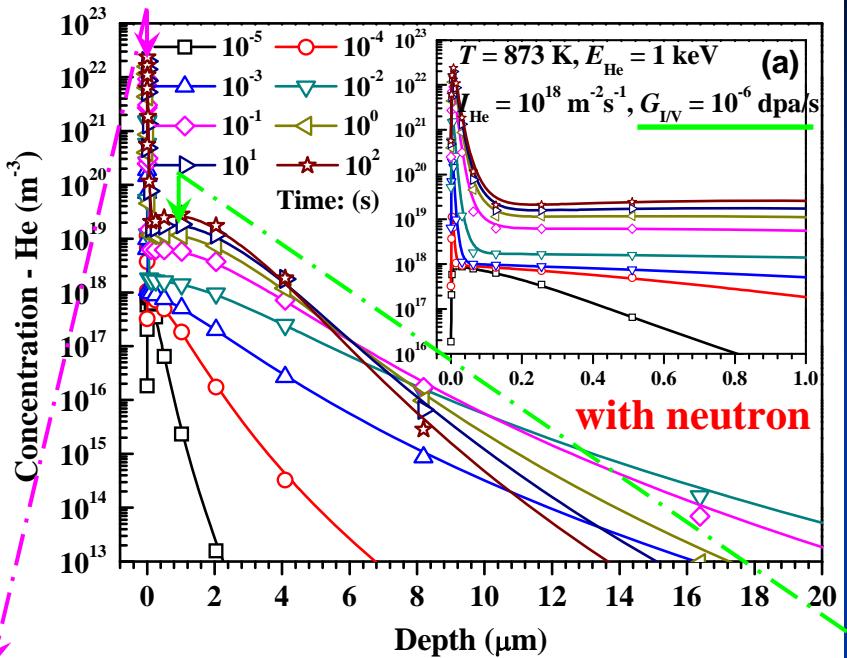
$\sim 0.013 \text{ eV}$



Iwakiri et al., J. Nucl. Mater. 283-287 (2000) 1134.

