The understanding of H/He irradiated in W by a multi-scale approach

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Outline

• Radiation Damage
• Multi-scale Modeling
• MC for the primary radiation
• Cluster Dynamics (CD) Model
• H/He in W
• Summary
Radiation damage

• Plasma-material interactions (PMI) in nuclear devices:

  Cause the surface reconstruction of plasma-facing materials (PFMs, W) to roughness or even more complex nanostructures (mounds, fuzz, bubbles, pores and blisters) & ion (D/T/He) retention and sputtering of PFMs & degradation of structural materials.

Radiation Damage

- **Radiation damages:** Fission & Fusion
- **Structural / PFM:** Fe, Be, C, W, Mo, Alloy, …;
- **High energy particles:** Electron (MeV), Ion (D/T/He…, eV-keV), Neutron (MeV);
- **Defects and impurities:** Point defects, loops/clusters, impurities, …;
- **Expts.:** SEM/TEM/NRA/RGA/RBS/TDS/APT… (steady state detection, Spatial scale);
- **Long-term evolution of microstructures?** (Time scale).

Radiation Damage

- Dynamical evolution of defects

Long-term (ps-y), multi-scale (nm-m) and multi-micromechanisms coupling process.

Lu et al., *Nucl. Fusion* 54 (2014) 086001;
Multi-scale Modeling

• **Challenge:** How to effectively couple atomic diffusion events with displacing and continuous processes at finite temperature.

• **Sequential multi-scale modeling:** MC + DFT/MD + CD
Multi-scale Modeling

Sequential multi-scale modeling:

**MC + DFT/MD + CD**

Multi-scale Modeling of Defect Evolution

- Primary Damage
- Dynamic Mechanism
- Long-term Evolution

LAMMPS, TRIM, IM3D, VASP, LAMMPS, MD++, RT-CD, IRadMat

**IM3D & IRadMat**
Monte Carlo simulation of primary radiation damage

- Primary radiation damage: **Ballistic phase**, in the range of \(~ nm\) and the time-scale of \(~\) sub-\(ps\); two types of collision – **binary & cascade/spike** collision.

- Until now radiation damage simulation codes (like SRIM) have been limited in ability to describe 3D geometry, computational efficiency, or both.

**Advantages: MC vs MD**

- Simple and high efficiency;
- Arbitrary 1D/3D structures;
- Accounting of electronic energy loss and multiple- and plural-scattering;
- No limitations in nanostructure sizes, ion energies, or availability of empirical inter-atomic potentials.
• IM3D: Primary radiation damage under ion irradiation

A 3D Parallel MC Code for Efficient Simulation of Primary Radiation Damage

Standard SRIM database
Fast database indexing technique
MPI parallel

Arbitrarily complex 3D structures
Efficiency ~ at least 2 orders higher

As accurate as SRIM
More efficient and universal


http://theory.issp.ac.cn/IM3D, MIT
• Verification of IM3D  
  more details in Li’s poster

• IM3D vs. SRIM for bulk  

• Ion depth-distributions under ion implantation with different energies

• V depth-distribution predicted by full-cascade and Kinchin-Pease models
• **IM3D:** Arbitrarily complex targets based on CSG/FETM methods
**Comparison of IM3D and SRIM**

### Software

<table>
<thead>
<tr>
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<tr>
<td>Scattering angles</td>
<td>MAGIC approximation</td>
<td>Fast database indexing</td>
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<tr>
<td>Geometries</td>
<td>1D bulk or multi-layers</td>
<td>Arbitrarily 3D geometries</td>
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<td>Computational Efficiency</td>
<td>Serial, low</td>
<td>2-3 orders faster for serial version, MPI parallel (&gt; 80%)</td>
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<tr>
<td>Defect distributions</td>
<td>1D depth-distributions</td>
<td>3D space-distributions, spatial correlation</td>
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> 700 citations per year

**Serial:** 2-3 orders higher

**Parallel:** ~ 80%

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• IM3D: Open source/Graphical interface

http://theory.issp.ac.cn/IM3D

Fluorine
18.998
Multi-scale Modeling

Sequential multi-scale modeling:

**MC + DFT/MD + CD**

Multi-scale Modeling of Defect Evolution

- Primary Damage
- Dynamic Mechanism
- Long-term Evolution

Tools:
- LAMMPS
- TRIM
- IM3D
- VASP
- LAMMPS MD++
- RT-CD
- IRadMat

**IM3D & IRadMat**
Cluster Dynamics (CD) Model

- **CD model** based on the mean-field rate theory is commonly employed to describe defect concentration evolution in a set of diffusion-reaction type master equations, by considering the generation, diffusion, reaction and absorption processes of point defects and clusters with a possible event list and rate coefficients in materials under thermal aging or irradiation.

