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Strategy of Materials Simulation and Recent Progress in China

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Rui Ding (IPP-CAS)
Hong-Bo Zhou (BUAA)
Yu-Hao Li (BUAA)
& NINUM3 team
For the contributions to this talk!

Outline

Strategy: Fusion materials simulation

Simulation platform of neutron irradiation

Summary

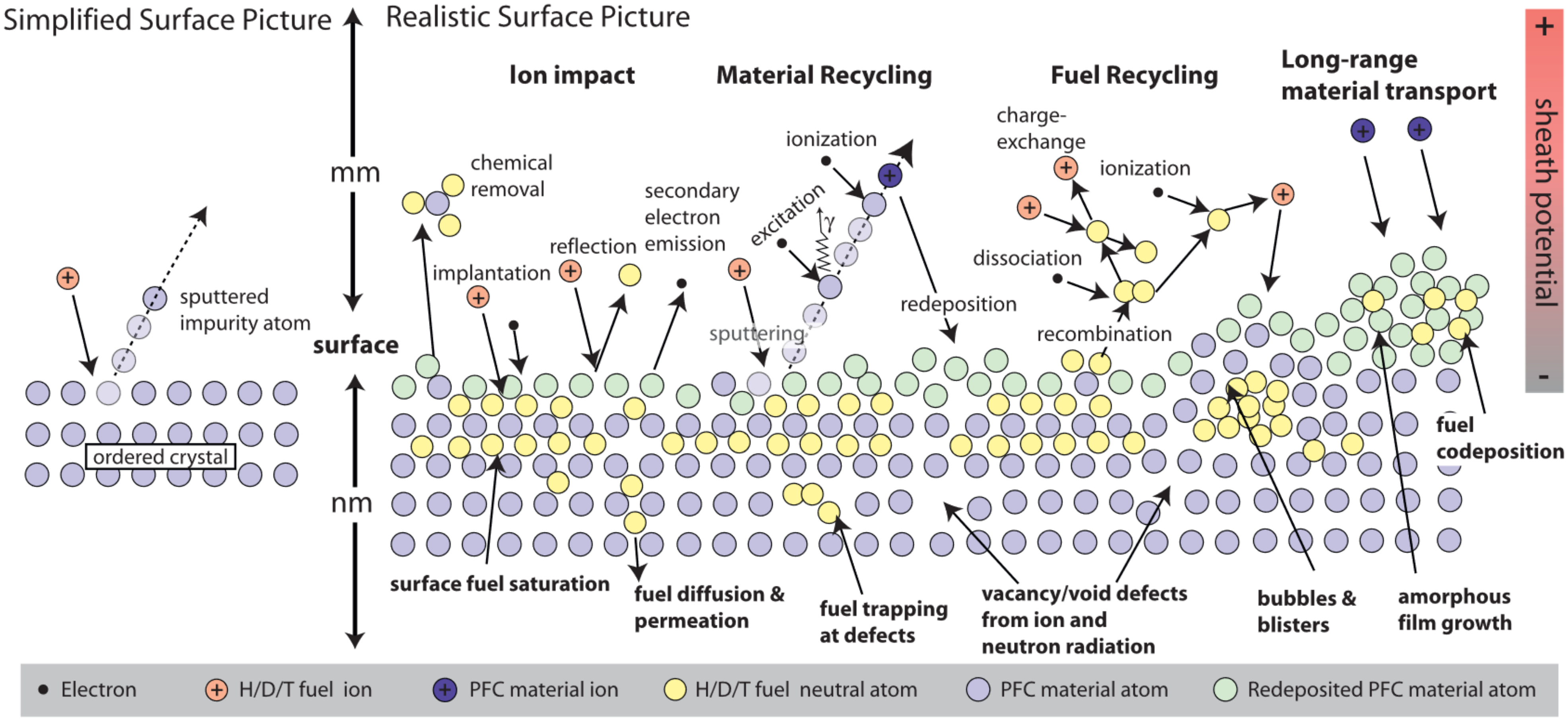
A Phased Roadmap for the Development of Fusion Reactor Materials in China

			2023-2030（to BEST/ITER-TBM）	2031-2040（to DEMO）	2041-2050（to PFPP）	
PFM/PFC	Pure Tungsten	FW & Divertor	1. Pure W performance and mass production stability are improved; 2. Complete > $10^{24}m^{-2}s^{-1}$ plasma irradiation, 20 MW m^{-2} heat load test and >2dpa fission neutron irradiation; 3. Obtain comprehensive key data on mechanical, thermal, irradiation, and H-isotope compatibility. 4.. Master the connecting process of W with heat sink, establish the production standard of pure W PFC, 5. Use CRAFT and BEST to evaluate the pure W divertor.	1. ~5 dpa fission neutron irradiation, > 1 dpa fusion neutron irradiation; 2. CRAFT, BEST, DEMO test; 3. Optimize the design and manufacturing process and improve the production standard.	1. Determine the PFC manufacturing process in PFPP; 2. Develop PFC on-line detection and *in-situ* repair technology.	Comprehensive Database of FRM
	Adv. W-based Materials	FW & Divertor	1. Large-scale fabrication process is determined, and cold state performance is completely tested; 2. High-flux plasma irradiation; 3. Complete >2 dpa fission neutron irradiation.	1. The output meets the needs of the demonstration reactor, and the production capacity of components is established; 2. ~5 dpa fission neutron irradiation, > 1 dpa fusion neutron irradiation; 3. Test of BEST and DEMO.	1. Determine a W-based material for PFPP; 2. R&D of advanced W-based materials for DEMO applications.	
	Liq. Metal PFM	FW & Divertor	1. Determine the material, structure and process of the first wall of flowing liquid metal; 2. Complete the test and analysis of the basic data of the first wall of flowing liquid metal; 3. High-flux plasma irradiation, substrate material > 2 dpa fission neutron irradiation.	1. Establish manufacturing standards for advanced liquid metal parts; 2. Study the synergistic effect of strong electromagnetism, high heat load and high particle flow; 3. The substrate material > 5 dpa fission neutron irradiation, BEST and DEMO test.	1. Fabrication of advanced liquid metal modules to meet PFPP requirements; 2. R&D of new flowing liquid metal wall structures for commercial applications.	
	Heat Sink	Divertor	1. Complete R&D of Cu-based heat sinks, determine the large-scale fabrication process, and complete the cold performance test 2. The connection process of new heat sinks with W was established; 3. >2 dpa neutron irradiation.	1. Determine the process of large-scale fabrication of plates and pipes; 2. >5 dpa fission neutron irradiation, BEST and DEMO test.	1. Identification of a Cu-based heat sink for PFPP; 2. R&D of new heat sinks for commercial applications.	
	C, other PFM	FW & Divertor	Continue to pay attention to R&D progress and explore breakthrough technology applications			
Structural M	RAFM Steel	FW & Blanket	1. Establish database of cold state (including welding); 2. Complete the certification of materials in nuclear industry and material manuals; 3. Complete 20 dpa fission nd ~5 dpa fusion neutron irradia. 1. BEST/ITER-TBM application evaluation; 2. Component manufacturing and standard certification.	1. Complete 30 dpa fission neutron and 10 dpa fusion neutron irradiation; 2. DEMO test to evaluate its application prospects.	Complete the application verification on DEMO	
	Adv. RAFM	FW & Blanket	1. Fabrication of 100 kg and cold state database; 2. Complete 5 dpa fission neutron irradiation. 1. R&D ton-scale fabrication technology; 2. BEST/ITER-TBM application evaluation; 3. Certification of materials for the nuclear industry.	1. Complete 20 dpa fission neutron and 10 dpa fusion neutron irradiation; 2. Establish industrial production processes, material manuals and component manufacturing standards; 3. DEMO test to evaluate its application prospects.	Complete the application verification on DEMO	
	ODS Steel	FW & Blanket	1. Ton-scale fabrication, complete cold state database; 2. 5 dpa fission neutron irradiation and preliminary database; 3. Establish an additive manufacturing blanket process. 1. Ton-scale industrial production, standardization system and quality certification; 2. Establish standard connection technology.	1. Complete the certification of materials in the nuclear industry and the establishment of material handbook, and component manufacturing standards; 2. 20 dpa fission neutron and 10 dpa fusion neutron irradiation; 3. DEMO is tested to evaluate its application prospects.	1. Irradiation of small specimen of >50 dpa with fusion neutron; 2. Complete the application verification on DEMO. Establish a comprehensive database of FRM irradiation and evaluate its commercial application	
	V Alloy	Liq. Li Blanket		1. According to the requirements of T-breeding Blanket, R&D in a timely manner; 2. Development of 100-kilogram fabrication technology and establishment of cold state database.		
	SiC	LLDC Blanket	Fabrication process R&D of FCI and performance tests of SiCf/SiC with low thermal and electrical conductivity, strong T resistance, appropriate toughness and radiation resistance of about 100 kg were completed. 1. Industrial production process and specification; 2. BEST-TBM application evaluation; 3.~5 dpa fission neutron irradiation.	1. Complete 10 dpa fission and 5 dpa fusion neutron irradiation; 2. Compatibility of liquid multiplier materials; 3. DEMO is tested to evaluate its application prospects. Fabrication process of SiC_f/SiC composites with about 100 kg of nuclear-grade pure silicon carbide, near-stoichiometric ratio, high thermal conductivity, high strength and toughness, radiation resistance and gas-tightness.	1. Irradiation of small specimen of >50 dpa with fusion neutron; 2. Complete the application verification on DEMO. Establish a comprehensive database of FRM irradiation and evaluate its commercial application	
Functional M	Be Be Alloy	Solid Blanket Solid Blanket	1. Master the fabrication process, mass production capacity, and reduce costs; 2. BEST/ITER-TBM application evaluation; 3. Complete 5 dpa fission neutron irradiation.	1. Complete the certification of materials in the nuclear industry and the establishment of material handbook,; 2. 10 dpa fission and 5 dpa fusion neutron irradiation; 3. DEMO is tested to evaluate its application prospects.	1. DEMO engineering test under actual working conditions; 2. > 30 dpa fission neutron irradiation performance assessment.	
	Li Ceramics	Solid Blanket	1. Ton-scale mass production capacity, and reduce costs; 2. BEST/ITER-TBM application evaluation; 3. Complete 5 dpa fission neutron irradiation.	1. Complete the certification of materials in the nuclear industry and the establishment of material handbook; 2. 10 dpa fission and 5 dpa fusion neutron irradiation; 3. DEMO is tested to evaluate its application prospects.	1. DEMO engineering test under actual working conditions, TBR>1; 2. > 30 dpa fission neutron irradiation performance assessment.	
	Pb-Li Liq FLiBe Molten	Liquid Blanket Liquid Blanket	1. Corrosion of structural materials and retardation technology; 2. Effect of 5 dpa fission neutron irradiation on material compatibility and hydrogen isotope behavior of structural materials; 3. Liquid metal flow and MHD effects.	1. Certification of materials in the nuclear industry, material handbook, and establish industrial production processes; 2. 10 dpa fission and 5 dpa fusion neutron irradiation; 3. DEMO is tested to evaluate its application prospects.	1. DEMO engineering test under actual working conditions, TBR>1; 2. > 30 dpa fission neutron irradiation performance assessment.	
	T Barrier	FW & Blanket	1. Master the fabrication process, PRF at 500°C > 1000; 2. >5 dpa fission neutron irradiation and evaluation of performance.	1. Certification of materials in the nuclear industry, material handbook, and establish industrial production processes; 2. DEMO is tested to evaluate its application prospects.	1. DEMO engineering test under actual working conditions; 2. > 20 dpa fusion neutron irradiation performance assessment.	
	Shielding M	VV	1. Master the engineering fabrication process of radiation shielding materials and components for BEST; 2. R&D of new high-performance radiation shielding materials.	1. BEST/DEMO test under actual working conditions; 2. R&D on industrial fabrication process and performance of new shielding materials.	DEMO engineering test under actual working conditions	
	Diagnosis M	First Mirror, etc	1. Neutron/gamma irradiation, plasma sputtering or high heat load assessment; 2. Determine the diagnostic materials for the fusion experimental reactor.	BEST/DEMO engineering test and in-situ cleaning or repair technology research under actual working conditions		
Irradiation Platform		Fusion N Source	1. Build a small fusion neutron source and 5-10 dpa fusion neutron irradiation for small specimen; 2. Completed the engineering design of fusion neutron source and started construction.	1. Complete 5-10 dpa fusion neutron irradiation of small specimen, and verify them with computational simulation; 2. Using the DEMO and fusion neutron source, 5-10 dpa irradiation for important components; 3. Upgrade the fusion neutron source, and start the construction of a medium-sized fusion neutron source.	1. Irradiation and evaluation of small specimen of 20-50 dpa; 2. 10-20 dpa Irradiation and evaluation of small components such as blanket with low-power DEMO reactor; 3. Irradiation of small specimen of 60-80 dpa.	
		Fission N & Triple-Ions	1. 10-20 dpa fast neutron irradiation; 2. Establish equivalent experimental methods for fusion, fission neutron and ion irradiation; 3. Establish a national standard for small specimen testing.	1. 20-30 dpa fission neutron irradiations; 2. Establish evaluation criteria for FRMs based on fission neutron and triple ion irradiation.	Systematical fission neutron irradiation (30 dpa) for different new materials to improve the irradiation performance data of various FRMs.	
		High Heat Load	1. Build the highest power electron gun and high heat load test platform; 2. Complete the high thermal load test of the full-size test piece of divertor and blanket components.	1. Design and build a high heat load test platform in the hot cell; 2. Evaluate the performance and life of the divertor and blanket components.		
		Plasma Bombard	1. Build a linear plasma device with the highest parameter level in the world; 2. Complete the plasma irradiation + steady-state heat flux synergy test of materials and modules; 3. Establish a screening standard for the plasma irradiation resistance of the FW material.	1. Design and build high-flux plasma irradiation conditions that can accept neutron irradiation activated samples; 2. Build a high-flux plasma irradiation facility that can use gram-scale tritium.	1. Plasma irradiation of high-dose fusion neutron irradiation material/component module: 2. Build advanced PFC full-scale module large-beam area plasma irradiation conditions; 3. Verify PFC in-situ repair technology.	
Simulation Platform		Fusion *vis* Fission	1. Establish the relationship between fission and fusion neutron irradiation; 2. Simulation and prediction of micro-macro effects of 10-20 dpa fusion neutron irradiation.	1. Establish a material evaluation system that includes organizational structure and mechanical and thermal properties; 2. Fusion neutron irradiation simulations of FRMs in 20-50 dpa.	1. Simulations of materials with fusion neutron irradiation at 50-100 dpa; 2. Establish a service performance evaluation and failure analysis system for blanket structural materials and PFMs.	
		PMI	1. Simulation of surface morphology evolution under H-isotope/helium plasma synergistic irradiation; 2. To investigate the sputtering etching of the wall surface under H-He synergistic irradiation.	1. Coupling the PSI simulation with the neutron irradiation; 2. Prediction synergistic effects of FRMs under hydrogen-helium and neutron irradiation.		

