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

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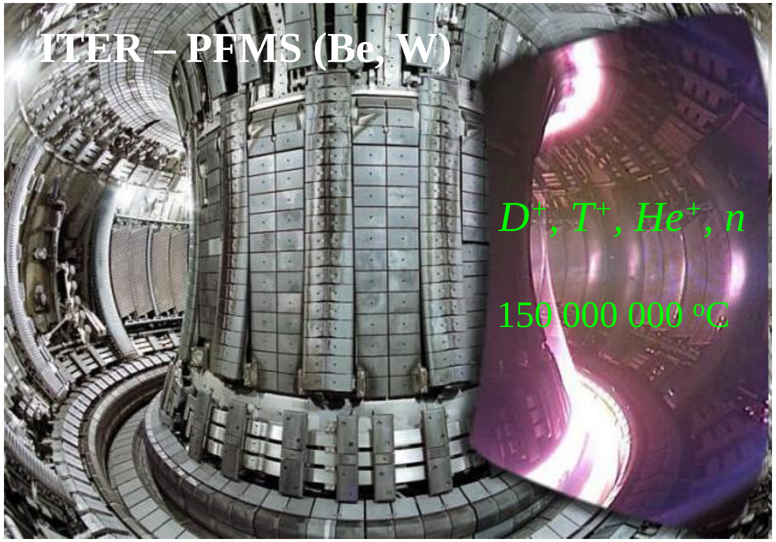
Outline

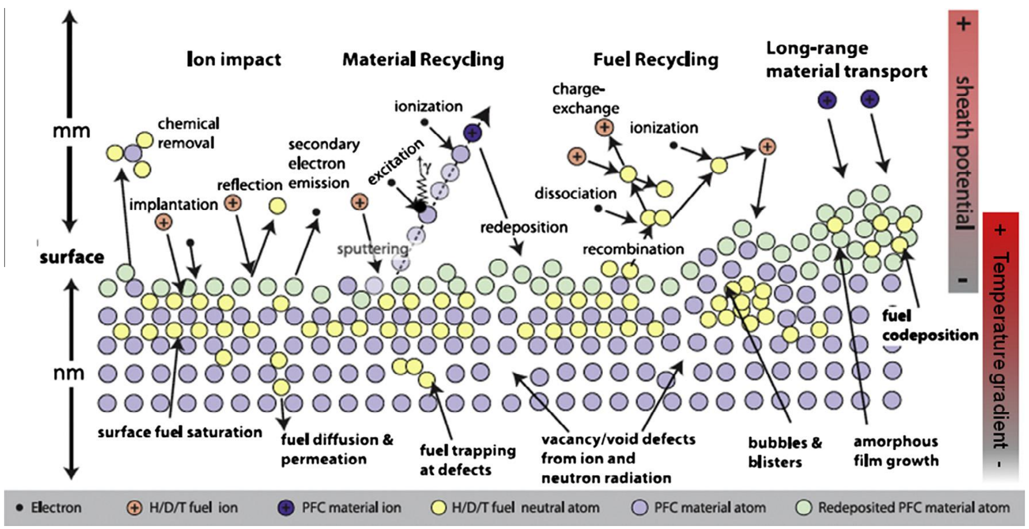
- Radiation Damage
- Multi-scale Modeling
- MC for the primary radiation
- Cluster Dynamics (CD) Model
- H/He in W
- Summary

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.

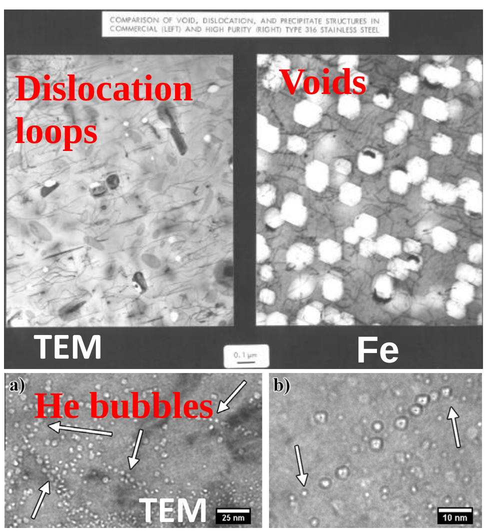


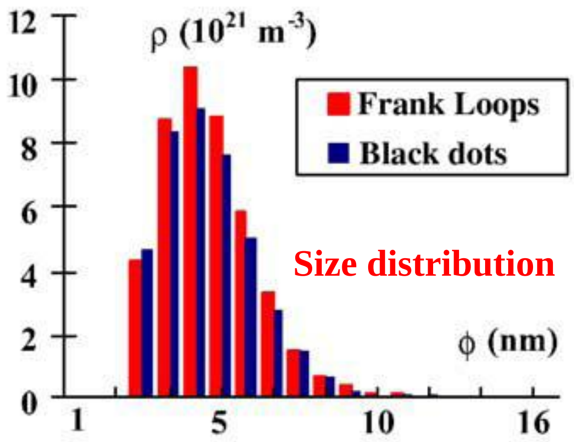


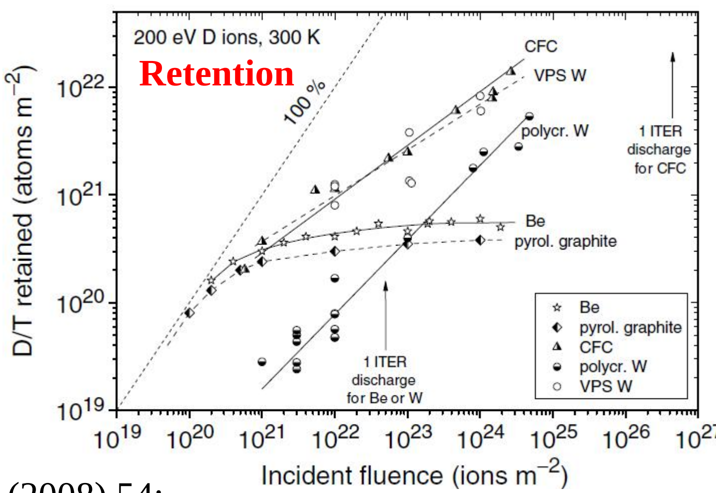
B.D. Wirth et al., *J. Nucl. Mater.* 463 (2015) 30.

Radiation Damage

- **Radiation damages:** Fission & Fusion
- **Structural / PFMs:** 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).





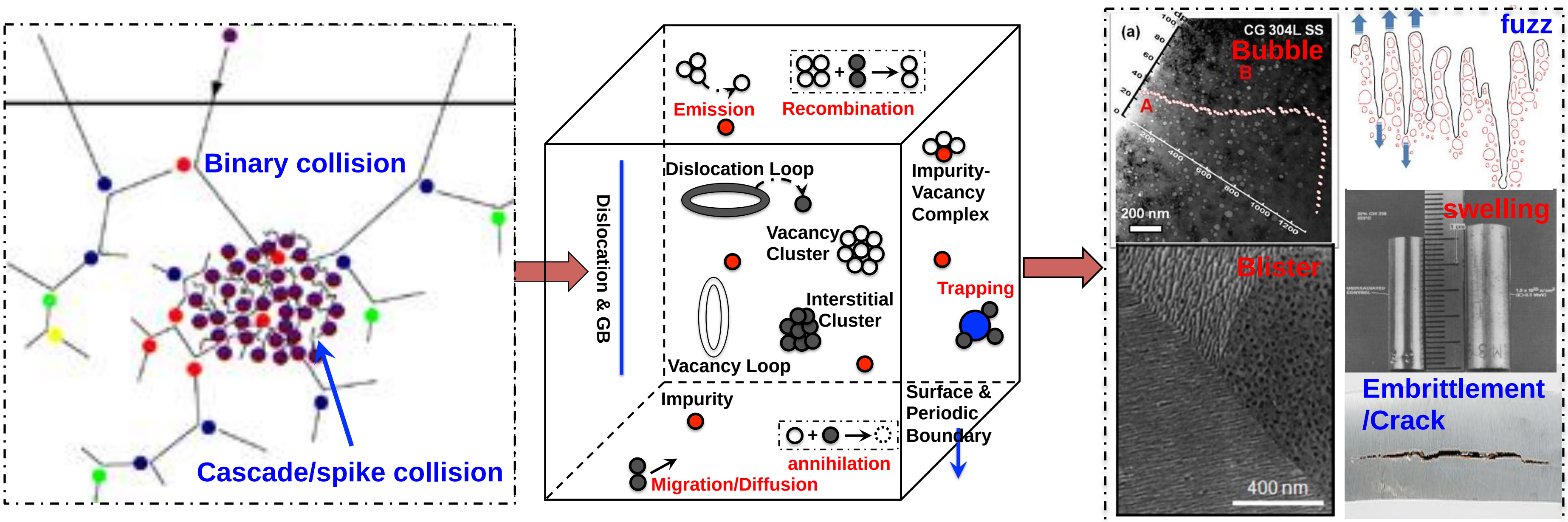


Samaras & Victoria, *Mater. Today*, 11 (2008) 54;
Li, et al., *J. Nucl. Mater.* 445 (2014) 165.

Radiation Damage

- **Dynamical evolution of defects**

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

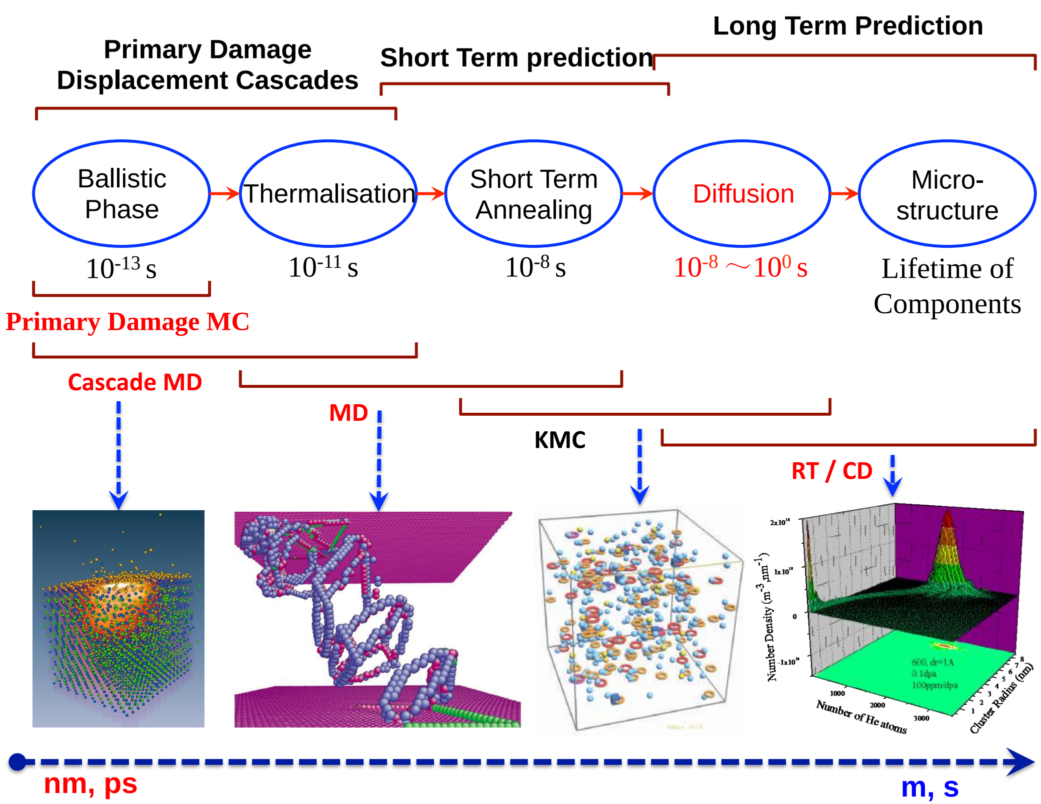


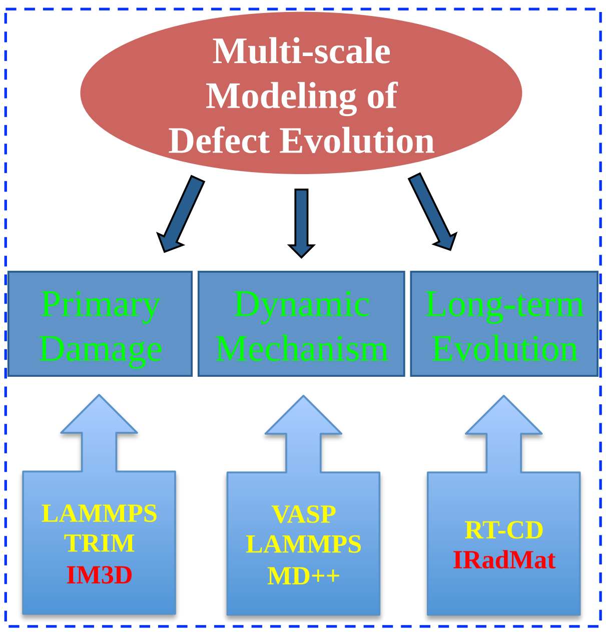
Defect production | **Defect evolution** | **Macroscopic damage**

Yip & Short, *Nature Mater.* 12 (2013) 774; Lu et al., *Nucl. Fusion* 54 (2014) 086001; Samaras & Victoria. *Mater. Today*, 11 (2008) 54; Nordlund, et al., *J. Phys. D: Appl. Phys.* 47 (2014) 224018.