- **History: Theory**
  - Van’t Hoff-Arrhenius law - reaction rate coefficients (1889)
  - Transition state theory (TST) - reaction rate/barrier (1932-1978)
  - Classical rate theory - Master equations (Kramer, 1940)

• **History:** Numerical algorithms of master equations (MEs)

• **Difficulties:** accuracy (no spatial correlation), efficiency (coupled ODEs) and stability (stiff system)

• **Acceleration or coarse-graining approximate algorithms:**
  - Discrete phase-cut method
  - Fokker-Plank approximation
  - K-method & Grouping method
  - Stochastic cluster dynamics
  - Hybrid method, etc.

• **Recent developments:** Multi-species, Space-resolved, Spatial correlation, …

Cluster Dynamics (CD) Model

- **Master equations**: IRadMat

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

**MC/MD/OKMC** 1D/3D space Rate coefficients (DFT/MD/Expt.)

- **Coarse-grained methods**: \( > 10^6 \rightarrow < 10^4 \) PDEs

**Fokker-Plank**

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

**Group method**

\[
C_{i,j}(x,y) = L_{0}^{i,j} + L_{1x}^{i,j}(x - \langle x \rangle_i) + L_{1y}^{i,j}(y - \langle y \rangle_j)
\]

**SRSCD** CD + KMC

Defect production & diffusion

Production:
- Electron: $e^-$ (MeV), Frenkel-pairs point defects
- Ion: $D^+, T^+, He^+$ ... (eV ~ keV), point defects + clusters
- Neutron: n (MeV), cascade, dislocation loops, vacancy clusters

Point defects $G(1)$:
- NRT model, cascade: $G^{NRT}$; $G^{NRT} (1 - \varepsilon_r)$
- Constant and uniform rate: neutron irradiation or transmutation
- SRIM/IM3D/MARLOWE: ions

Size distribution function $G(x)$:
- MD cascade: size/space distribution
- KMC annealing defect size/space distribution: IM3D + OKMC

Diffusion: Finite difference approximation with non-uniform mesh

$$\frac{\partial^2 C^j_{\theta}}{\partial z^2} |_{\theta = 1, l_2, v, x} = \frac{2}{(1 + \delta)h} \left( \frac{C^j_{\theta} - C^j_{\theta}}{\delta h} - \frac{C^j_{\theta} - C^{j-1}_{\theta}}{h} \right)$$

### Reaction and absorption

#### Reaction event-list & Rate coefficients: DFT/MD/Expt.

Dissociative absorption:

\[ k_{V_n+\theta}^+ |_{\theta=I,I_2,He} = 4\pi r_{V_n} D_{\theta}, \]

\[ \gamma_n^- = 4\pi r_{V_{n-1}} D_V \exp\left(-E_{V_n-V}^b / k_B T\right) \]

\[ \theta + GB \rightarrow GB-\theta, \theta = I, V, H, He \ldots \]

\[ K_{GB}^\theta = S_m^\theta \left( \frac{\sqrt{S_m^\theta d}}{2} \coth \frac{\sqrt{S_m^\theta d}}{2} - 1 \right) \times \left( 1 + \frac{S_m^\theta d^2}{12} - \sqrt{S_m^\theta d} \coth \frac{\sqrt{S_m^\theta d}}{2} \right)^{-1} \]

\[ \theta + DL \rightarrow DL-\theta, \theta = I, V, H, He \ldots \]

\[ K_{DL}^\theta = \rho Z_{DL}^\theta \]


**He in W:**

\[ I, I_2, V, He, I_n, V_n, He_n, He_n I, He_m V_n, DL, GB \]

**H in W/Be:**

\[ I, I_2, V, H, I_n, HI, H_m V \big|_{m\leq 8}, DL, GB \]

\[ I + V \rightleftharpoons 0; \]
\[ I + I_n \rightleftharpoons I_{n+1}; \]
\[ I + V_n \rightarrow V_{n-1}; \]
\[ I + He_n \rightleftharpoons He_n I; \]
\[ I + He_m V_n \rightleftharpoons He_m V_{n-1}; \]
\[ I_2 + I_n \rightleftharpoons I_{n+2}; \]
\[ I_2 + V_n \rightarrow V_{n-2}; \]
\[ I_2 + He_m V_n \rightarrow He_m V_{n-2}; \]
\[ V + I_n \rightleftharpoons I_{n-1}; \]
\[ V + V_n \rightleftharpoons V_{n+1}; \]
\[ V + He_n \rightleftharpoons He_n V; \]
\[ V + He_n I \rightarrow He_n V; \]
\[ V + He_m V_n \rightleftharpoons He_m V_{n+1}; \]
\[ He + V_n \rightleftharpoons He V_n; \]
\[ He + He_n \rightleftharpoons He_{n+1}; \]
\[ He + He_n I \rightleftharpoons He_{n+1} I; \]
\[ He + He_m V_n \rightleftharpoons He_{m+1} V_n; \]
\[ \theta + D \rightarrow D\theta; \]
\[ \theta + S \rightarrow S\theta; \]

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H/He Retention under Ion Irradiation

A1. H/He retention in plasma-facing materials (PFMs)

- **Plasma-surface interaction (PSI)**: Defect accumulation, D/T/He retention, embrittlement, swelling, bubbles, etc.