Roadmap: Fusion materials modeling & simulation

	2020s (to BEST, ITER-TBM)	2030s (to DEMO)	2040s (to PFPP)
Neutron irradiation	1. Establish the relationship between fission and fusion neutron irradiation; 2. Simulation and prediction of micro-macro effects of 10-20 dpa fusion neutron irradiation.	1. Establish a material evaluation system that includes structure and mechanical/thermal properties; 2. Fusion neutron irradiation simulations of FRMs in 20-50 dpa.	1. Simulations of materials with fusion neutron irradiation at 50-100 dpa; 2. Establish a service performance evaluation and failure analysis system for blanket structural materials and PFMs.
Plasma-wall interactions	1. Simulation of surface morphology evolution under H-isotope/helium plasma synergistic irradiation; 2. To investigate the sputtering etching of the wall surface under H-He synergistic irradiation.	1. Coupling the PSI simulation with the neutron irradiation; 2. Prediction synergistic effects of FRMs under hydrogen-helium and neutron irradiation.	

Modeling of plasma-wall interactions



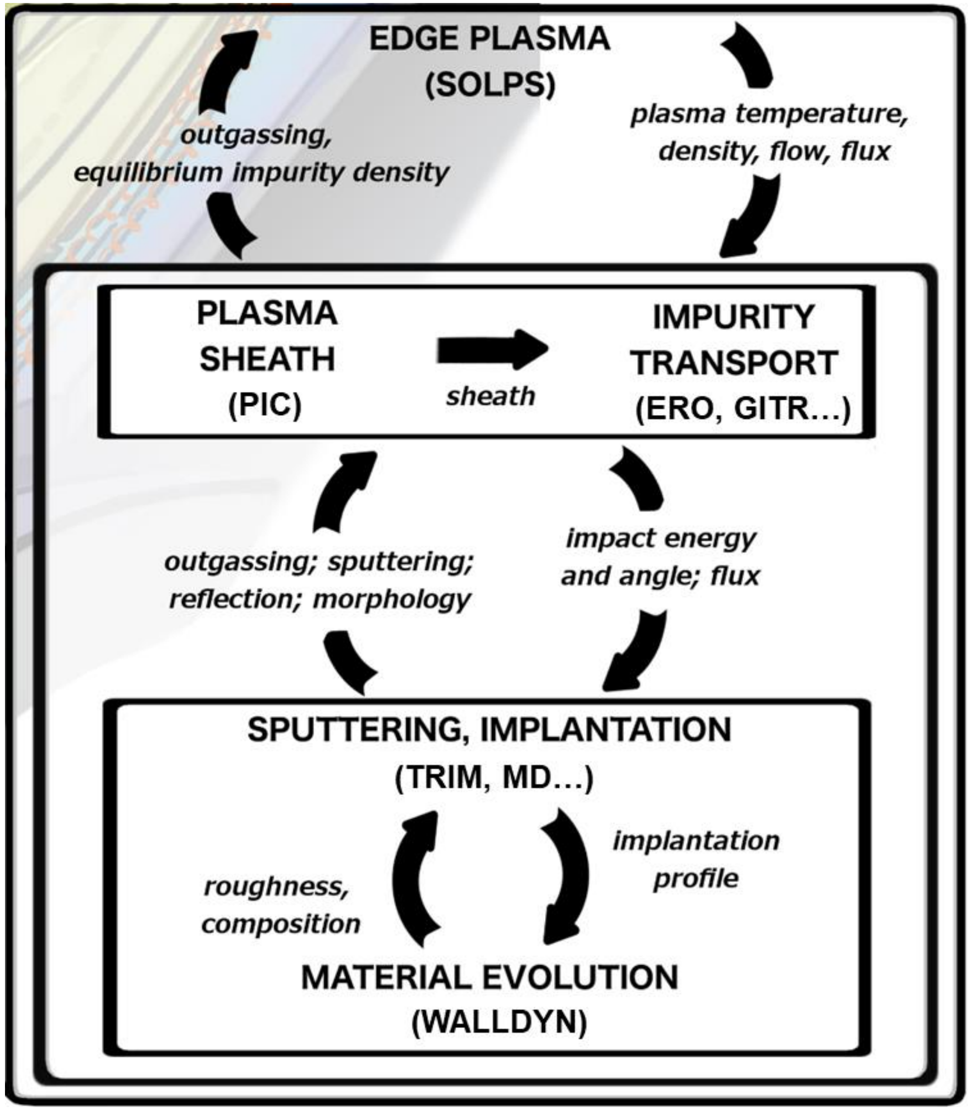
B.D. Wirth, et al. MRS Bulletin 36 (2011) 216-222