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**



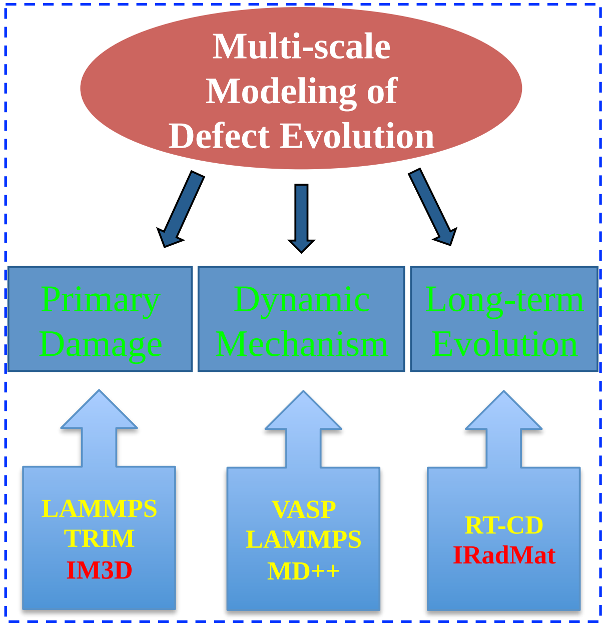


IM3D & IRadMat

Multi-scale Modeling

Sequential multi-scale modeling:

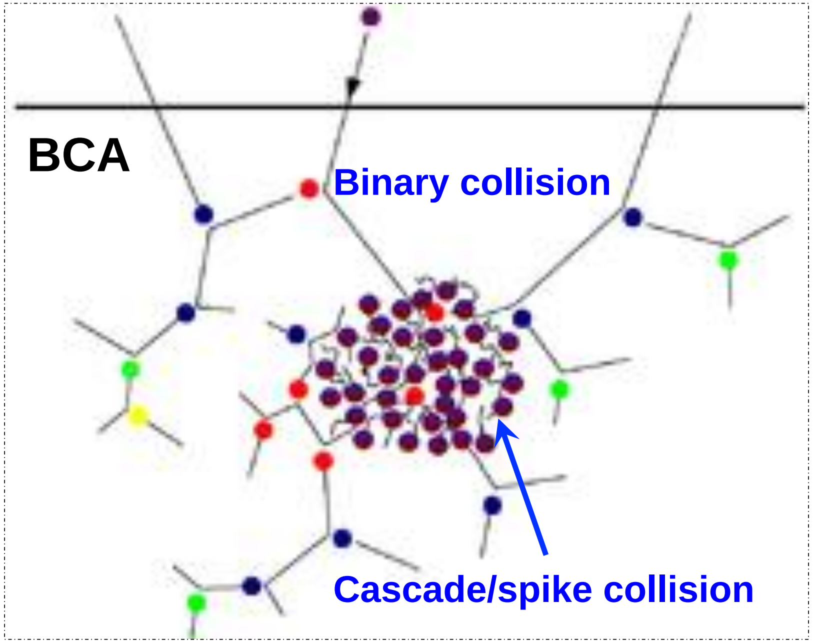
MC + DFT/MD + CD



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.

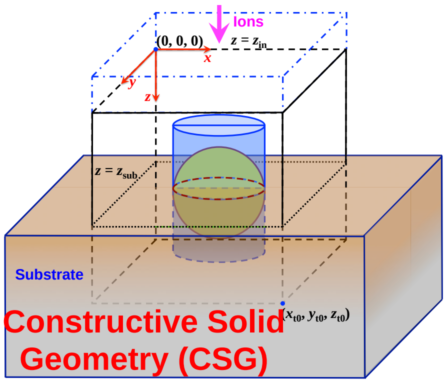


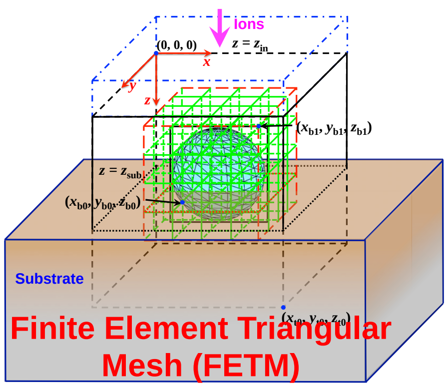
Advantages: MC vs MD

- 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





Arbitrarily complex 3D structures

+

Standard SRIM database

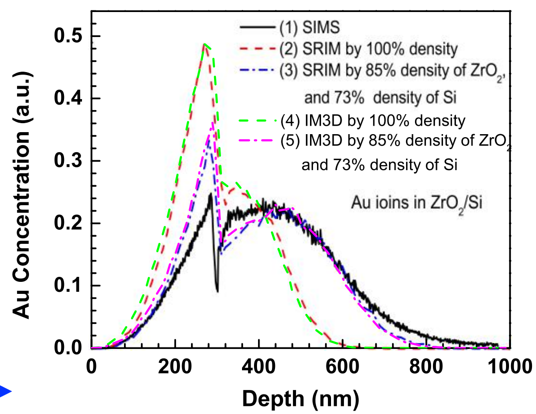
Fast database indexing technique

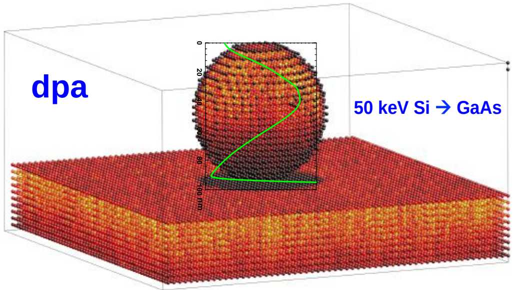
MPI parallel

→

C & MPI

Efficiency ~ at least 2 orders higher





As accurate as SRIM

More efficient and universal

Li , *Sci. Rep.* 5 (2015) 18130.

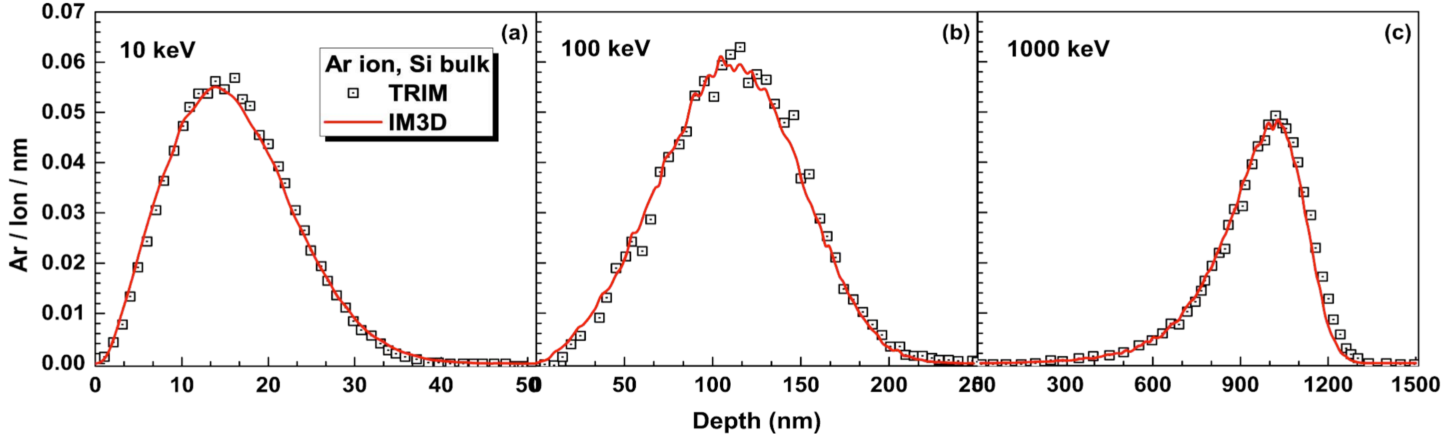
http://theory.issp.ac.cn/IM3D, MIT

- **Verification of IM3D** more details in Li's poster

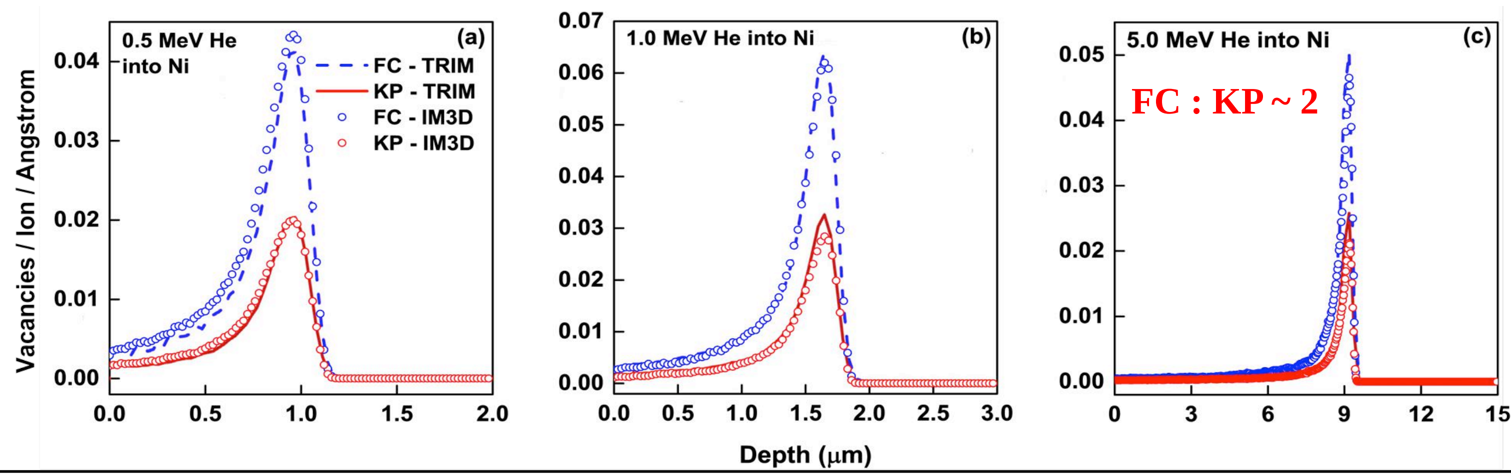
- **IM3D vs. SRIM for bulk**

Borschel et al., *Nucl. Inst. Meth. Phys. Res. B* 269 (2011) 2133.
Stoller et al., *Nucl. Inst. Meth. Phys. Res. B* 310 (2013) 75.