- **SRIM/IM3D** (initial distributions of defects) + CD (long-term evolution)

• CD v.s. Expts.

• Depth distribution of H/He in PFMS
• Retention – H/He Fluence
• Retention – Temperature, desorption

Ning, J. Nucl. Mater. 430 (2012) 20;
• Different behaviors of H/He retention in W/Be

• The competition between capture and drift-diffusion processes & the difference in binding energies between H-H and He-He determine the retention behavior of H and He in W/Be.

Li, J. Nucl. Mater. 431 (2012) 26;
A2. Effect of grain size on the behavior of H/He retention in W

- Larger He bubbles intend to accumulate at interfaces/GBs, with less He retention and damages left in grain interior.

- Higher H retention occurs in nanocrystalline W comparing to coarse-grained W


Zhao, Nucl. Fusion 57 (2017) 086020.
- Effect of grain size on the behavior of H/He retention in W

- H/He retention increases dramatically with decreasing grain size, due to the enhancement of H/He trapped in GBs.

- For W based PFM s coarse-grained crystals should be selected in practice.

A3. H/He retention & radiation damage under practical conditions

- Effects of Pre-irradiation & ion energy/flux/fluence
- Synergistic irradiation of ions and neutron: $G_{\text{I/V}} = 10^{-6} \text{ dpa/s}$
- First wall & Divertor


• **Synergistic radiation effects of He ions and neutrons**

• The defects produced by neutron irradiation prevent He diffusion into bulk, leading to He retention in near surface area and He total retention increase

• **First wall** – surface retention and damage

**Divertor** – bulk retention and damage

\[ G_{\text{I/V}} = 10^{-6} \text{ dpa/s} \]

Defect Evolution under neutron Irradiation

- Defect production by neutron irradiation in CD
- Point defects \( G(1) \): \( G_{I/V} = 10^{-6} \) dpa/s
- Size distribution function \( G(x) \): MD, MC - OKMC (IM3D + MMonCa)


Zhao, *to be published.*
A4. Radiation tolerance in nano-crystalline (NC) materials

- Anti-irradiation of NC materials: Under what conditions?

Han et al., Acta. Mater. 60 (2012) 6341.

I-V recombination & I emission


• **Effect of diffusion bias on radiation tolerance of Fe/W with different grain sizes**

• **Diffusion bias**: the ratio of mean diffusion distance per unit time between SIAs and vacancies.

\[
B_D \equiv -\log\left(\sqrt{D_V/D_1}\right)
\]

- Steady-state chemical rate theory

\[
C_V = \frac{1}{B_V}\left(\sqrt{A_V^2d^{-4} + 2B_VK - A_Vd^{-2}}\right)
\]

\[
A_V = 57.6D_V; \quad B_V = \frac{8\pi}{a^2}D_V\left(\frac{D_V}{D_1}\right)\left(1 + \frac{D_1}{D_V}\right)
\]

**Non-steady states (ns - ∞): Diffusion bias?**

**Steady state (t = ∞)**

No effect of diffusion bias
From non-steady states to the steady state

\[ C_V = \frac{1}{B_V} \left( \sqrt{A_V d^{-4} + 2B_V K} - A_V d^{-2} \right) \]

\[ C_V / C_{V_0} \]

\[ E_{V_m} = 0.67 \text{ eV} \]

\[ E_{V_m} = 1.66 \text{ eV} \]

Zhao & Wei, to be published.
Summary-I

- Well established software for radiation defect behavior

- Inducing simple mathematic treatments

Sequential multi-scale modeling:

MC + DFT/MD + CD
Summary-II

Employ the sequential multi-scale modeling approach ($\text{MC+DFT/MD+CD}$) to study the dynamical behaviors of defects from atomic scale to mesoscale and from $ps$ to years.

• H/He retention under ion irradiation
  - Behaviors of H/He retention in poly-crystalline and nano-crystalline W/Be-based PFM s are revealed under practical irradiation conditions.

• Defect accumulation under neutron irradiation
  - Diffusion bias suppresses radiation resistance in nano-crystalline materials.
Thanks for your attention!