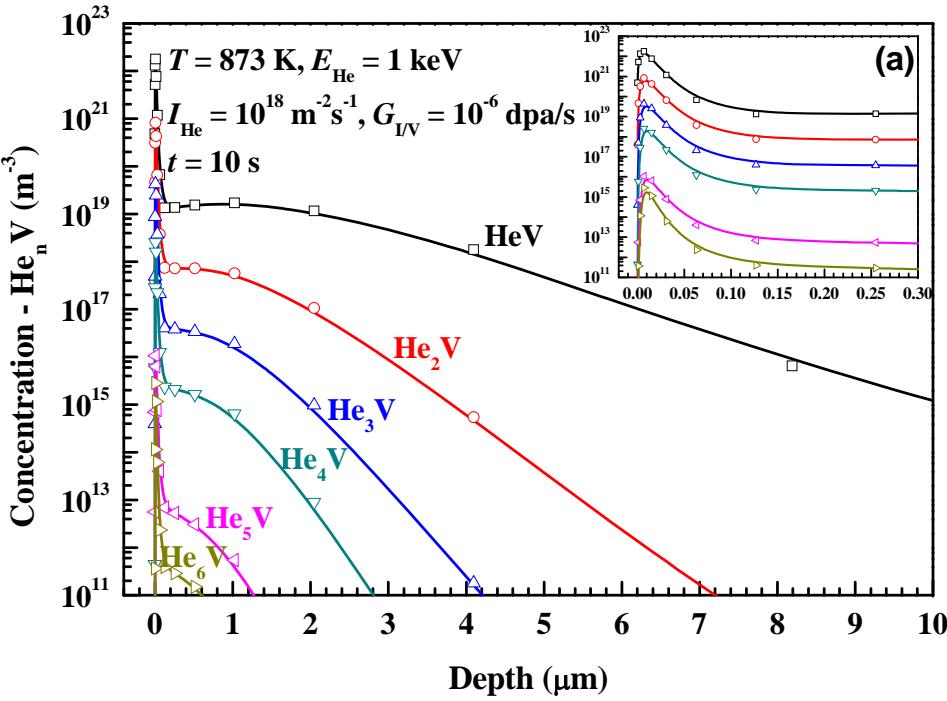
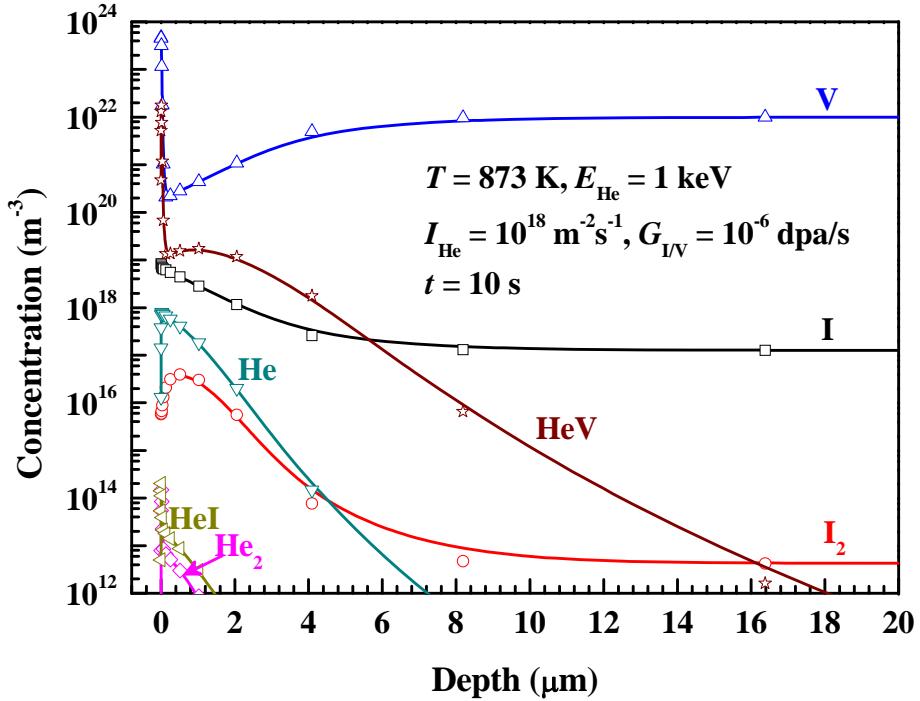
Case 1: first wall