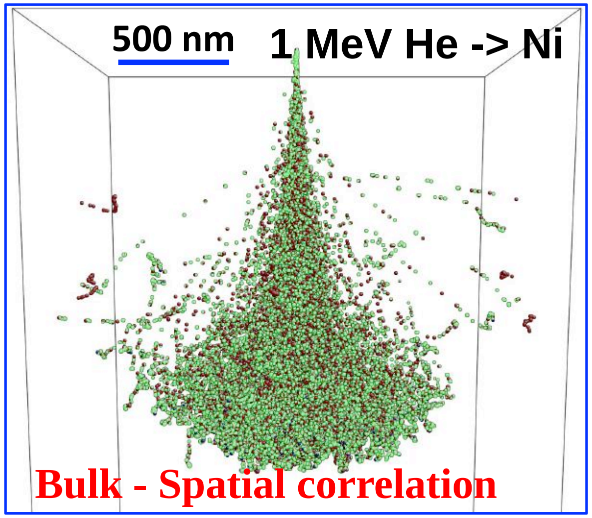
- Ion depth-distributions under ion implantation with different energies

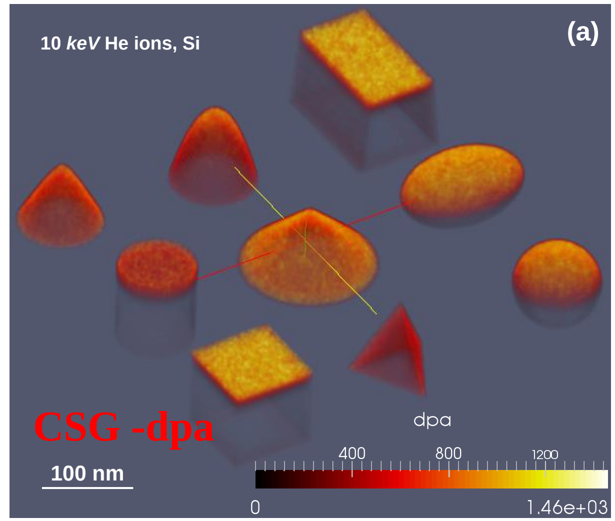


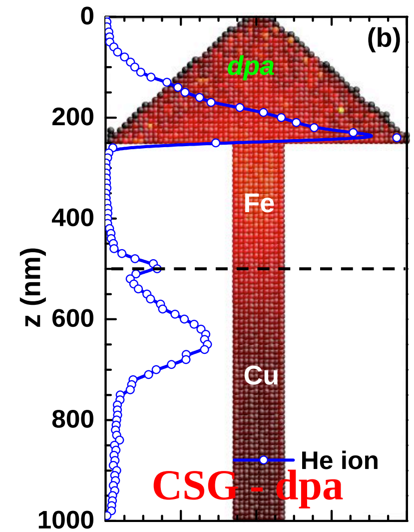
- V depth-distribution predicted by full-cascade and Kinchin-Pease models

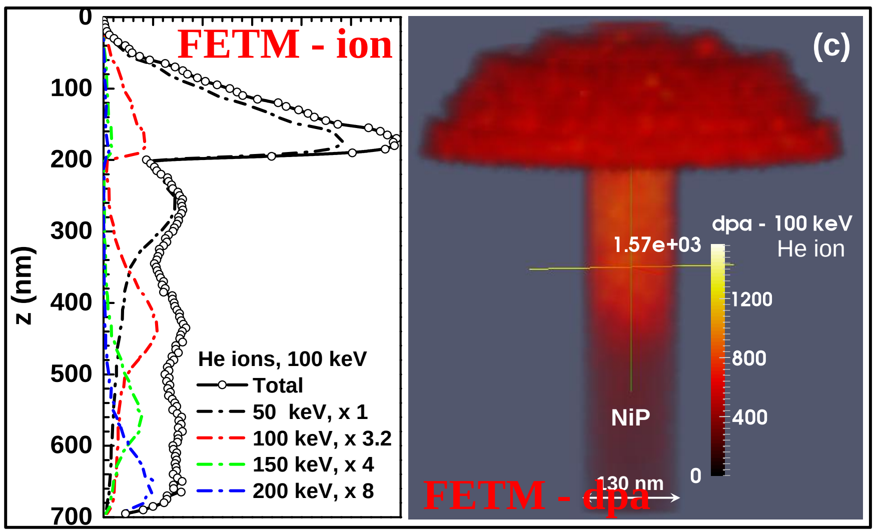


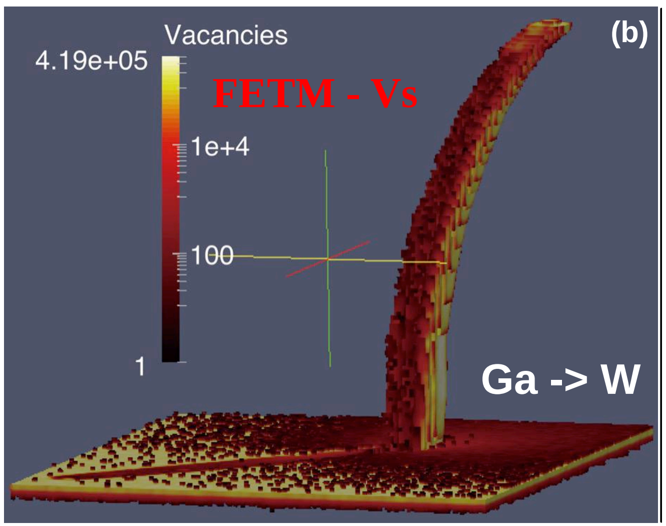
• IM3D: Arbitrarily complex targets based on CSG/FETM methods





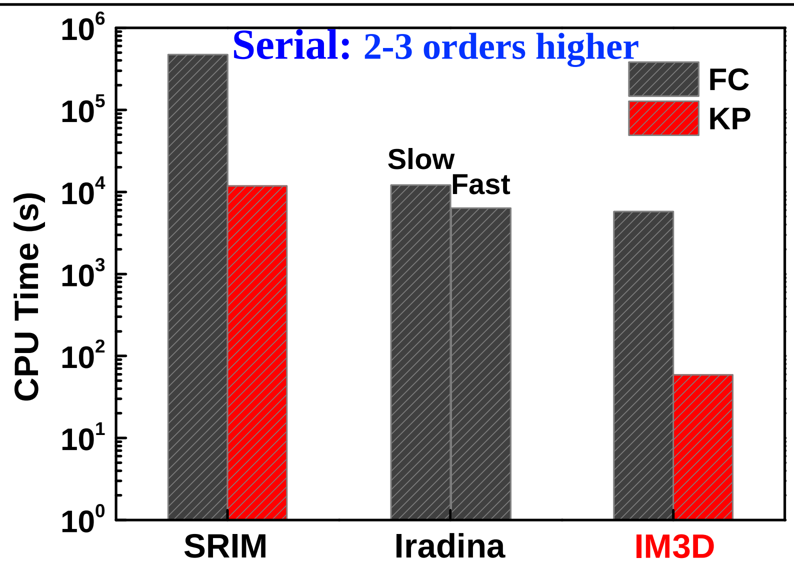


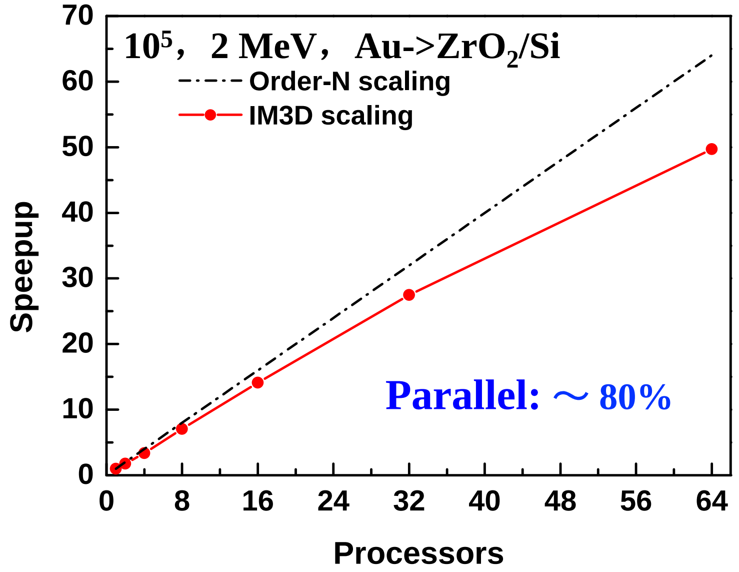




• Comparison of IM3D and SRIM

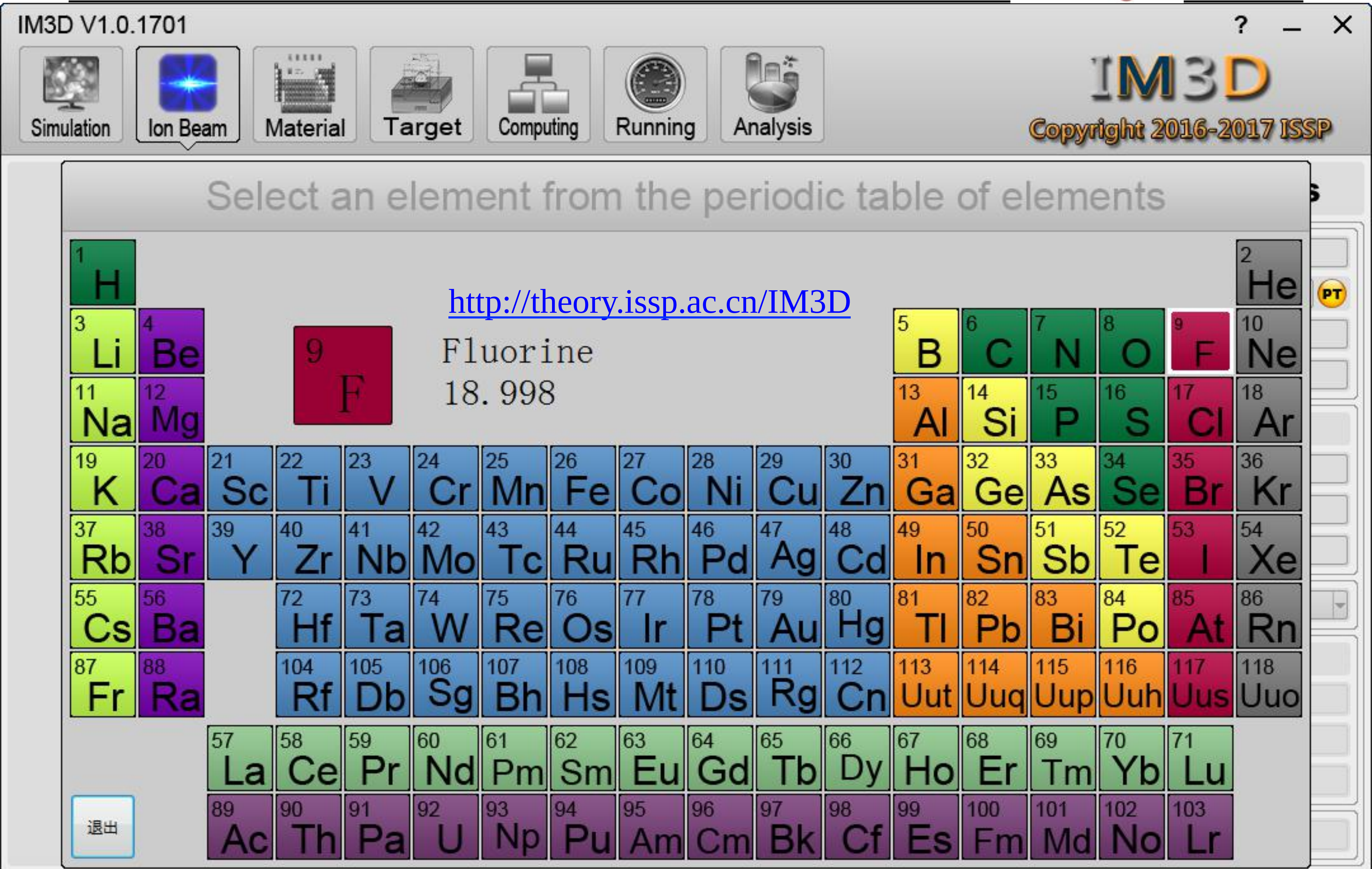
Li, Sci. Rep. 5 (2015) 18130.





