Cluster Dynamics Modeling of Defect Evolution in Neutron-irradiated Tungsten for Fusion Applications

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ABSTRACT

Tungsten is considered the most promising plasma-facing material, which can be exposed to high neutron loads at high temperature. However, a significant number of defects, such as dislocation loops, voids, and precipitates, are generated in W under neutron irradiation, leading to the degradation of its material properties. This study employed a cluster dynamics model that incorporates the one-dimensional migration of dislocation loops to simulate defect evolution in single-crystal and polycrystalline W under neutron irradiation at 600 – 1200 ℃, and compared the results with experimental data obtained from the BR2 reactor. A general agreement with experimental results was achieved, and the underlying causes of the observed discrepancies were analyzed.

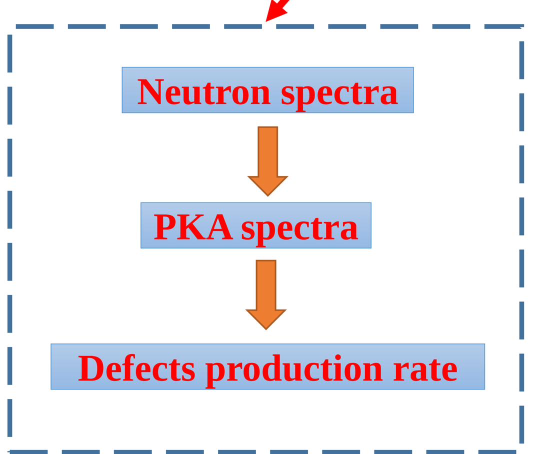
BACKGROUND

- Tungsten (W) is the primary plasma-facing material in fusion reactors, which suffers from microstructural defects such as dislocation loops, voids and transmutation precipitates, leading to severe property degradation.
- Experimental studies are costly and limited. While cluster dynamics (CD) models are key for simulating long-term defect evolution.
- There is a lack of simulations capable of directly and accurately comparing complex defect evolution processes in W. (rapid migration of dislocation loops , effects of transmutation-induced precipitates).
- This study uses a CD model that accounts for the rapid one-dimensional migration of dislocation loops and clusters larger than 10 nm. The simulation results are compared with experiments conducted on both single crystal and polycrystalline W in the BR2 reactor.

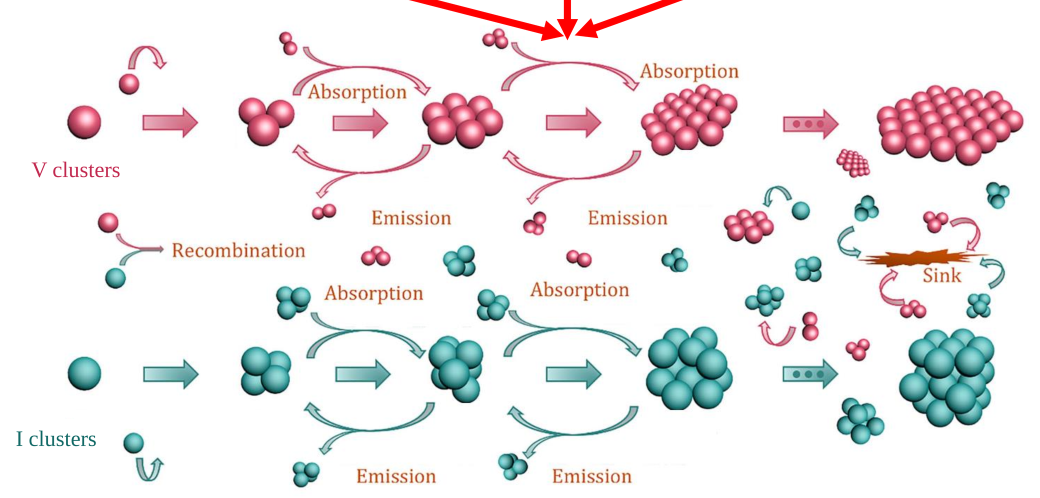
METHODS

- CD, based on the rate theory, is a mesoscale approach used to model the evolution of defects in materials.

$$\frac{dC_x}{dt} = G_x + \sum_{(y,z)} (R_{y+z\to x} - R_{x\to y+z}) - \sum_{(y,z)} (R_{x+y\to z} - R_{z\to x+y}) + L_x$$



Source term



Reaction and sink term [1]