Depth distribution of *He* in *W*



Case 1: first wall

W, 10 s



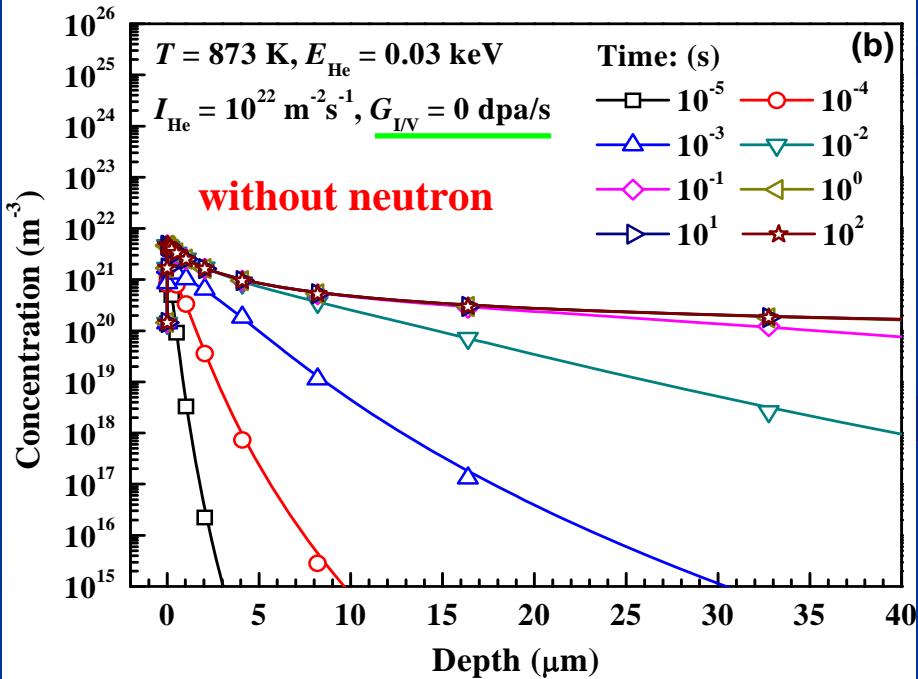
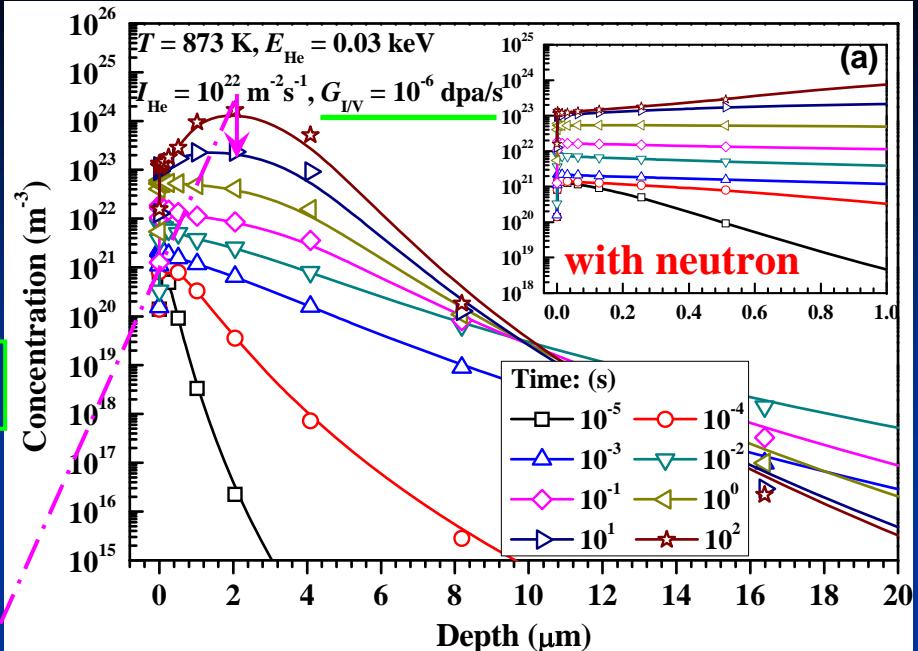
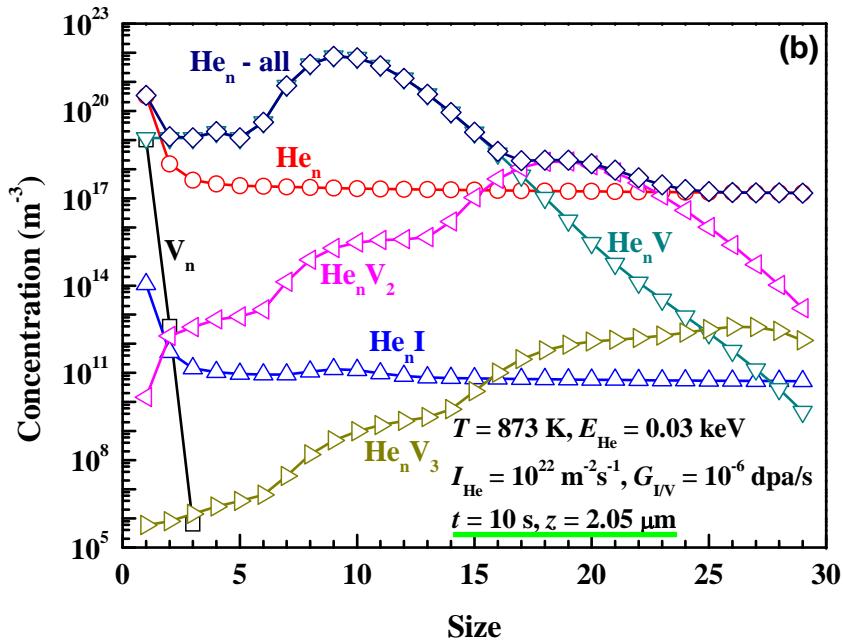
Concentrations of mobile defects & *He*-vacancy complexes along with depth