Edge plasma + Plasma-wall interactions + Materials (surface & bulk)

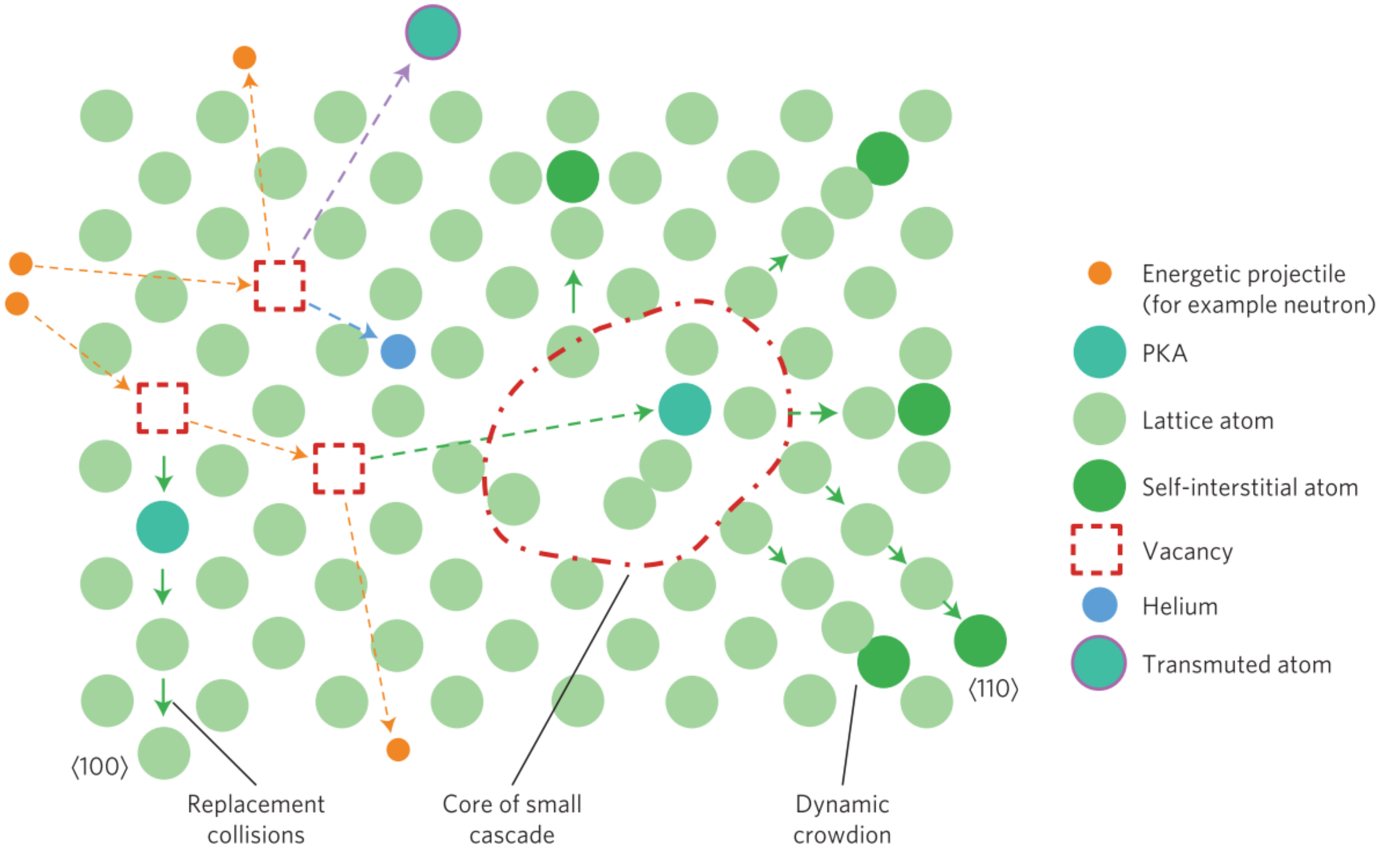
Erosion/Surface morphology/Property degradation/Hydrogen isotopes retention

Integrated modeling for plasma-wall interactions

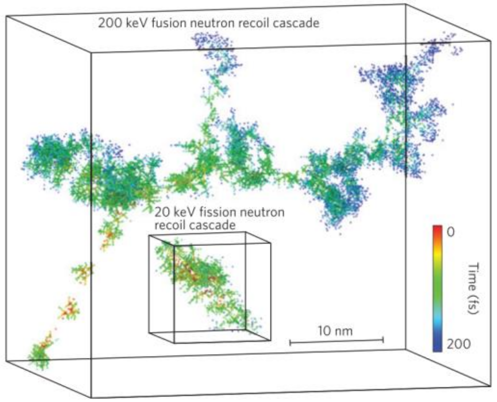
- **Coupling different codes (materials – edge – core)**
  - SOLPS – PIC – ERO/GITR
  - ERO/GITR – TRIM/MD
  - TRIM/MD – WALLDYN
  - SOLPS – ONETWO (core plasma)
- **Database:**
  - Materials, A&M data
- **Code development within integrated frameworks**



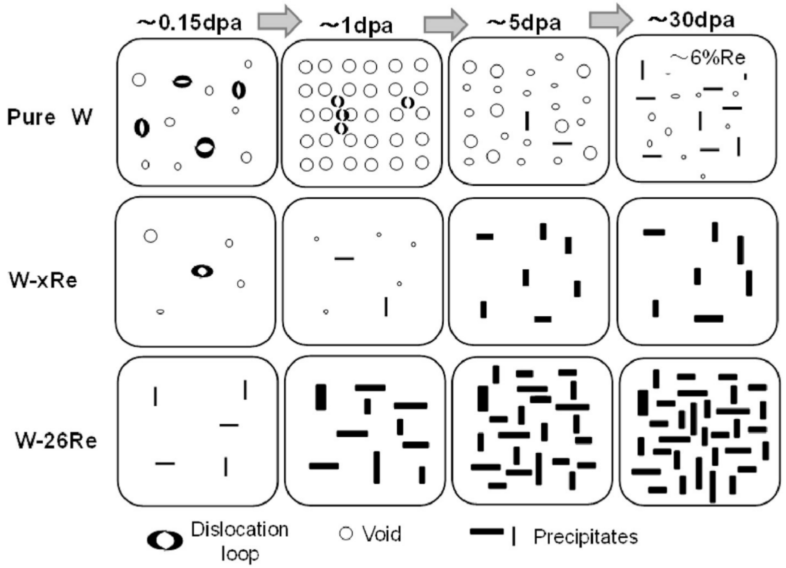
Modeling of neutron irradiation damage



Displacement cascade



Transmutation effects



Displacement defects + **Transmutations elements**

Defects production & evolution → Property degradation → Materials failure

Knaster et al. Nature Phys 12 (2016) 424-434; Hasegawa et al. J Nucl Mater 471 (2016) 175.

Benchmark of simulation platform

- **Irradiation Experiments**
  - More fission neutron irradiation experiments: HFETR, CMRR, SINQ
  - Triple beam ion irradiation (H+He+heavy ions synergy)
- **Facilities**
  - EAST, HL-3 Tokamak
  - CRAFT, BEST
  - CFETR
  - IFMIF-DONES

Outline

Strategy: Fusion materials simulation

Simulation platform of neutron irradiation

Summary

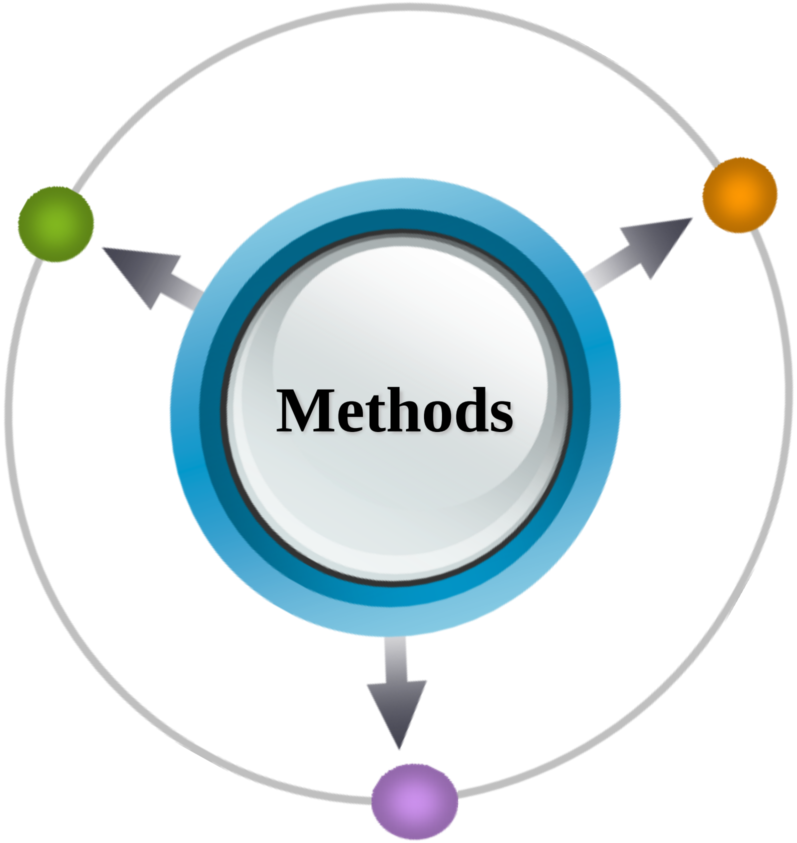
Investigation of neutron irradiation damage