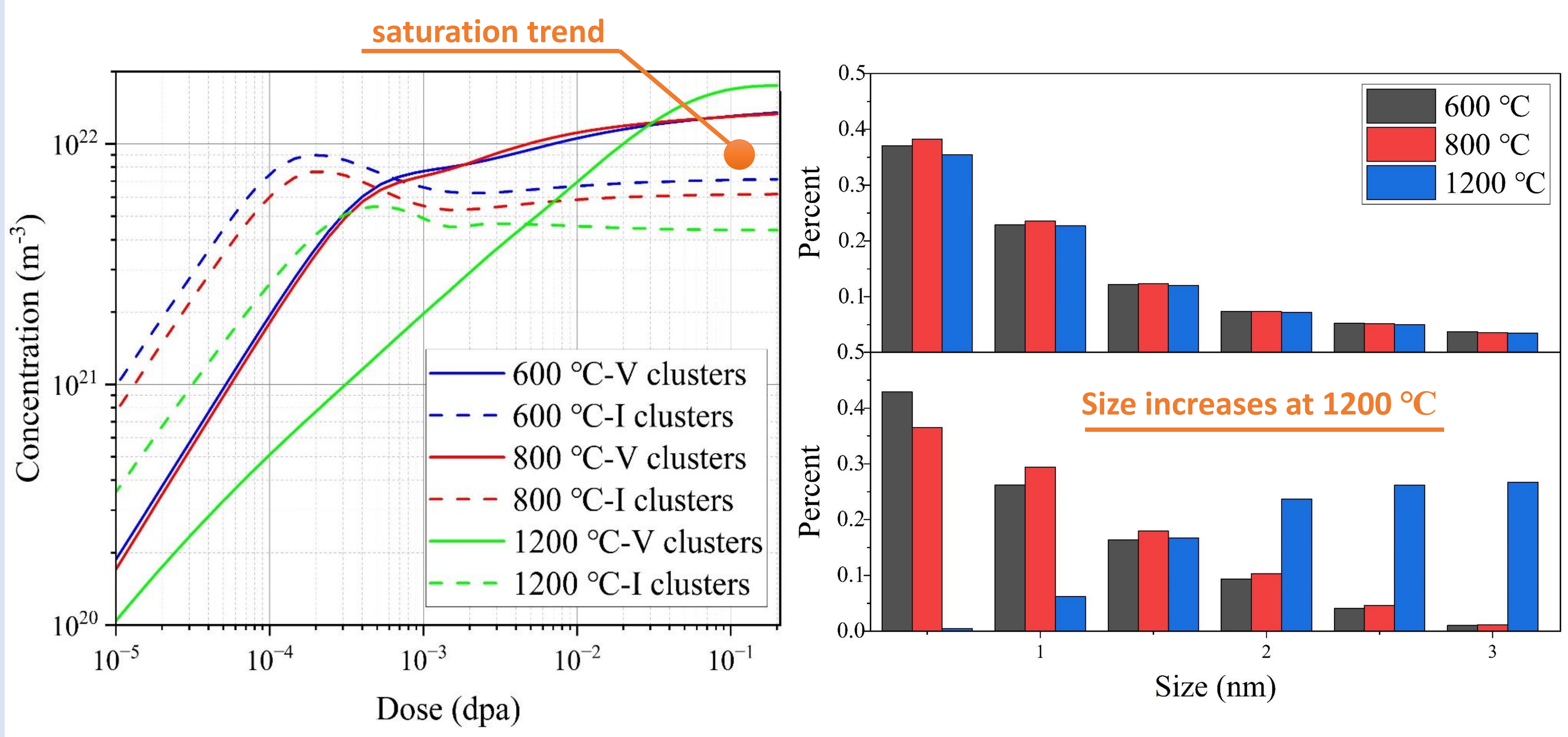
- The reaction rates employed in this work are cited from Reference [2]

Reaction	Reaction rate coefficient k^+/k^-
Clustering reactions	
$V_x + V_y \to V_{x+y}$; $V_x + I_y \to V_{x-y}$ or I_{y-x} (3D SIA)	$4\pi(r_x + r_y)(D_x + D_y)$
$I_x + I_y \to I_{x+y}$ (3D + 3D SIA)	$4\pi Z_{int}(r_x + r_y)(D_x + D_y)$
$V_x + I_y \to V_{x-y}$ or I_{y-x} (1D SIA)	$(4\pi r_x + 2\pi r_y)D_x + \pi^2(r_x + r_y)^4 D_y C_x$
$I_x + I_y \to I_{x+y}$ (3D + 1D SIA)	$Z_{int}(4\pi r_x + 2\pi r_y)D_x + Z_{int}^4\pi^2(r_x + r_y)^4 D_y C_x$
$I_x + I_y \to I_{x+y}$ (1D + 1D SIA)	$Z_{int}^4\pi^2(r_x + r_y)^4(D_x C_y + D_y C_x)$
Dissociation reactions	
$I_{x+1} \to I_x + I$; $V_{x+1} \to V_x + V$; $I_{x+1} \to I_{x+2} + V$	$\frac{k^+}{\Omega}\exp(\frac{-E_b^+}{k_B T})$