Software	SRIM http://www.srim.org	IM3D http://theory.issp.ac.cn/IM3D
Scattering angles	MAGIC approximation	Fast database indexing
Geometries	1D bulk or multi-layers	Arbitrarily 3D geometries
Computational Efficiency	Serial, low	2-3 orders faster for serial version, MPI parallel (> 80%)
Defect distributions	1D depth-distributions	3D space-distributions, spatial correlation
	> 700 citations per year	More efficient and general

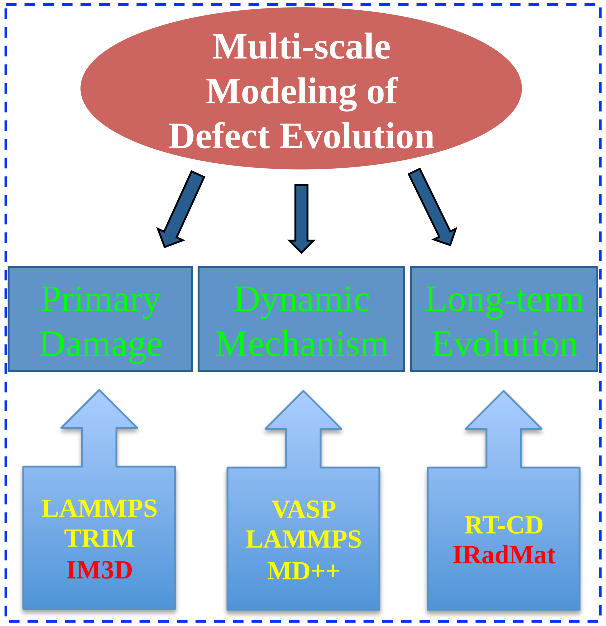
- IM3D: Open source/Graphical interface



Multi-scale Modeling

Sequential multi-scale modeling:

MC + DFT/MD + CD



IM3D & IRadMat

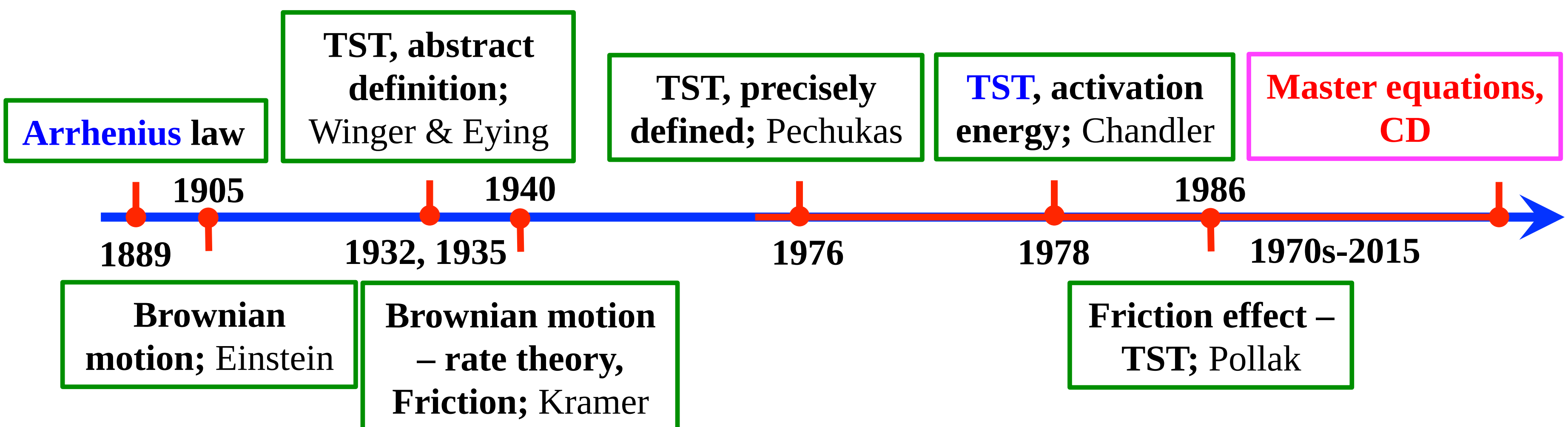
Cluster Dynamics (CD) Model

- **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

Pollak & Talkner, *Chaos* 15 (2005) 026116.

  - 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)



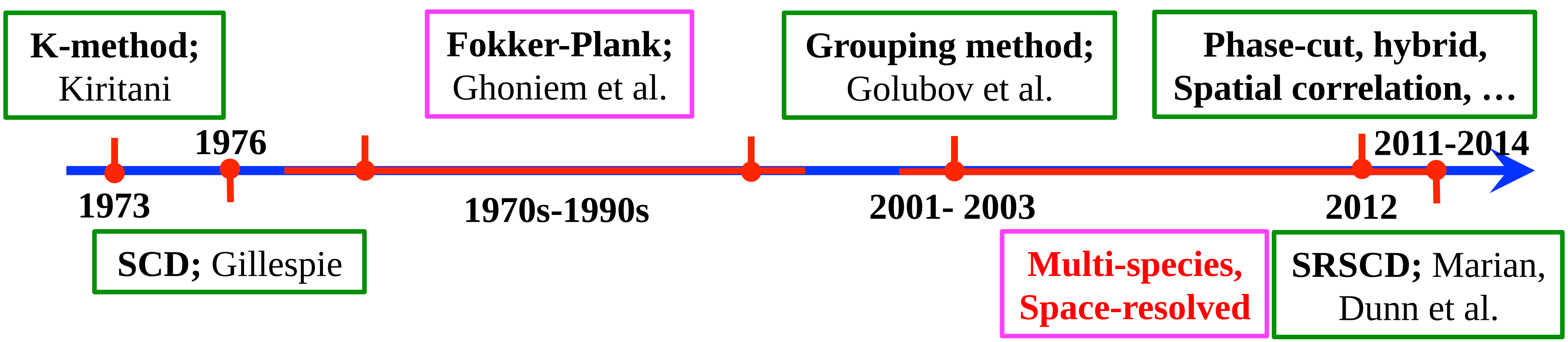
- **History:** Numerical algorithms of mater equations (MEs)

- **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.

Kiritani, *J. Phys. Soc. Japan* 35 (1973) 95;
Gillespie, *J. Comput. Phys.* 2 (1976) 403;
Ghoniem et al., *J. Nucl. Mater.* 92 (1980) 121;
Golubov et al., *Philos. Mag. A* 81 (2001) 643;
Marian & Bulatov, *J. Nucl. Mater.* 415 (2011) 84;
Gherardi et al., *Comput. Phys. Commun.* 183 (2012) 1966;
Xu et al., *Appl. Phys. Lett.* 102 (2013) 011904;
Ortiz et al., *Phys. Rev. B* 80 (2009) 134109;
Dunn et al., *J. Nucl. Mater.* 443 (2013) 128.

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



Cluster Dynamics (CD) Model

- **Master equations:** IRadMat

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

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

Primary Damage & DFT/MD/Exp. Paras → Rate Theory CG Methods → Space/Time/Size-Distribution of Defects

- **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

$$C_{i,j}(x,y) = L_0^{i,j} + L_{1x}^{i,j}\left(x - \langle x \rangle_i\right) + L_{1y}^{i,j}\left(y - \langle y \rangle_j\right)$$

SRSCD **CD + KMC**

Li, *Commu. Comput. Phys.* 11 (2012) 1547; Golubov et al., *Philos. Mag. A* 81 (2001) 643; Marian & Bulatov, *J. Nucl. Mater.* 415 (2011) 84.

- **Defect production & diffusion**

- **Production:** Marian et al., *J. Nucl. Mater.* 462 (2015) 409.
  - 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}; $G^{NRT}\left(1-\varepsilon_r\right)$
  - 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

$$\frac{\partial^2 C_\theta^j}{\partial z^2}\Big|_{\theta=I,I_2,V,X} = \frac{2}{(1+\delta)h}\left(\frac{C_\theta^{j+1}-C_\theta^j}{\delta h}-\frac{C_\theta^j-C_\theta^{j-1}}{h}\right)$$

Li, *Commu. Comput. Phys.* 11 (2012) 1547.

• Reaction and absorption

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

$$k^{+}_{V_n+\theta}\big|_{\theta=I,I_2,He}=4\pi r_{V_n}D_\theta,$$

$$\gamma_n^{-}=4\pi r_{V_{n-1}}D_V\exp\left(-E^b_{V_n-V}\Big/k_BT\right)$$

$\theta+GB\rightarrow GB\text{-}\theta,\ \theta\ =\ I,\ V,\ H,\ He\ ...$

$$K^{\theta}_{GB}=S^{\theta}_{m}\left(\frac{\sqrt{S^{\theta}_{m}}d}{2}\coth\frac{\sqrt{S^{\theta}_{m}}d}{2}-1\right)\times\left(1+\frac{S^{\theta}_{m}d^2}{12}-\frac{\sqrt{S^{\theta}_{m}}d}{2}\coth\frac{\sqrt{S^{\theta}_{m}}d}{2}\right)^{-1}$$

$\theta+DL\rightarrow DL\text{-}\theta,\ \theta\ =\ I,\ V,\ H,\ He\ ...$

$$K^{\theta}_{DL}=\rho Z^{\theta}_{DL}$$

Bullough et al., *J. Nucl. Mater.* 90 (1980) 1.

Li, *Commu. Comput. Phys.* 11 (2012) 1547;
Ning, *Inter. J. Modern Phys. C* 23 (2012) 1250042;
Hu, *RSC Adv*. 5 (2015) 65750.

He in W:

I, I_2, V, He, I_n, V_n, He_n, He_nI, He_mV_n, DL, GB

$$\begin{aligned}
&I+V\rightleftharpoons 0;\\
&I+I_n\rightleftharpoons I_{n+1};\\
&I+V_n\rightarrow V_{n-1};\\
&I+He_n\rightleftharpoons He_nI;\\
&I+He_mV_n\rightleftharpoons He_mV_{n-1};\\
&I_2+I_n\rightleftharpoons I_{n+2};\\
&I_2+V_n\rightarrow V_{n-2};\\
&I_2+He_mV_n\rightarrow He_mV_{n-2};\\
&V+I_n\rightleftharpoons I_{n-1};\\
&V+V_n\rightleftharpoons V_{n+1};\\
&V+He_n\rightleftharpoons He_nV;\\
&V+He_nI\rightarrow He_n;\\
&V+He_mV_n\rightleftharpoons He_mV_{n+1};\\
&He+V_n\rightleftharpoons HeV_n;\\
&He+He_n\rightleftharpoons He_{n+1};\\
&He+He_nI\rightleftharpoons He_{n+1}I;\\
&He+He_mV_n\rightleftharpoons He_{m+1}V_n;\\
&\theta+D\rightarrow D\theta;\\
&\theta+S\rightarrow S\theta;
\end{aligned}$$

H in W/Be:

I, I_2, V, H, I_n, HI, $H_mV\big|_{m\le8}$, DL, GB

$$\begin{aligned}
&I+V\rightleftharpoons 0;\\
&I+I_n\rightleftharpoons I_{n+1};\\
&I+H\rightleftharpoons HI;\\
&I+H_mV\rightarrow mH;\\
&I_2+I_n\rightleftharpoons I_{n+2};\\
&I_2+V\rightarrow I;\\
&V+I_n\rightleftharpoons I_{n-1};\\
&V+H\rightleftharpoons HV;\\
&V+HI\rightarrow H;\\
&H+H_mV\rightleftharpoons H_{m+1}V;\\
&I+L\rightarrow LI;\\
&I_2+L\rightarrow LI_2;\\
&V+L\rightarrow LV;\\
&H+L\rightarrow LH;
\end{aligned}$$