Reactor experiments

- **Lack of fusion neutron sources**
- **Fast/mixed neutron reactors**

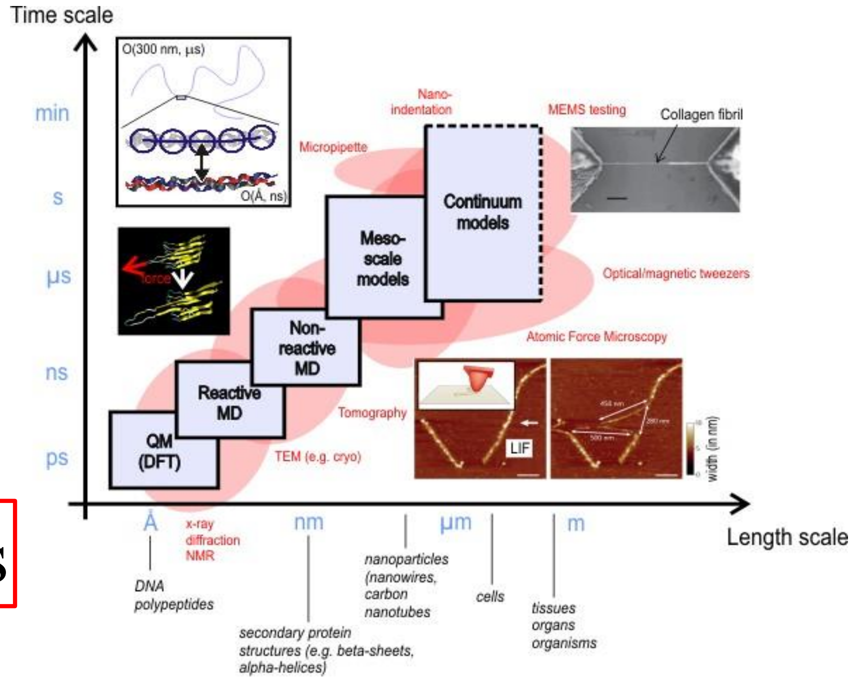
Reactor service conditions

- A limited number of reactors
- Unable to conduct single factor studies
- Under extreme conditions



Laboratory experiments

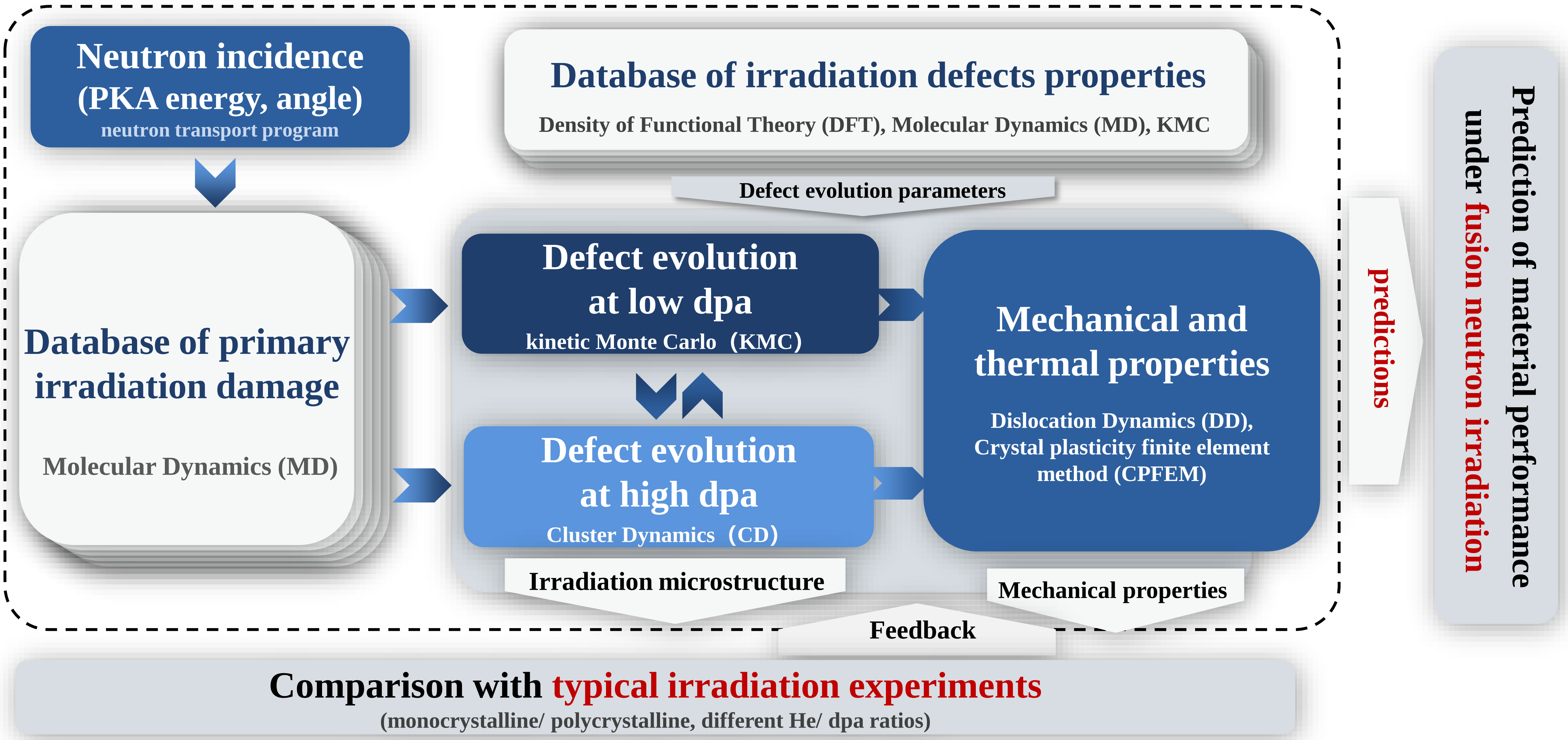
- **Heavy-ion irradiation**
- **Proton irradiation**



Computational simulations

- **Multiscale modeling**

Neutron Irradiation of Nuclear Fusion Materials: Multiscale Modeling Platform



Research team

- **Team Composition**
  - 12 Universities
  - 5 Institutes

- **Computing Platform**
  - National Supercomputing Center Changsha
  - Heavy Ion Research Facility at Lanzhou
  - National engineering research center for isotope
  - National Energy Fast Reactor Engineering R&D (Experimental) Center
  - China Nuclear Data Center
  - State Key Laboratory of Metal Matrix Composites
  - State Key Laboratory of Software Development Environment
  - Hunan Provincial Key Laboratory of Nuclear Equipment Reliability Technology
  - Beijing Key Laboratory of Advanced Nuclear Materials and Physics
  - Key Laboratory of Advanced Technologies of Materials, Ministry of Education
  - Shanghai Cloud Computing Joint Laboratory
  - Shanghai Key Laboratory of Scalable Computing and Systems

Research team

Project meeting, Shanghai, September 20, 2023

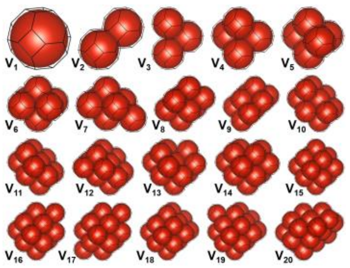
2018-2023, funded by National Magnetic Confined Fusion Energy R&D Program, MOST

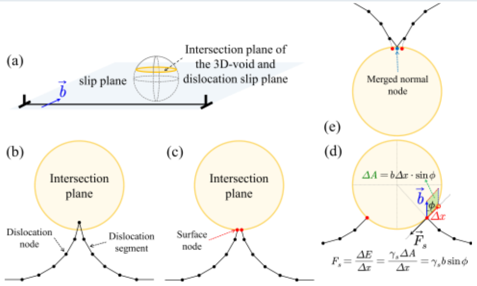
Tasks *(5dpa, 2018.12-2023.11)*

	Task	PI	Affiliation
Task 1	**Structure of primary irradiation damage and hydrogen-helium effect**	Deng Huiqiu	**Hunan University** Shandong University Sichuan University Hebei University of Technology
Task 2	**Thermodynamics and kinetic behavior of irradiation defects**	Kong Xiangshan	**Institute of Solid Physics, Chinese Academy of Sciences** University of Science and Technology of China Southwest Jiaotong University
Task 3	**Kinetic Monte Carlo simulation of irradiation microstructure evolution**	Zhou Hong-Bo	**Beihang University** Huazhong University of Science and Technology/North China Electric Power University Beijing Institute of Applied Physics and Computational Mathematics
Task 4	**Cluster dynamics simulation of irradiation microstructure evolution**	He Xinfu	**China Institute of Atomic Energy** Institute of Plasma Physics, Chinese Academy of Sciences University of Science and Technology Beijing
Task 5	**Calculation of mechanical and thermal properties based on irradiated microstructure**	Shen Yao	**Shanghai Jiao Tong University** Dalian University of Technology/Xi'an Jiaotong University

Platform

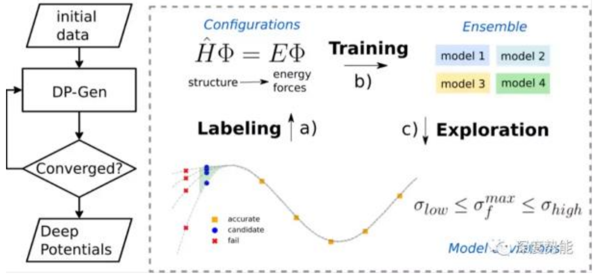
Models





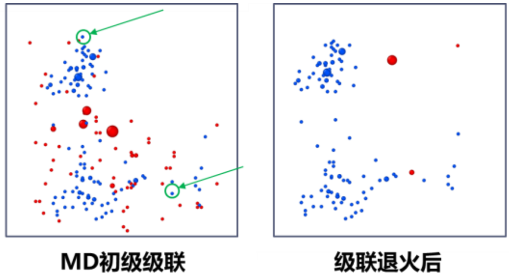
18 models: Defect evolution and performance prediction