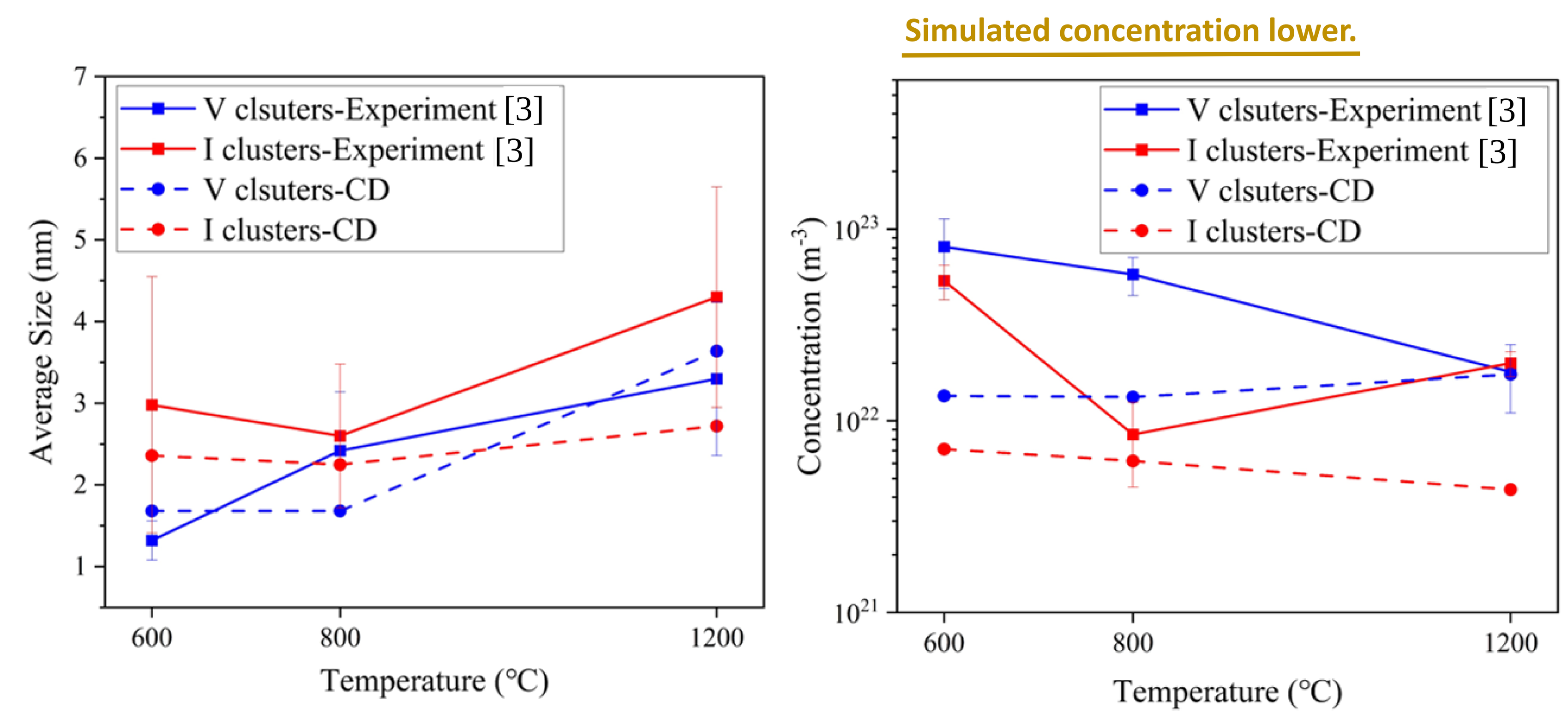
OUTCOME

Single crystal W simulation

- 600, 800, and 1200 ℃ up to 0.2 dpa in the BR2 reactor



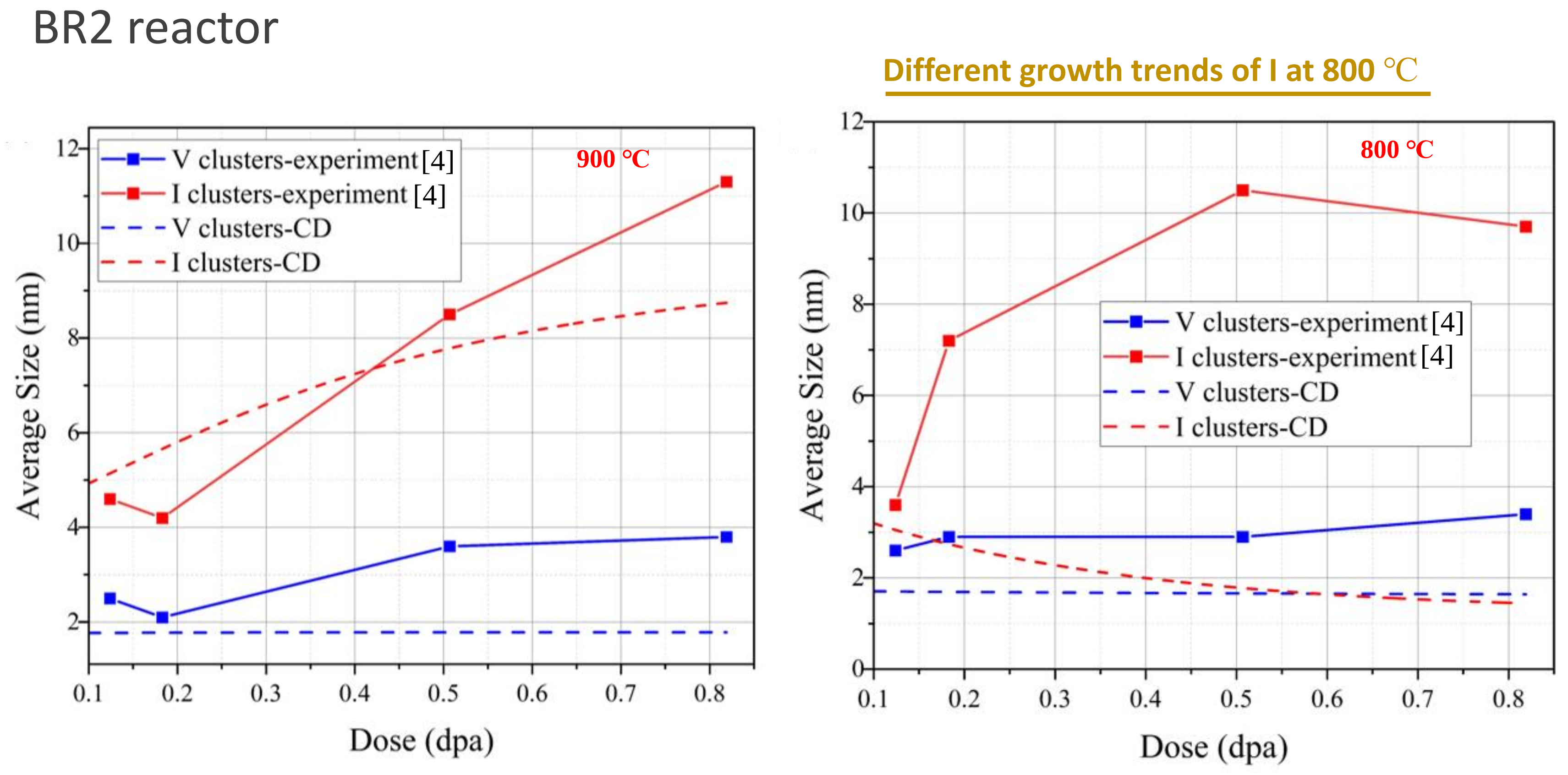
Total defect concentration and Size distribution (Size > 0.5 nm)



Comparison of average size and concentration with experiment

Polycrystalline W simulation

- 800 and 900 ℃ with doses of 0.124, 0.183, 0.507, and 0.819 dpa for the BR2 reactor



Relationship between average size and irradiation dose

REFERENCES

[1] XIONG, Y. et al., A Review of Cluster Dynamics in Studying Radiation Damage: Dominant Factors and Practical Implications, JOM 76 10 (2024) 5785.
[2] DUNN, A.Y., CAPOLUNGO, L., MARTINEZ, E., CHERKAOUI, M., Spatially resolved stochastic cluster dynamics for radiation damage evolution in nanostructured metals, Journal of Nuclear Materials 443 1–3 (2013) 128.
[3] DUBINKO, A. et al., Microstructure and hardening induced by neutron irradiation in single crystal, ITER specification and cold rolled tungsten, International Journal of Refractory Metals and Hard Materials 98 (2021) 105522.
[4] KLIMENKOV, M. et al., Influence of transmutation-induced Re/Os content on defect evolution in neutron-irradiated W, Journal of Nuclear Materials 592 (2024) 154950.

CONCLUSION

- The simulation results demonstrate general agreement with the experimental data.
- Discrepancies are observed between the simulation and experimental results, specifically in the overall magnitude of defect concentration and the size of clusters in polycrystalline tungsten at lower temperatures.
- Further model improvements are necessary and will likely focus on cluster migration rates and the influence of transmutation-induced precipitates.