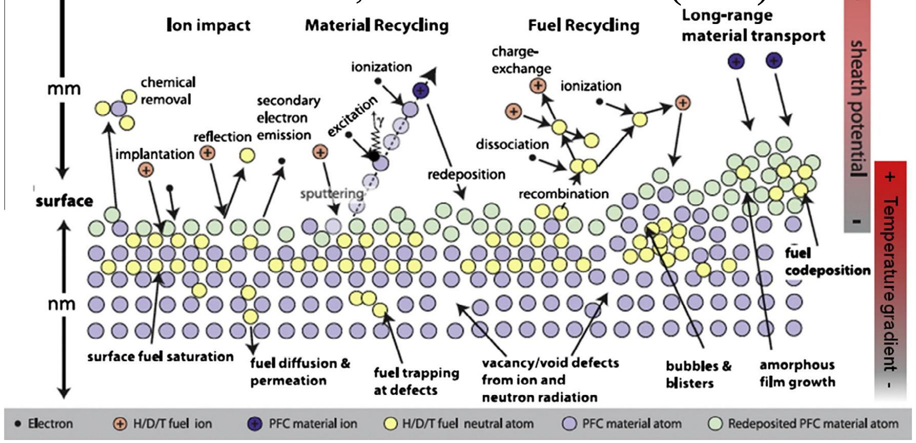
H/He Retention under Ion Irradiation

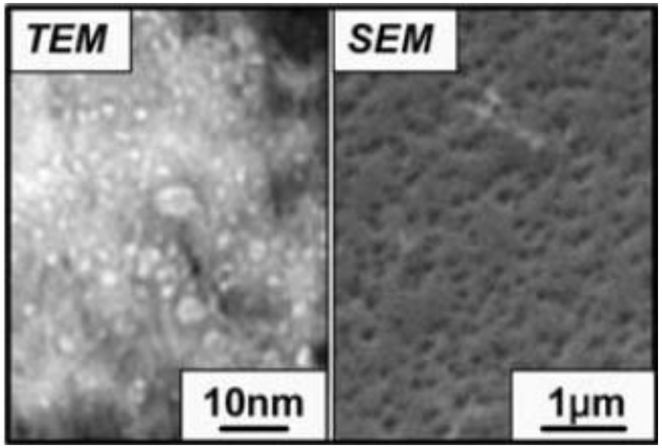
A1. H/He retention in plasma-facing materials (PFMs)

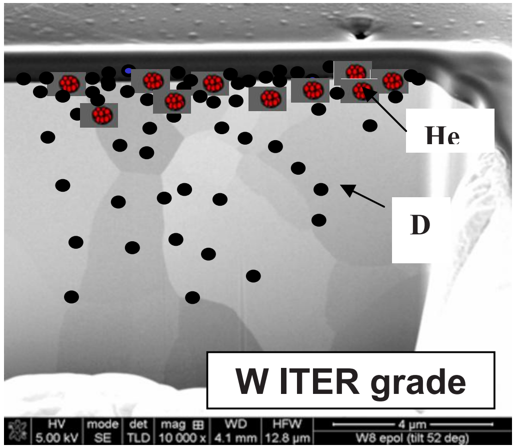
- **Plasma-surface interaction (PSI) :** Defect accumulation, D/T/He retention, embrittlement, swelling, bubbles, etc.

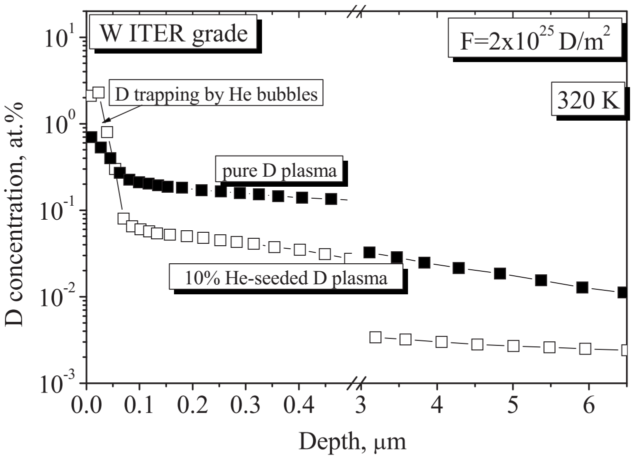
- SRIM/IM3D (initial distributions of defects) + CD (long-term evolution)

Wirth et al., *J. Nucl. Mater.* 463 (2015) 30.





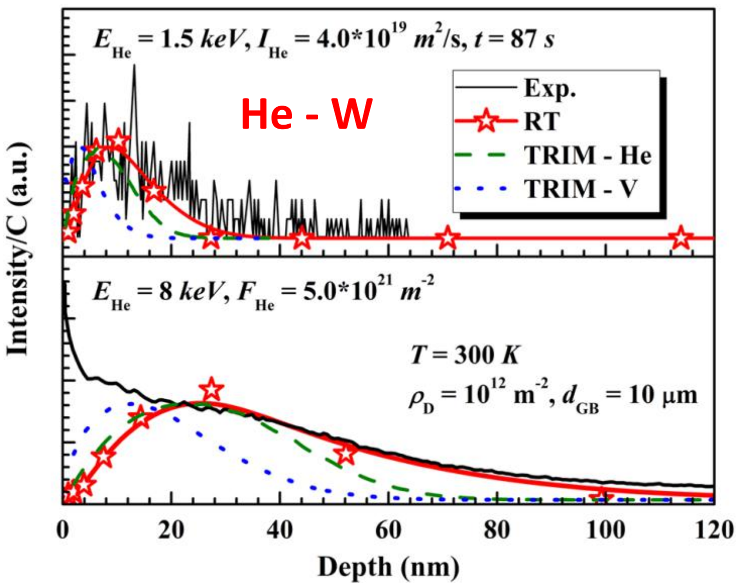


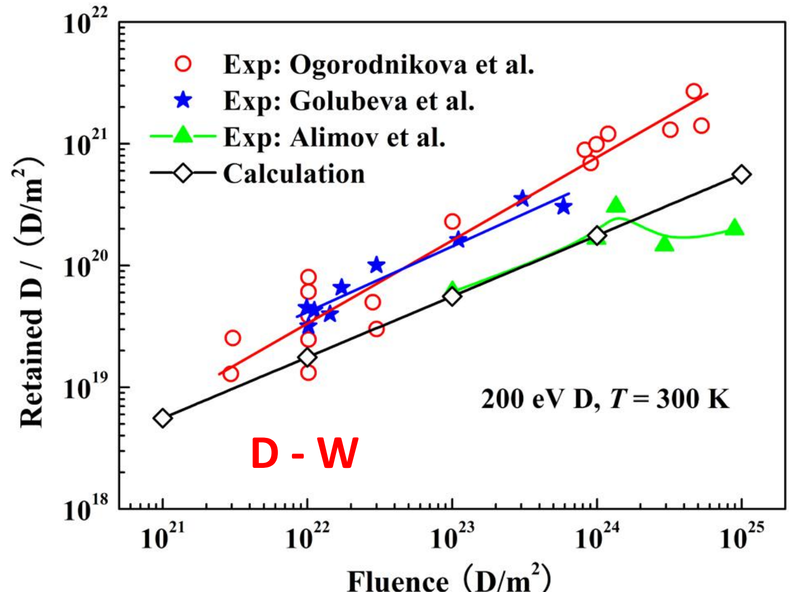


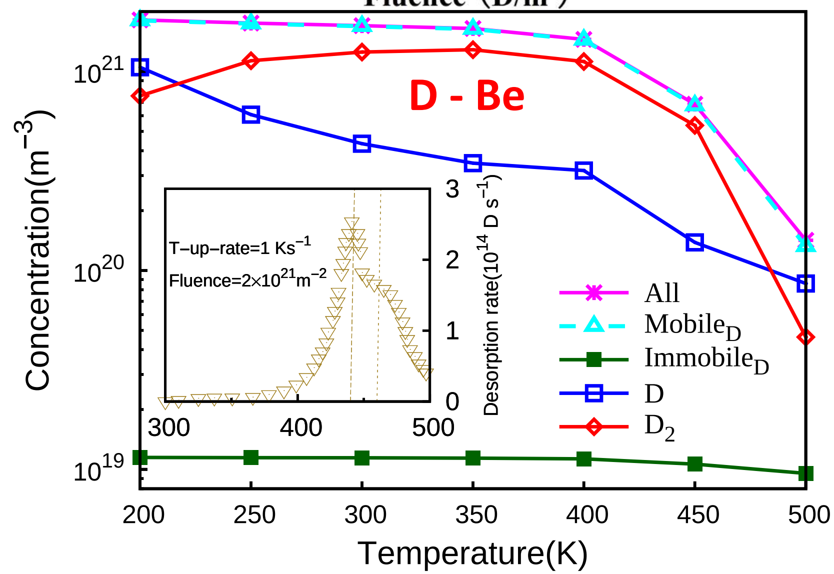
Ogorodnikova et al., *J. Appl. Phys.* 109 (2011) 013309; Tokitani et al., *J. Nucl. Mater.* 337–339 (2005) 937.

• CD v.s. Expts.

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





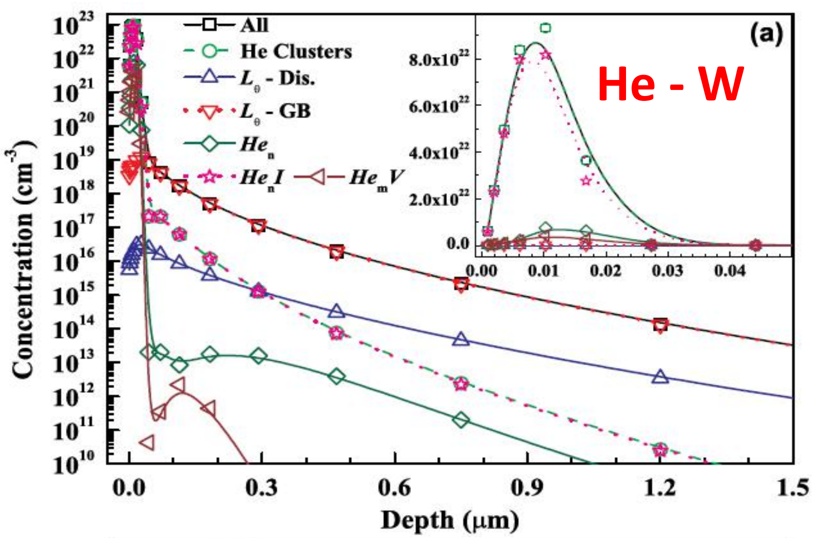


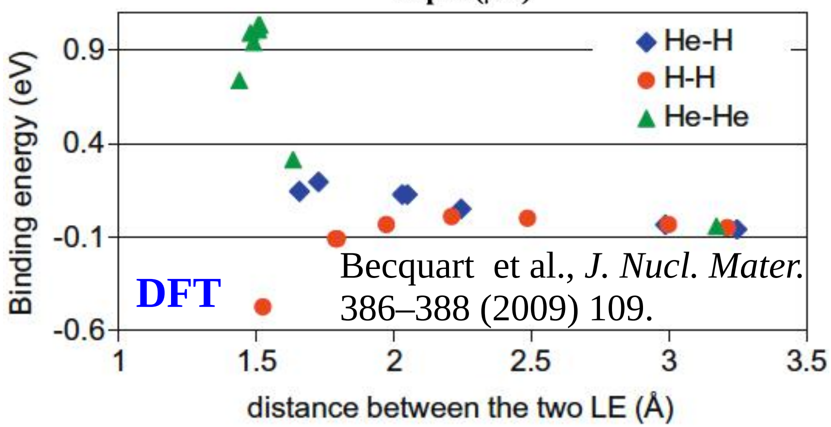
Li, *Commu. Comput. Phys.* 11 (2012) 1547;
Ning, *J. Nucl. Mater.* 430 (2012) 20;
Hu, *RSC Adv.* 5 (2015) 65750.

• Different behaviors of H/He retention in W/Be

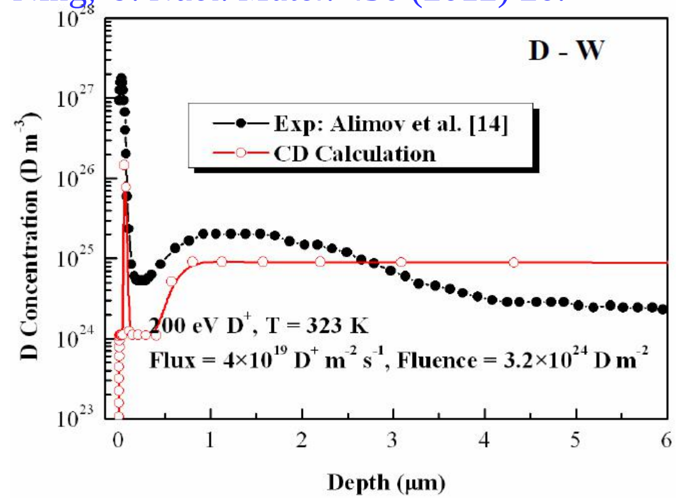
- The competition between capture and drift-diffusion processes & the difference in binding energies between H-H and He-He determine the retention behavior of H and He in W/Be.