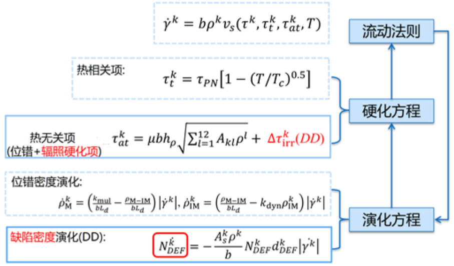
Potentials



10 potentials: Tungsten-based interatomic potential

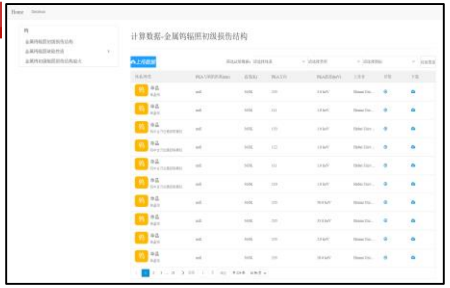
Methods





4 methods: data transfer

Database



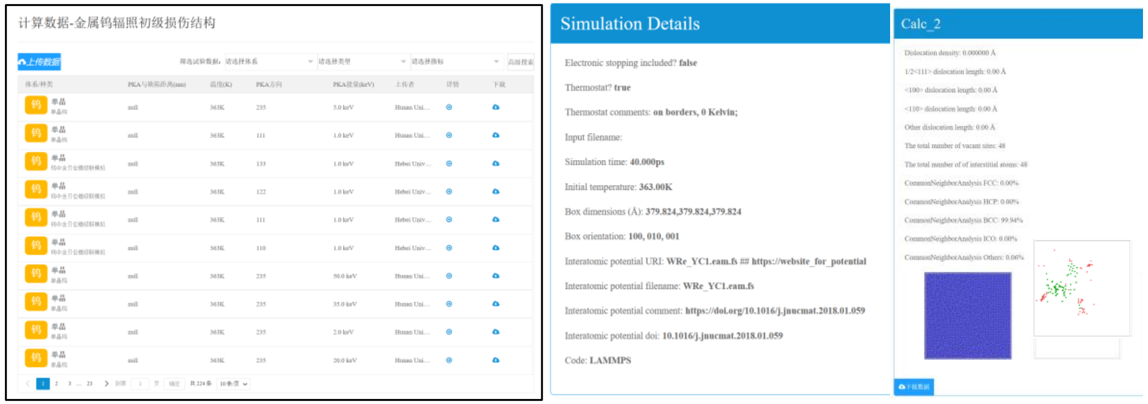
3 databases: Defect production and evolution parameters

Codes

13 codes: Neutron irradiation damage simulation

Databases of defect production and evolution

Displacement cascade database



Includes single crystal/dislocations/GBs/H/He

5462 data records

Defect property database

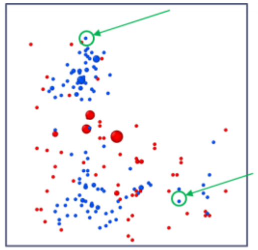
Includes vacancy/SIA/GBs/dislocations/H/He

9407 data records

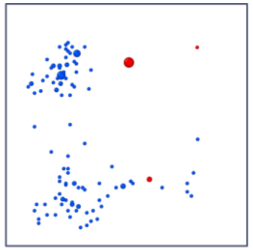
联合开发

Website: *http://115.25.142.9:8000/database/index*

Cascade annealing database



Primary damage



After annealing

- 13 annealing moments, 100 times per cascade
- **Total amount of data**

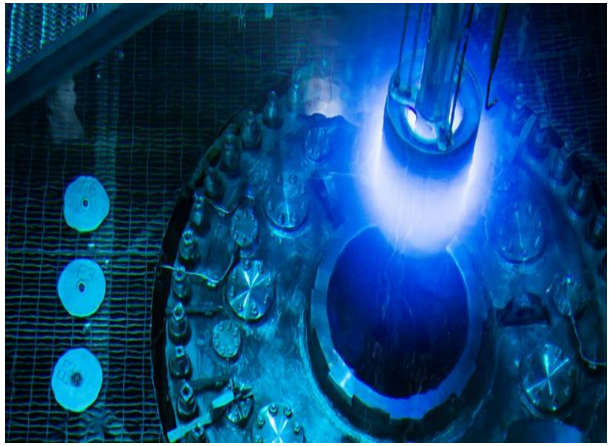
Single crystal： > 2400×100×13 data

Includes H/He： > 500×100×13 data

Neutron Irradiation of Nuclear Fusion Materials: Multiscale Modeling

NINUM³

Validations: Irradiation experiments (W as model material)