Case 2: divertor

$30\text{eV}, 10^{22} \text{m}^{-2} \text{s}^{-1}$

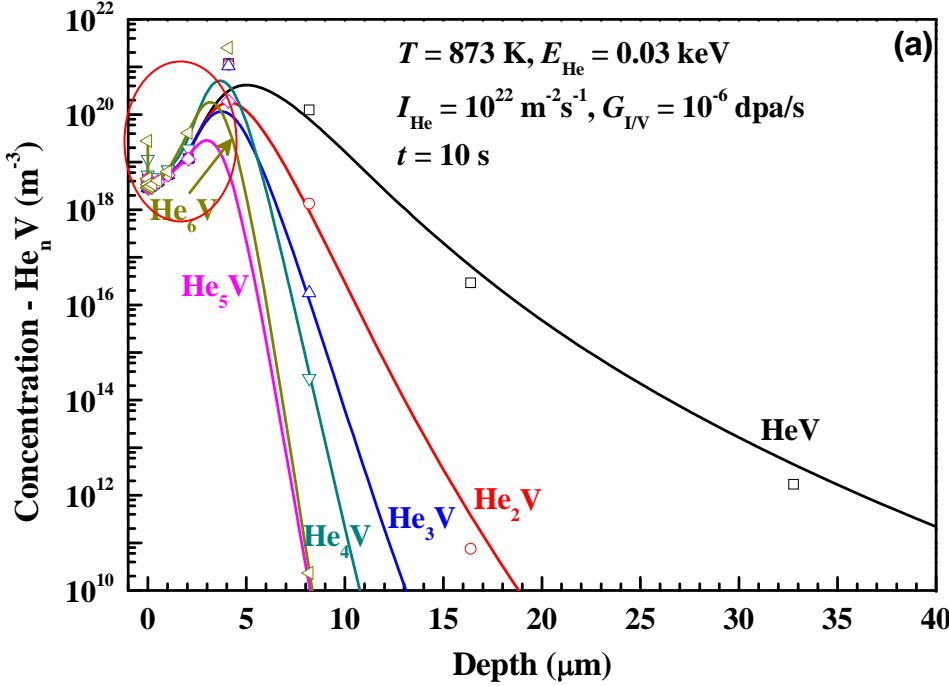
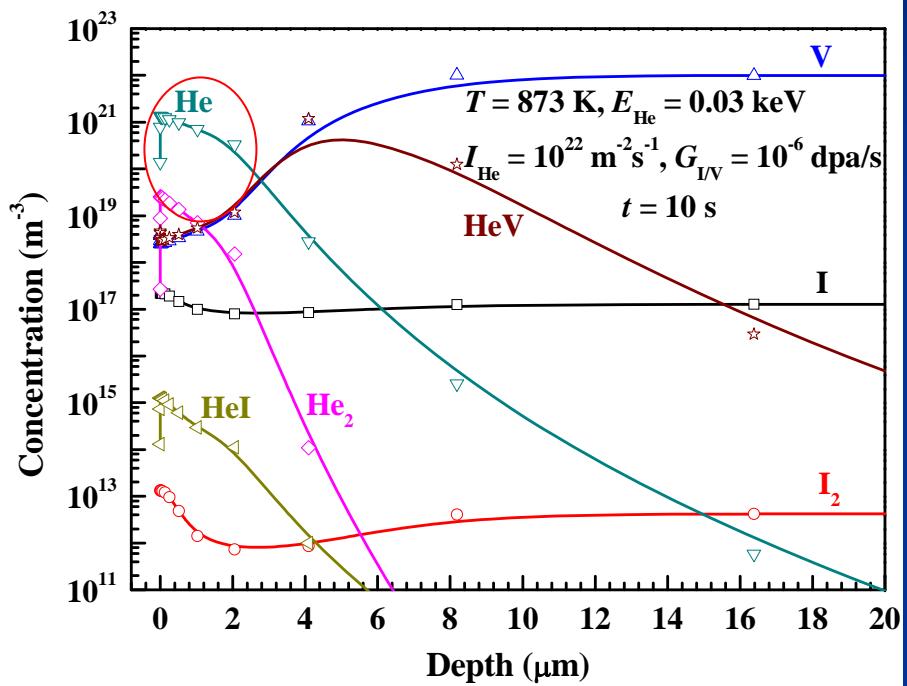
Depth distribution of He in W

Concentrations of deferent types of He with the cluster sizes



Case 2: divertor

W, 10 s



Concentrations of mobile defects & *He*-vacancy complexes along with depth

Conclusions

1. Cluster dynamics model:
 - involving different types of objects;
 - adopting up to date parameters & complex reaction processes;
 - considering the diffusion process along with depth;
 - including the synergistic effects of He and neutron irradiations.
2. The competition of the tapping and diffusion effects dominates the behaviors of *He* atoms in *W*.

The trapping effect of *He* atoms mainly comes from the reaction with vacancies and self-accumulation, leading to nearly all of the *He* concentration staying near surface.

The diffusion effect of mobile defects (like *He*) makes the distribution profile extend to the depth far from surface.
3. The trapping effect plays a dominant role for the case of *He* plasma with higher energy and lower flux while the diffusion effect plays a dominant role for the case of *He* plasma with lower energy and higher flux.

Thanks for your attention!