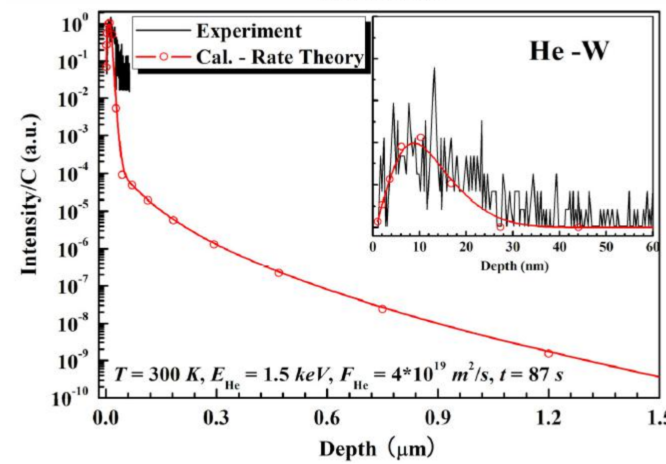
Li, *J. Nucl. Mater.* 431 (2012) 26;
Ning, *J. Nucl. Mater.* 430 (2012) 20.





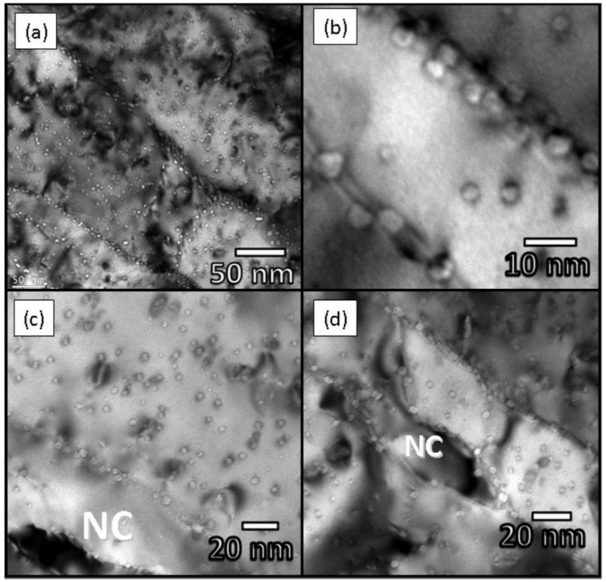
Becquart et al., *J. Nucl. Mater.* 386–388 (2009) 109.





A2. Effect of grain size on the behavior of H/He retention in W

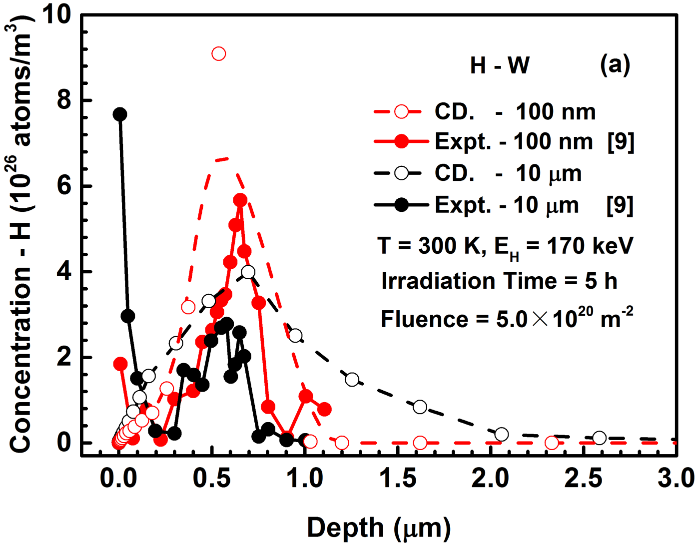
- Larger He bubbles intend to accumulate at interfaces/GBs, with less He retention and damages left in grain interior.
- Higher H retention occurs in nanocrystaline W comparing to coarse-grained W

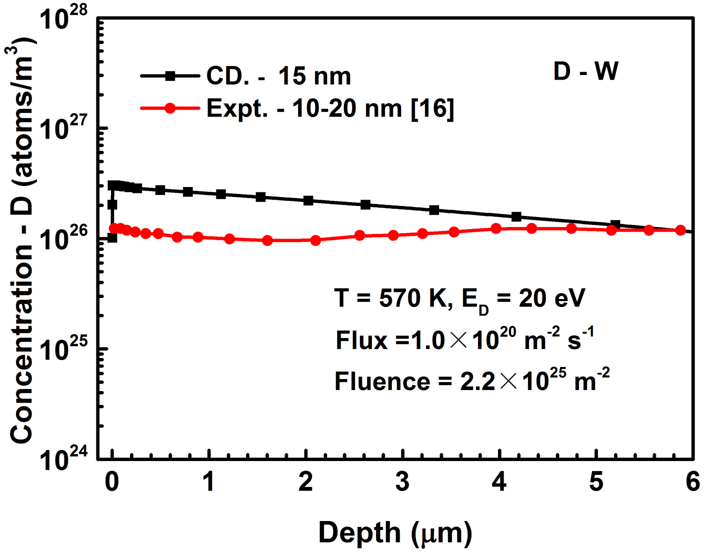


El-Atwani et al., *Sci. Rep.* 4 (2014) 4716.

González et al., *Nucl. Fusion* 55 (2015) 113009.

Zhao, *Nucl. Fusion* 57 (2017) 086020.

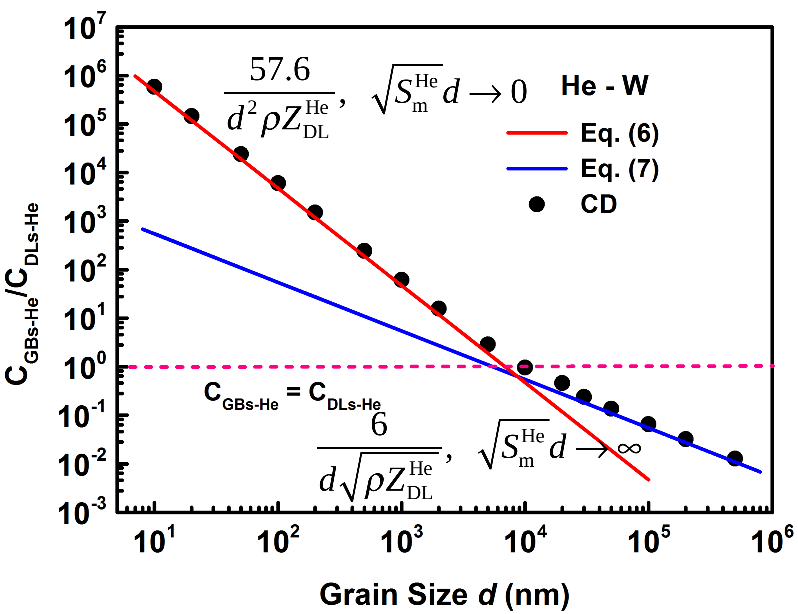


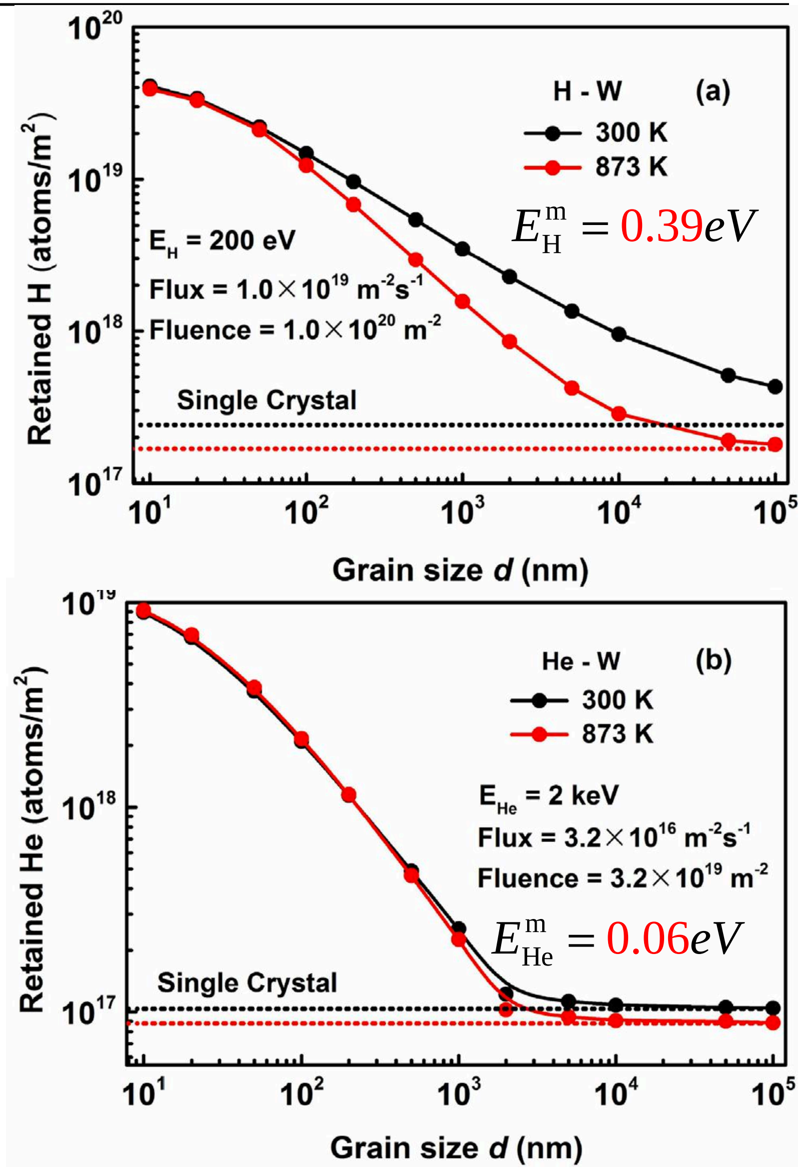


• Effect of grain size on the behavior of H/He retention in W

- H/He retention increases dramatically with decreasing grain size, due to the enhancement of H/He trapped in GBs.
- For W based PFMs coarse-grained crystals should be selected in practice.

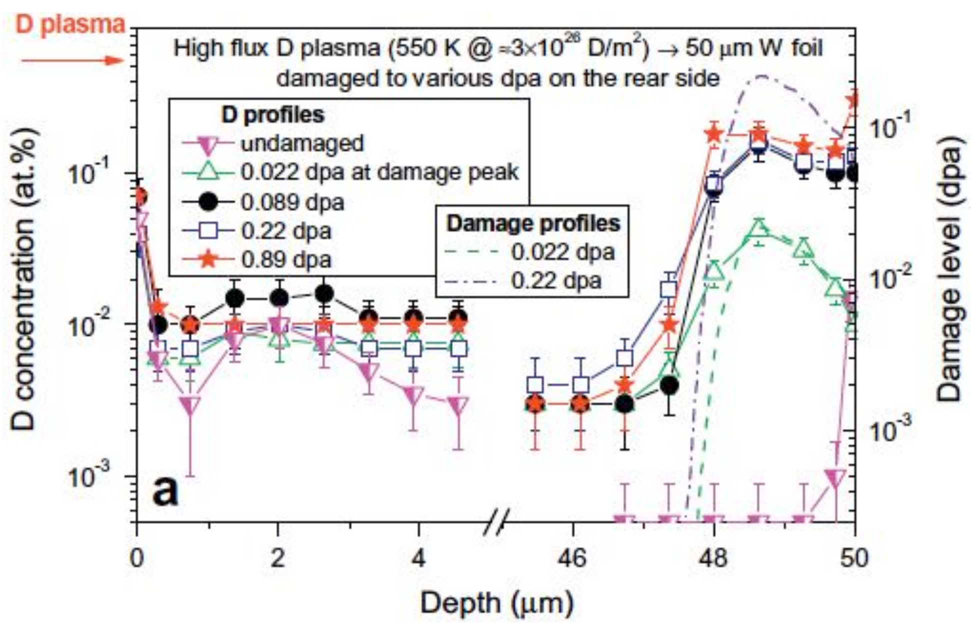
Zhao, *Nucl. Fusion* 57 (2017) 086020.