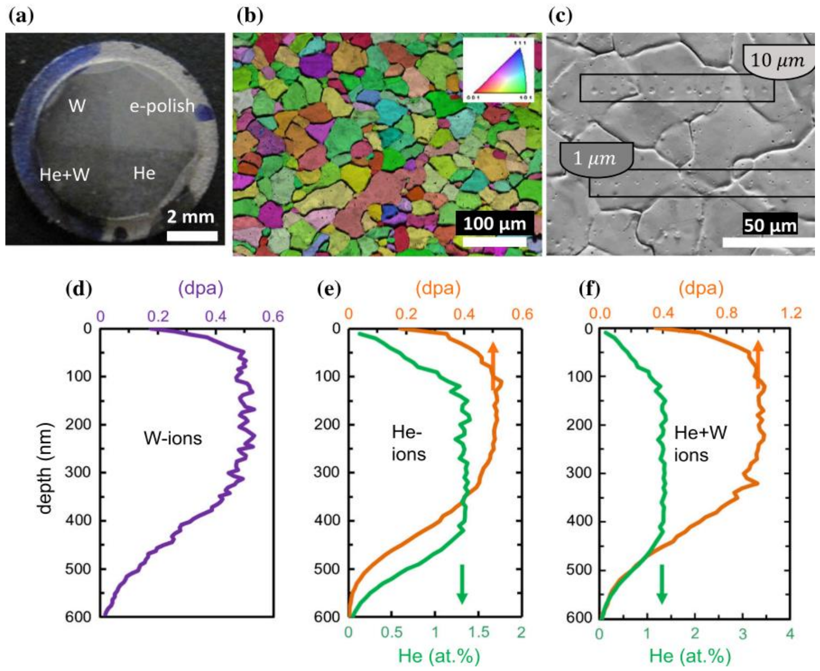
HFIR reactor

0.004 dpa @ 363 K

0.02 dpa @ 733 K

BR2 reactor

0.2 dpa @1073 K



Void & dislocation loop

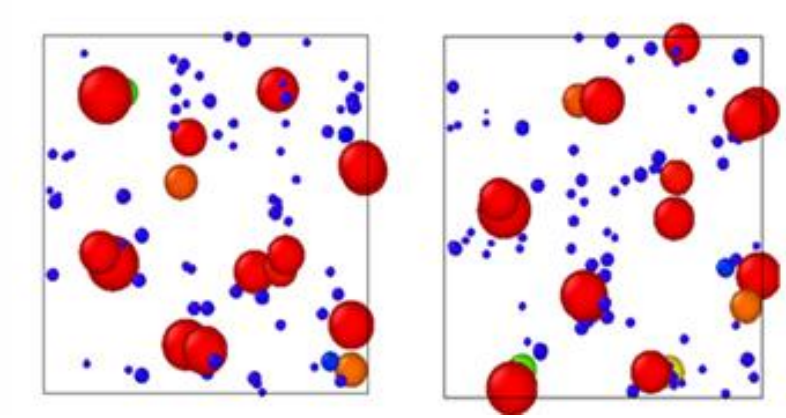
① number density

② size

\+

Hardness increment

Validation



Reproduce void lattice formation process

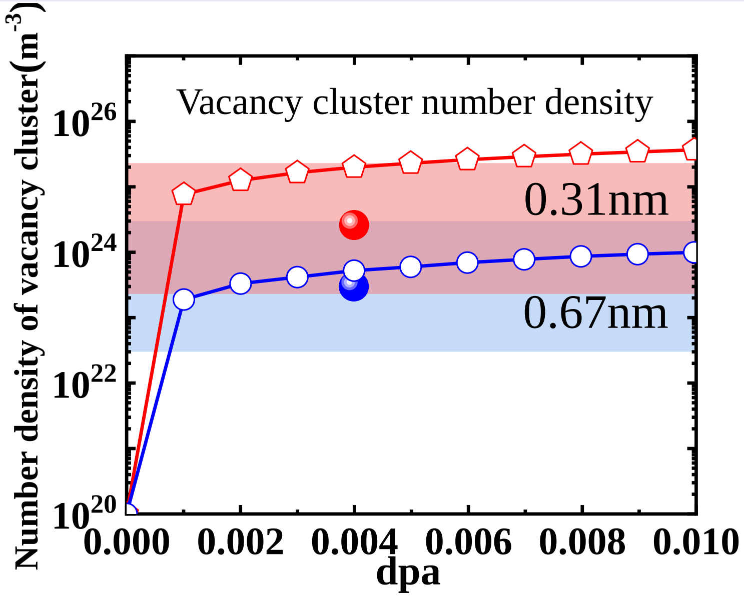
by neutron irradiation

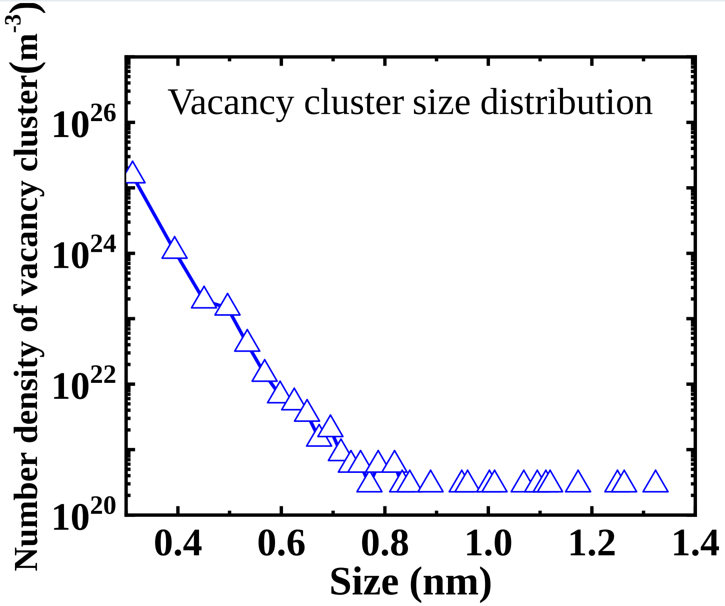
He+W ion irradiation

0.5dpa+0.25dpa

He: 1.5at%, 0.02 He/dpa

Validation ①: Neutron irradiation in HFIR *0.004 dpa @ 363 K*





Based on the microstructure

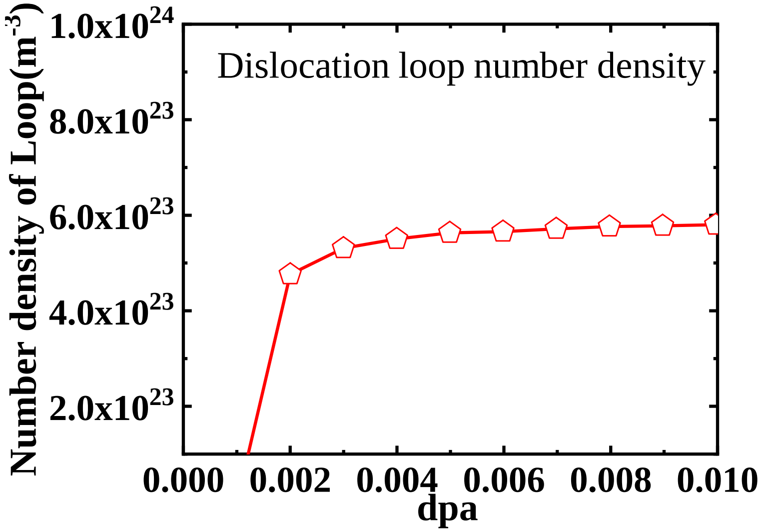
DD and CPFEM models are used to predict

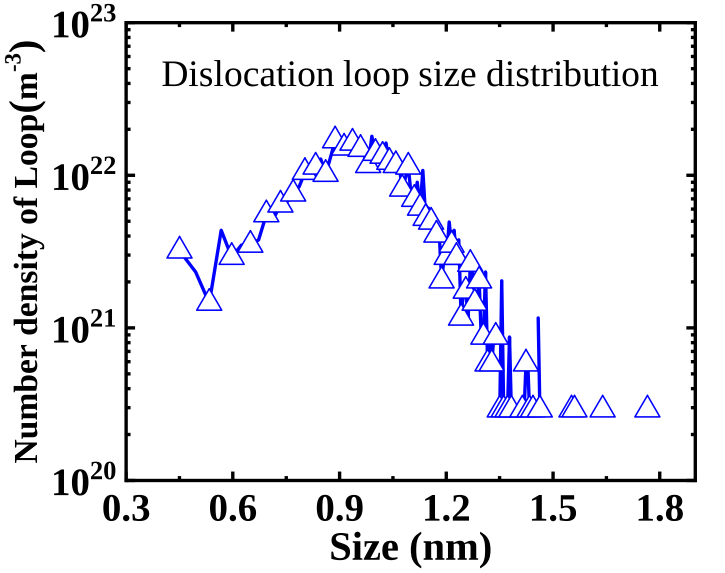
the hardness increment after irradiation

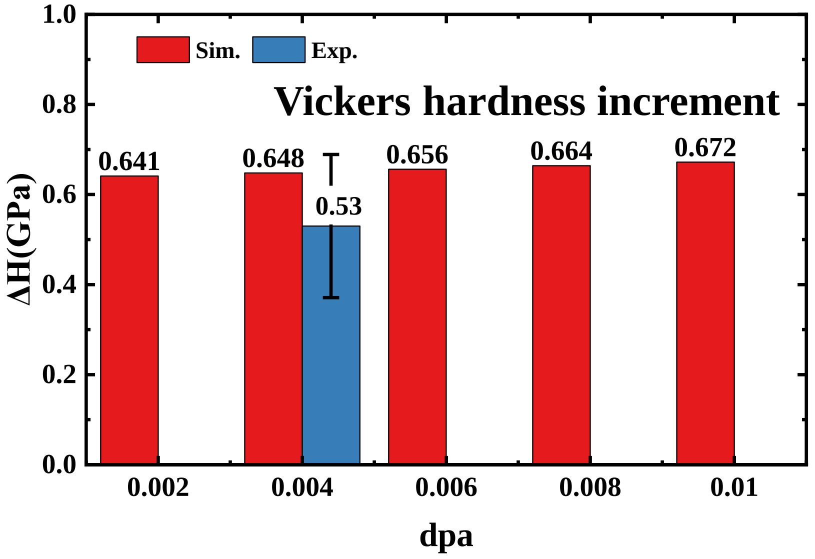
$$\Delta\tau_{\text{irr}} = \left[(\tau_{\text{Loop}})^{1.5} + (\tau_{\text{Void}})^{1.5} \right]^{\frac{2}{3}}$$

$$\tau_{\text{Loop}} = \alpha_L(D) Gb \left(N_L^k\right)^{2/3} D_{L,\text{eff}}$$

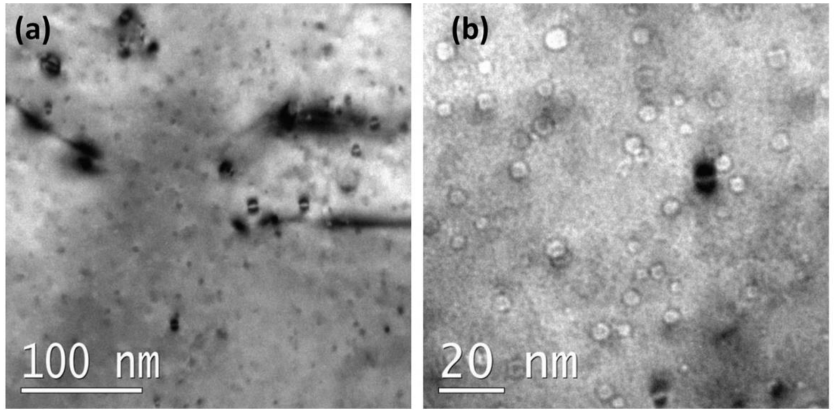
$$\tau_{\text{Void}} = \alpha_V(D) Gb N_V^{2/3} D_{V,\text{eff}}$$





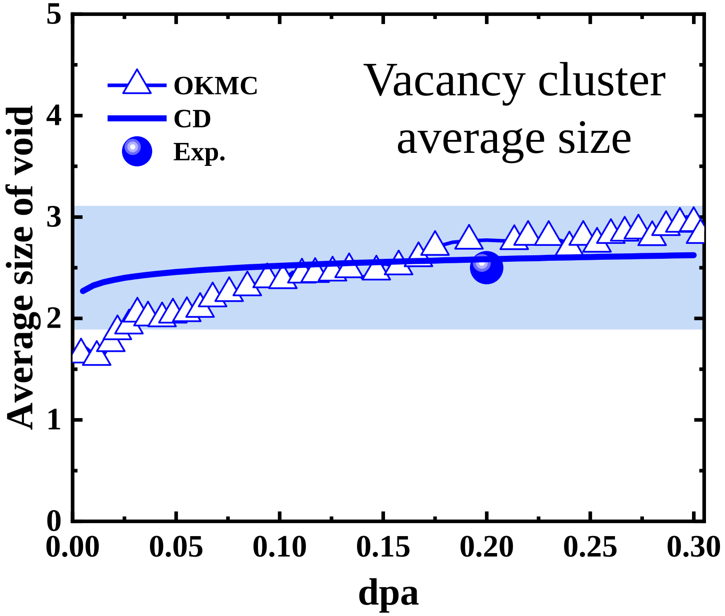


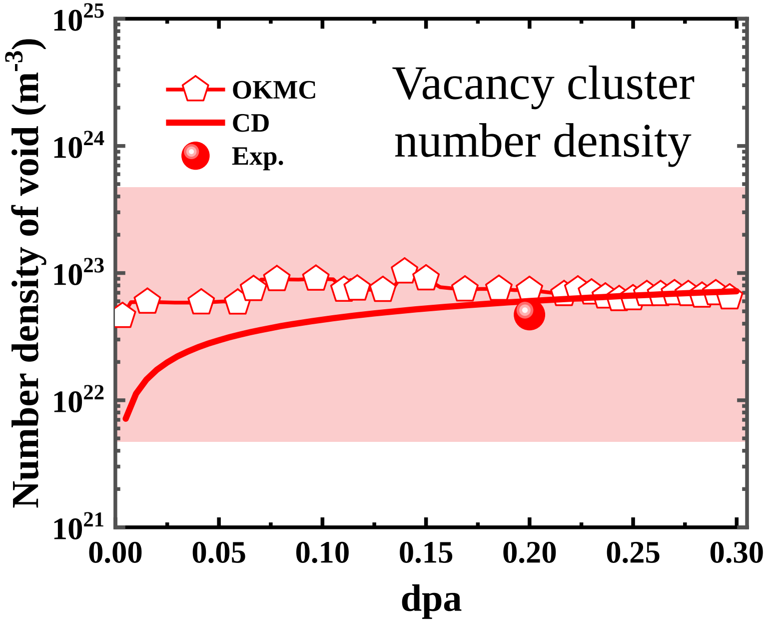
Validation ②: Neutron irradiation in BR2 *0.2 dpa @1073 K*

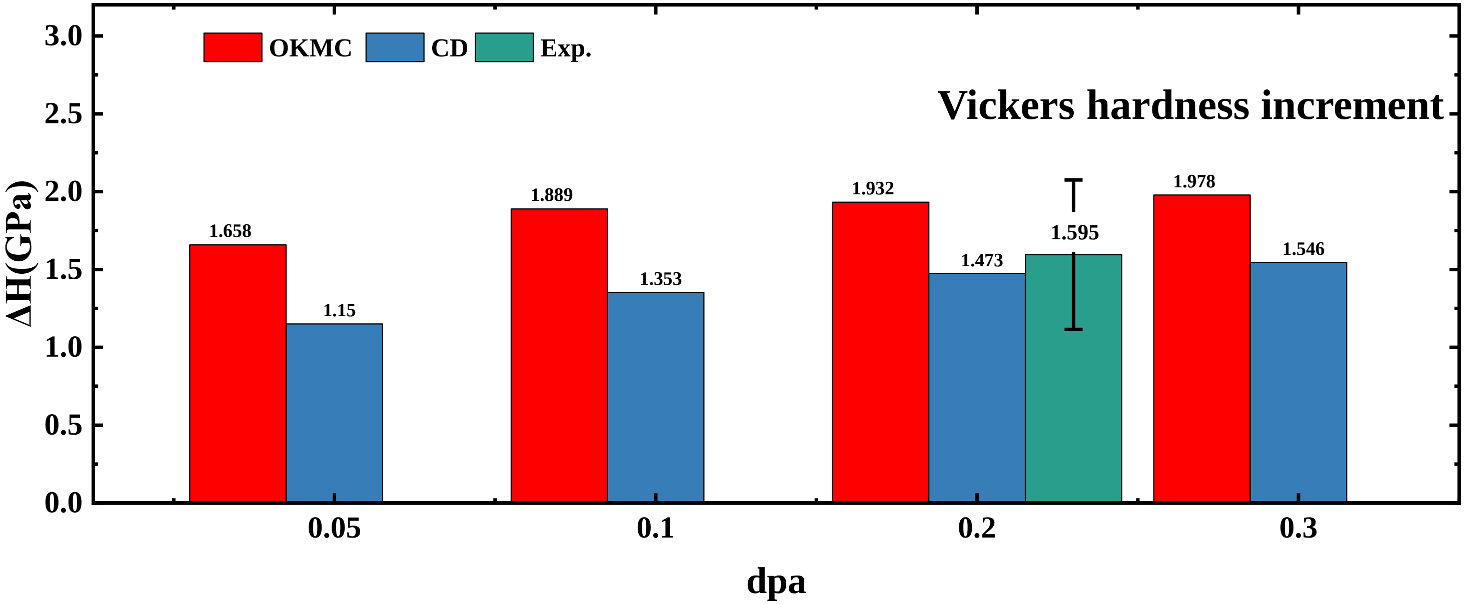


TEM images

BR2 reactor







Validation ③: He+W ion sequential irradiation

Quantifying the mechanical effects of He, W and He + W ion irradiation on tungsten with spherical nanoindentation

Jordan S. Weaver[1], Cheng Sun[2,3], Yongqiang Wang[2], Surya R. Kalidindi[4], Russ P. Doerner[5], Nathan A. Mara[1,6,*], and Siddhartha Pathak[7,*]

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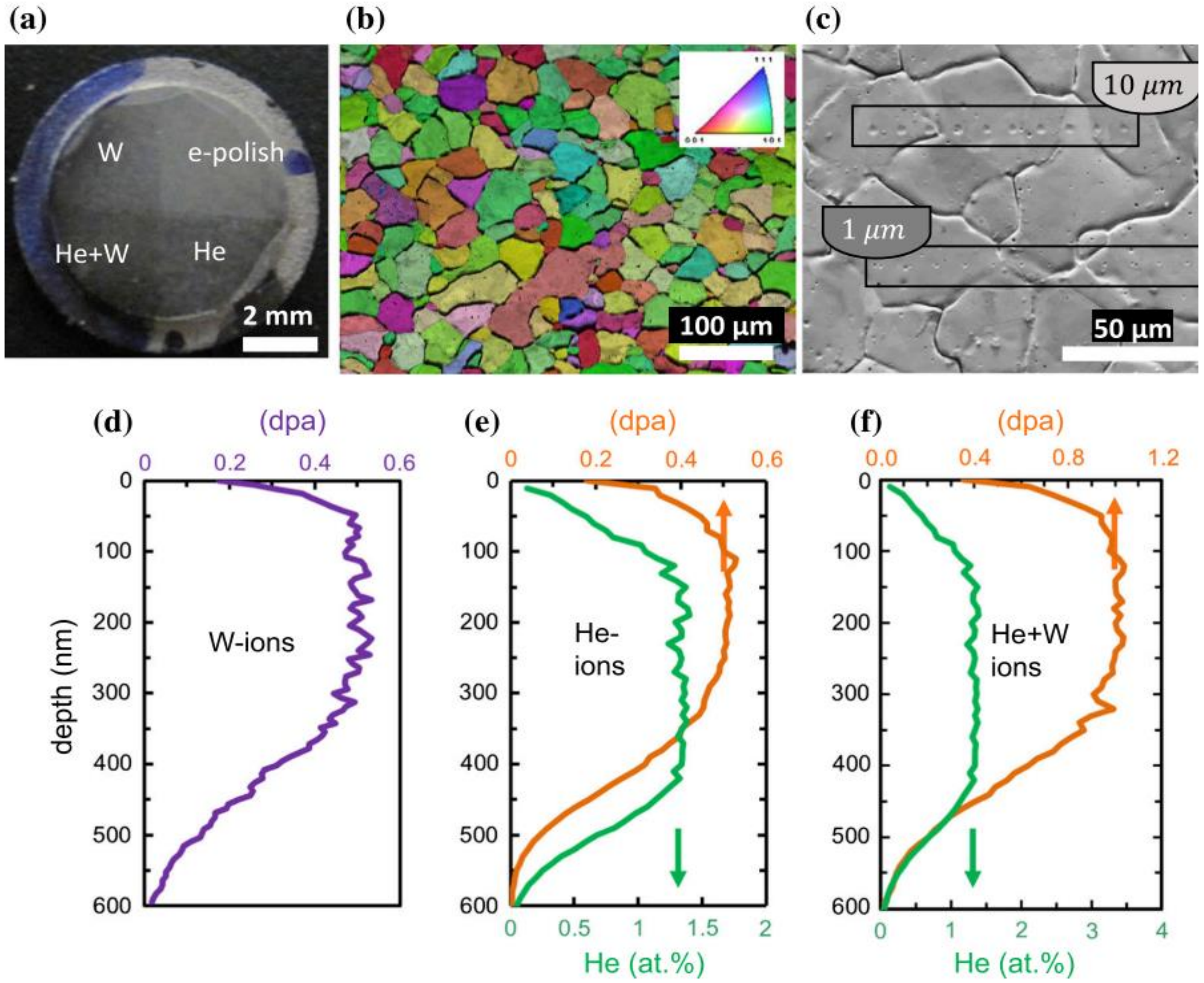
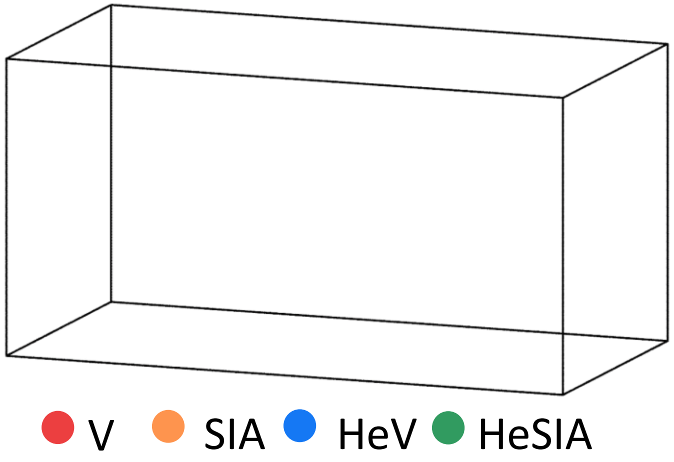
[2] Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, NM, USA
[3] Materials and Fuels Complex, Idaho National Laboratory, Idaho Falls, ID, USA