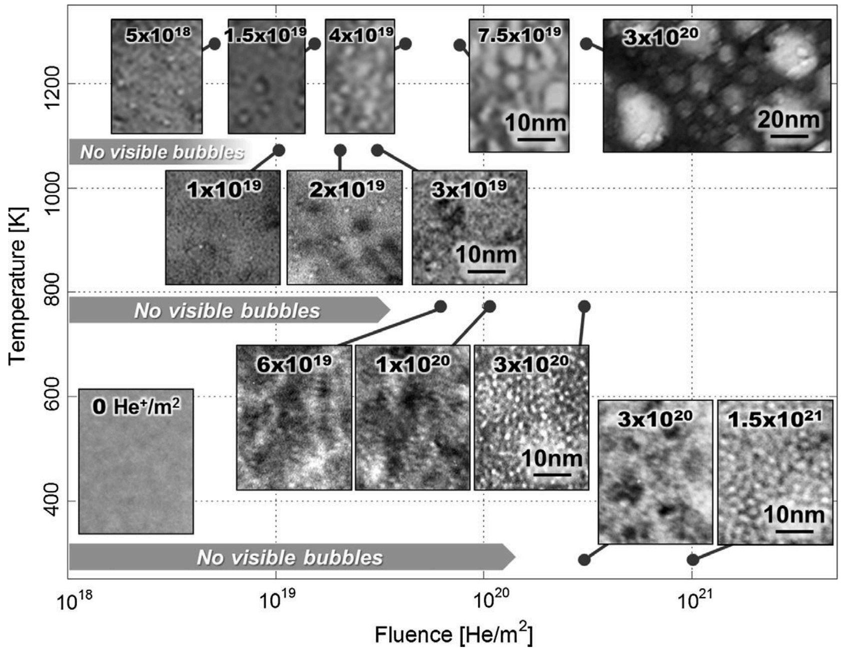


A3. H/He retention & radiation damage under practical conditions

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



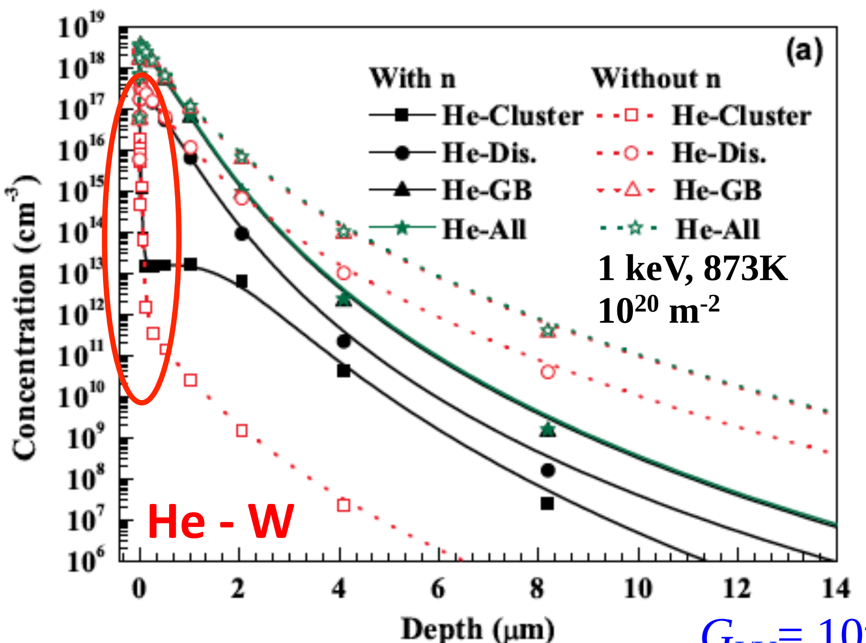
Alimov et al., *J. Nucl. Mater.* 441 (2013) 280.



Miyamoto et al., *J. Nucl. Mater.* 463 (2015) 333.

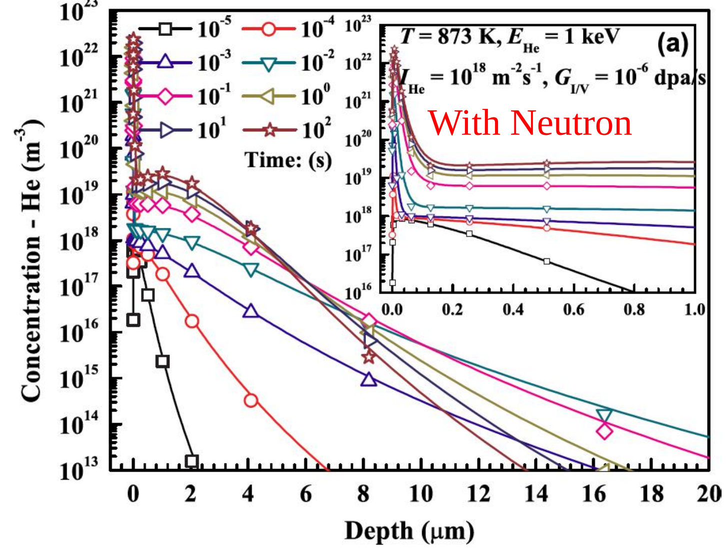
• Synergistic radiation effects of He ions and neutrons

- 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

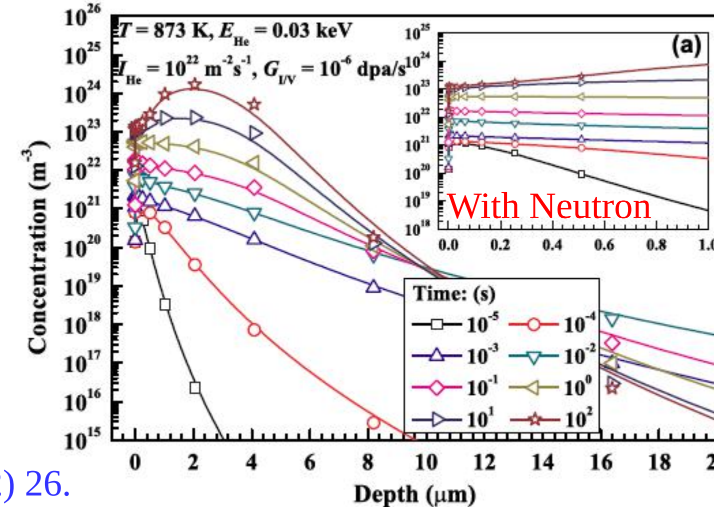


$G_{I/V}$ = 10^{-6} dpa/s

First Wall He, $1keV, 10^{18} m^{-2}s^{-1}$



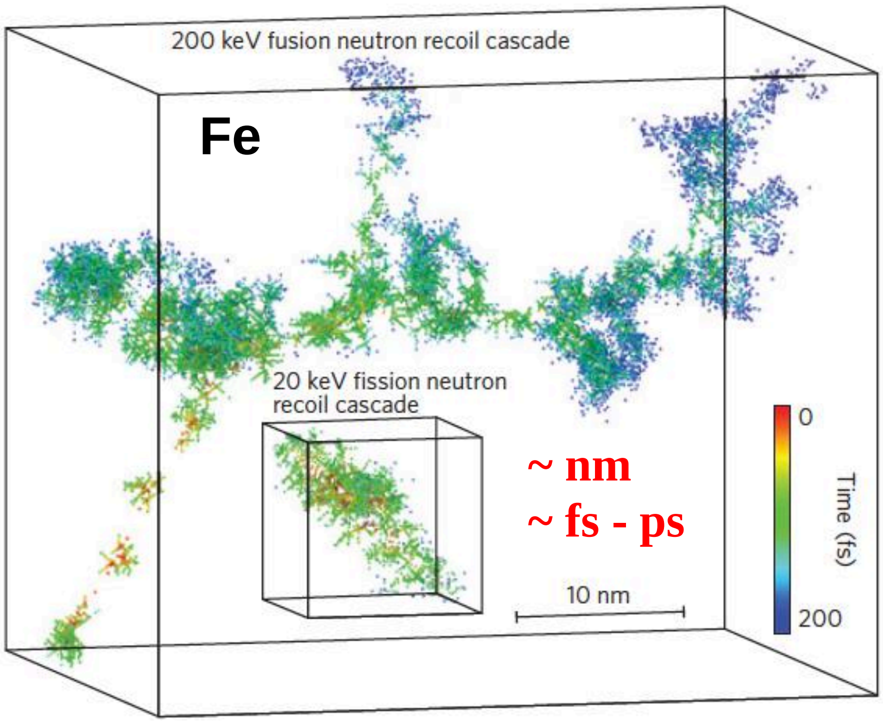
Divertor He, $30eV, 10^{22} m^{-2}s^{-1}$



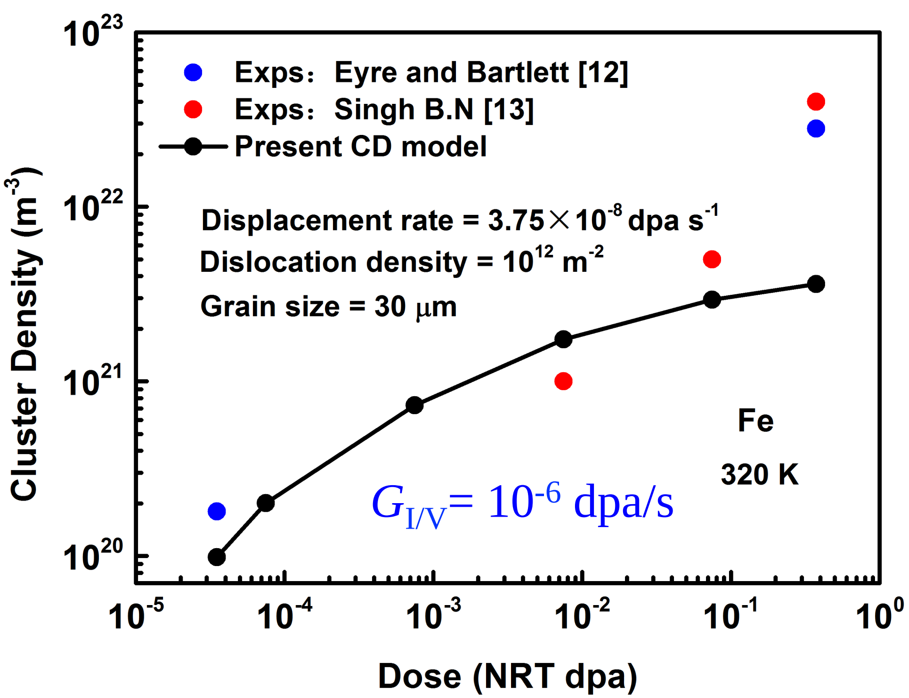
Li, *Commu. Comput. Phys.* 11 (2012) 1547; *J. Nucl. Mater.* 431 (2012) 26.

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)



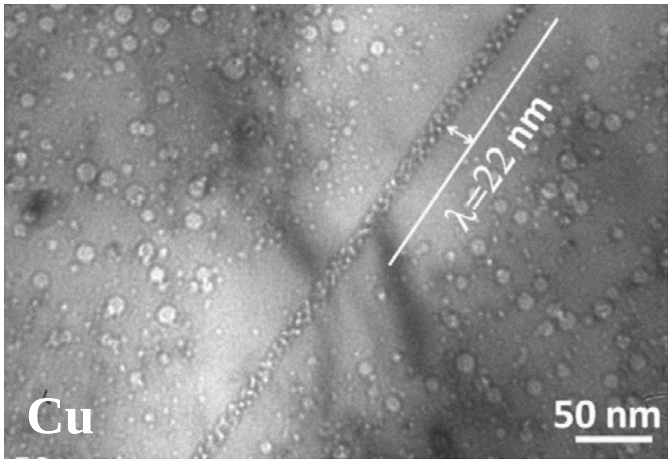
Knaster et al., *Nat. Phys.* 12 (2016) 424.



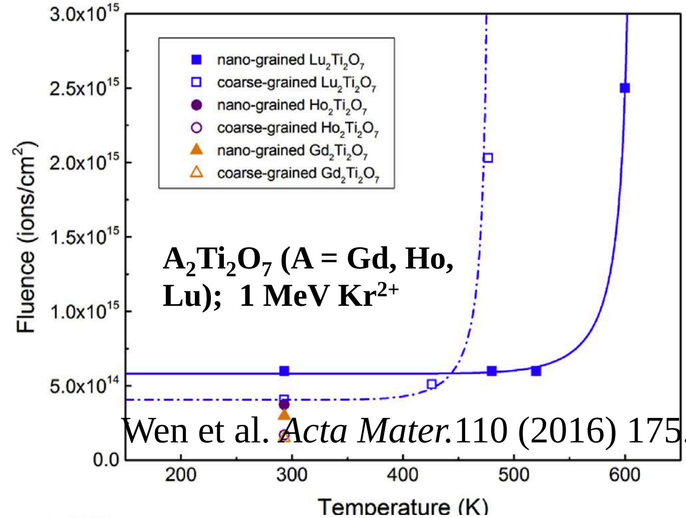
Zhao, *to be published.*

A4. Radiation tolerance in nano-crystalline (NC) materials

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

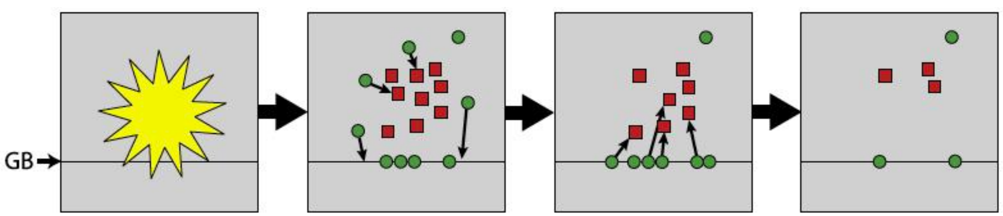


Han et al., *Acta. Mater.* 60 (2012) 6341.

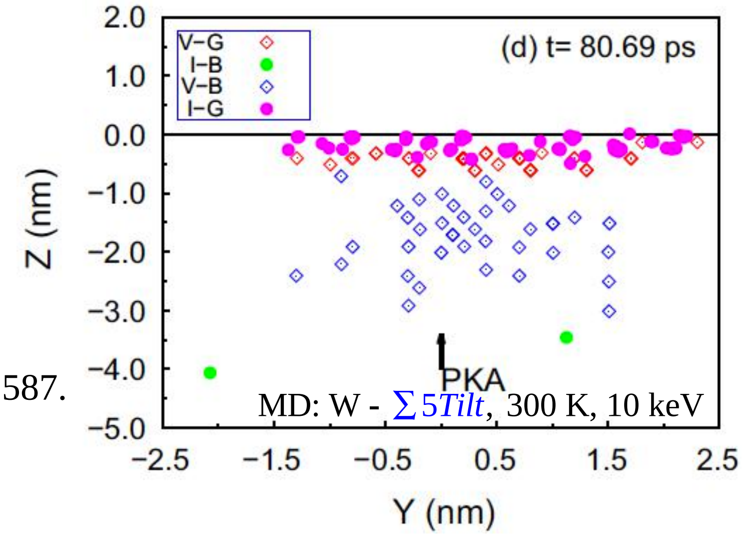


Wen et al. *Acta Mater.* 110 (2016) 175.

I-V recombination & I emission



Bai et al., *Science* 327 (2010) 1631; Ackland, *Science* 327 (2010) 1587.



MD: W - Σ5*Tilt*, 300 K, 10 keV

Zhang, *J. Nucl. Mater.* 458 (2015) 138.

• 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.

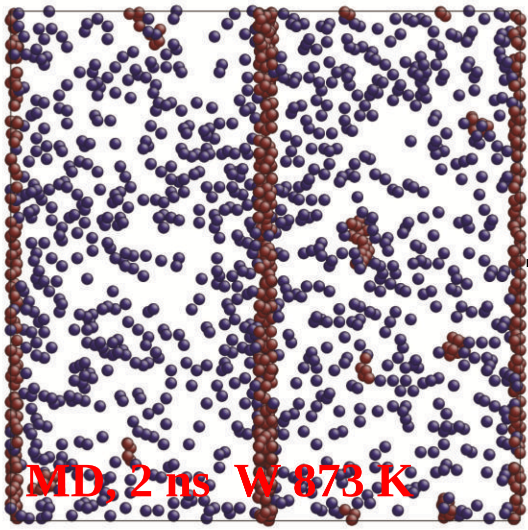
$$B_D \equiv -\lg\left(\sqrt{D_V / D_I}\right)$$

- Steay-state chemical rate theory

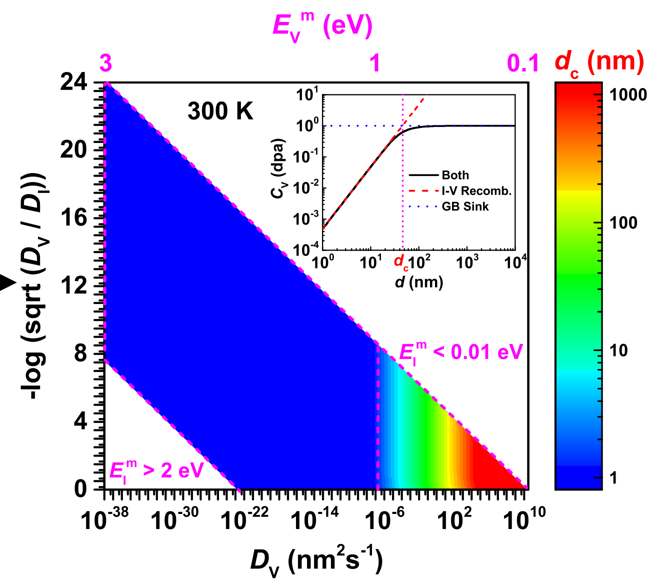
Shen, *Nucl. Instr. Meth. B* 266 (2008) 921.

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

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



From ns to infinite time-scales, what are the effects of the diffusion bias and grain sizes on materials radiation tolerance?



Extreme non-steady state (ns)

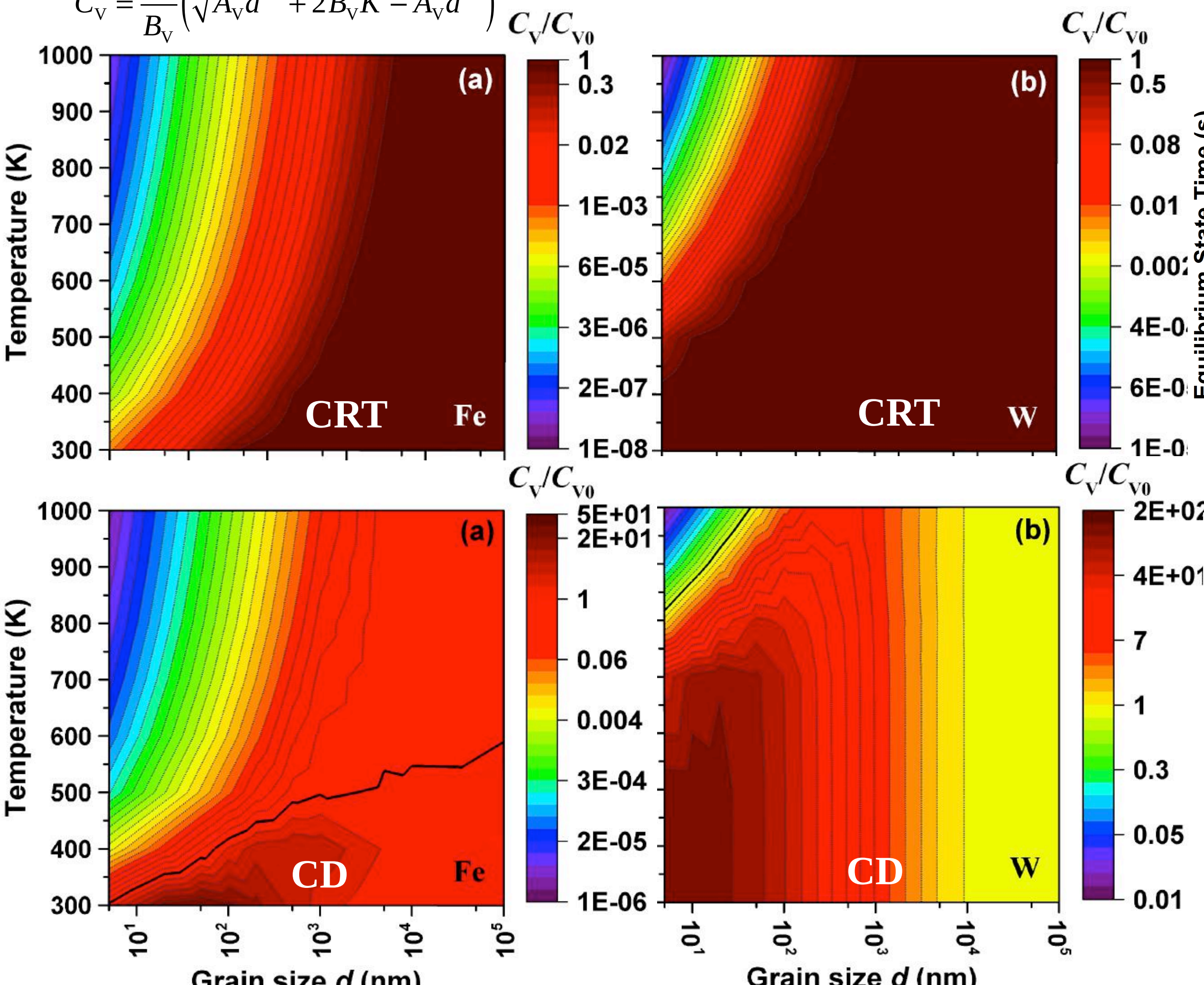
Non-steady states (ns - ∞): Diffusion bias?

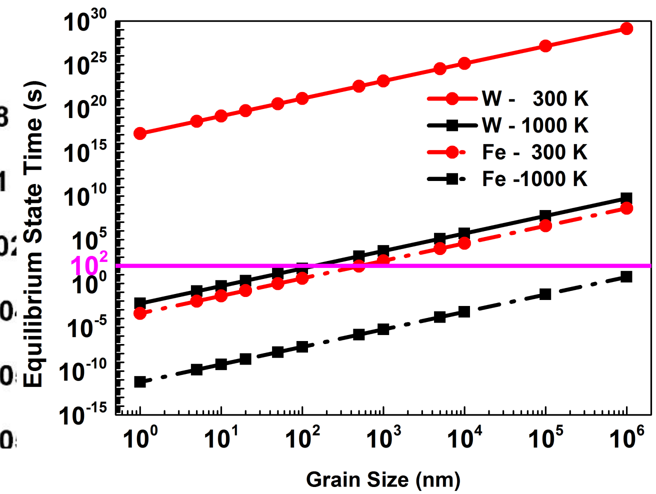
Steady state ($t = \infty$)
No effect of diffusion bias

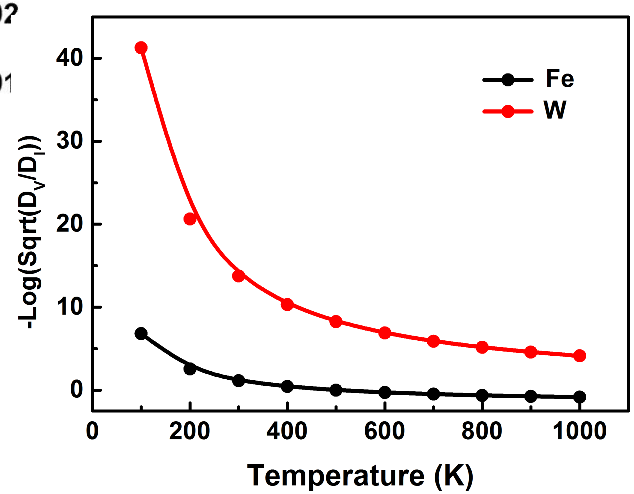
- **From non-steady states to the steady state**

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

Zhao & Wei, *to be published*.







E_v^m = 0.67 eV E_v^m = 1.66 eV

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 (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 PFMs are revealed under practical irradiation conditions.

- **Defect accumulation under neutron irradiation**

  - Diffusion bias suppresses radiation resistance in nano-crystalline materials.

Thanks for your attention!