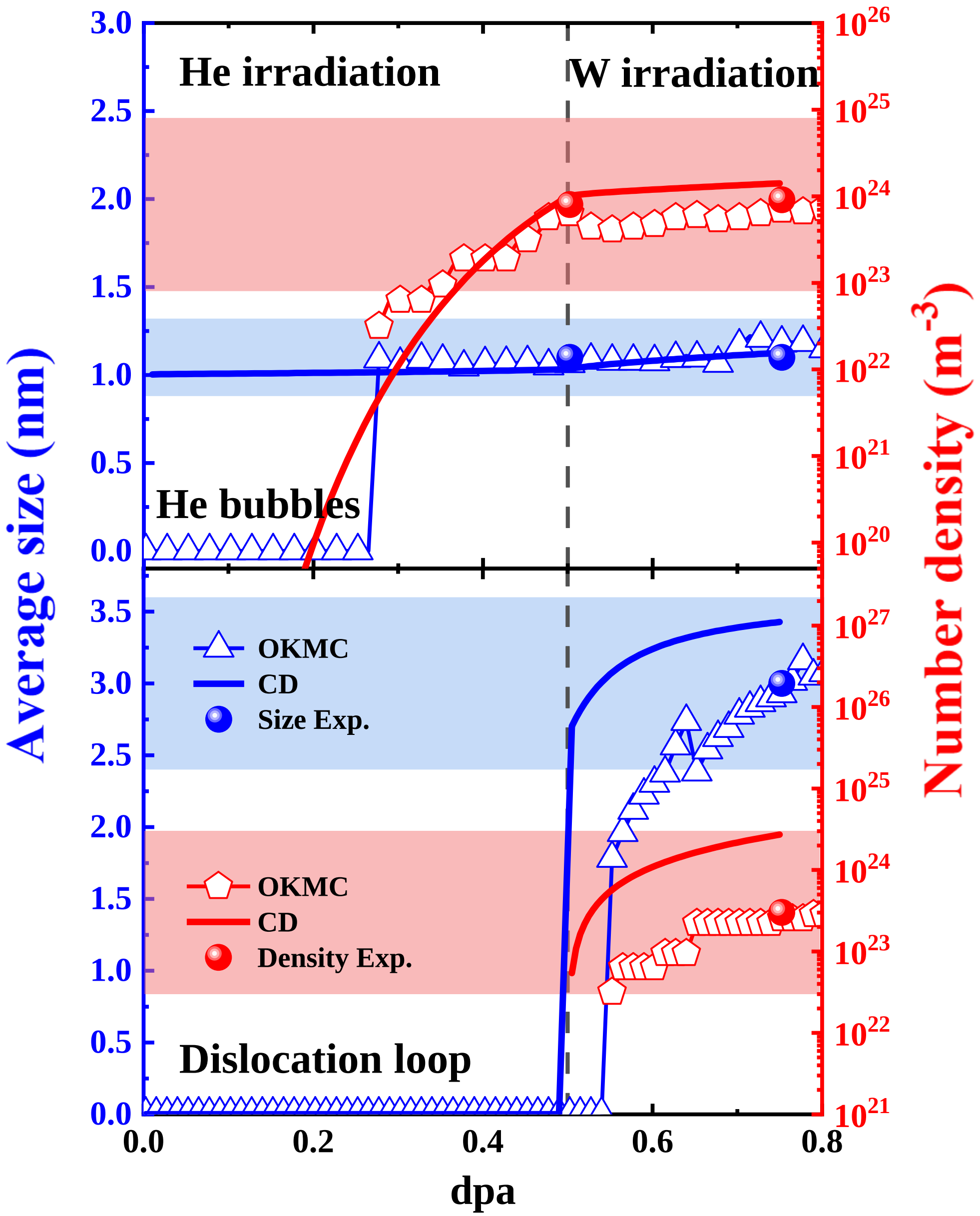


- **W material:** Room temperature, 35μm grain size
- He, W, and He+W sequential irradiation, **0.5dpa+0.25dpa** uniform damage region
- **He concentration: 1.5at%, 0.02 He/dpa**

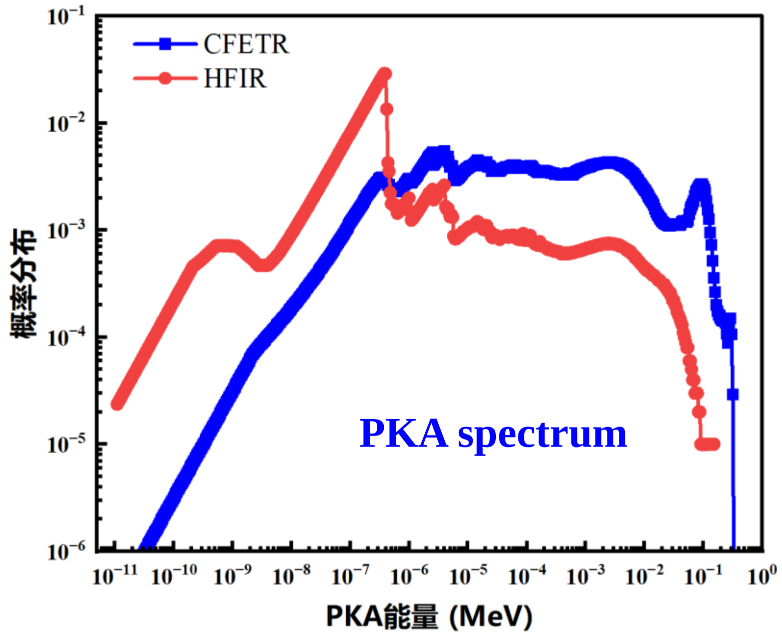
He+W ion sequential irradiation *0.75 dpa @ 363 K*

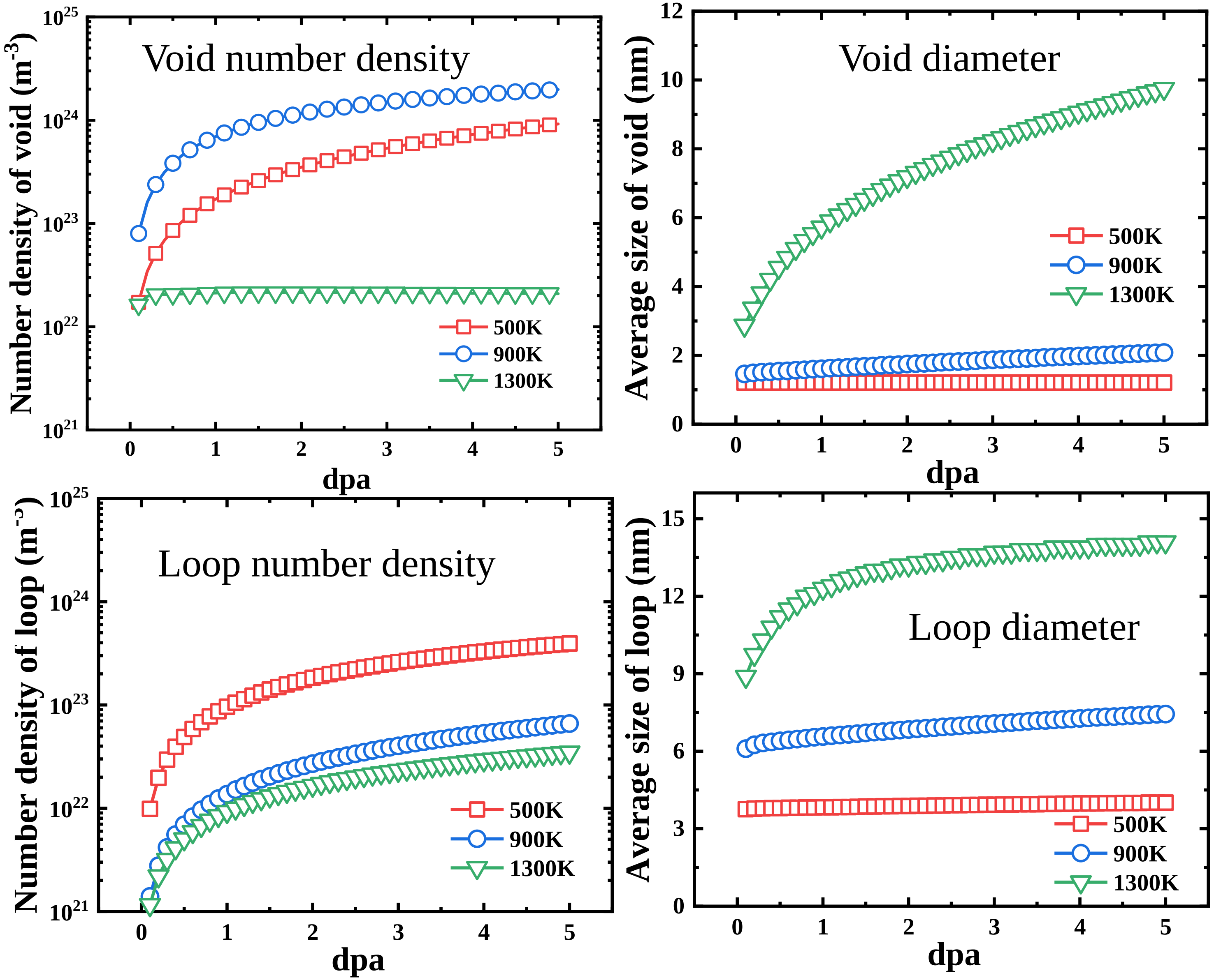


	He bubbles		*Dislocation loop*		*Void*	
	Diameter (nm)	Number density (10^{23} m^{-3})	Diameter (nm)	Number density (10^{23} m^{-3})	Diameter (nm)	Number density (10^{23} m^{-3})
Exp.-He	1.1	8.5	-	-	-	-
OKMC-He	**1.04**	**5.5**	-	-	-	-
CD-He	**1.03**	**9.9**	-	-	-	-
Exp.-He+W	1.1	9.1	3	3	-	-
OKMC-He+W	**1.18**	**6.94**	**2.92**	**2.52**	1.49	5.67
CD-He+W	**1.04**	**7.77**	**3.4**	**27**	1.39	3.7



Prediction CFETR：*5dpa, microstructure*





- Number density and average size: both gradually increases with irradiation dose.
- Temperature significantly increases the average size of voids/dislocation loops.

Outline

Strategy: Fusion materials simulation

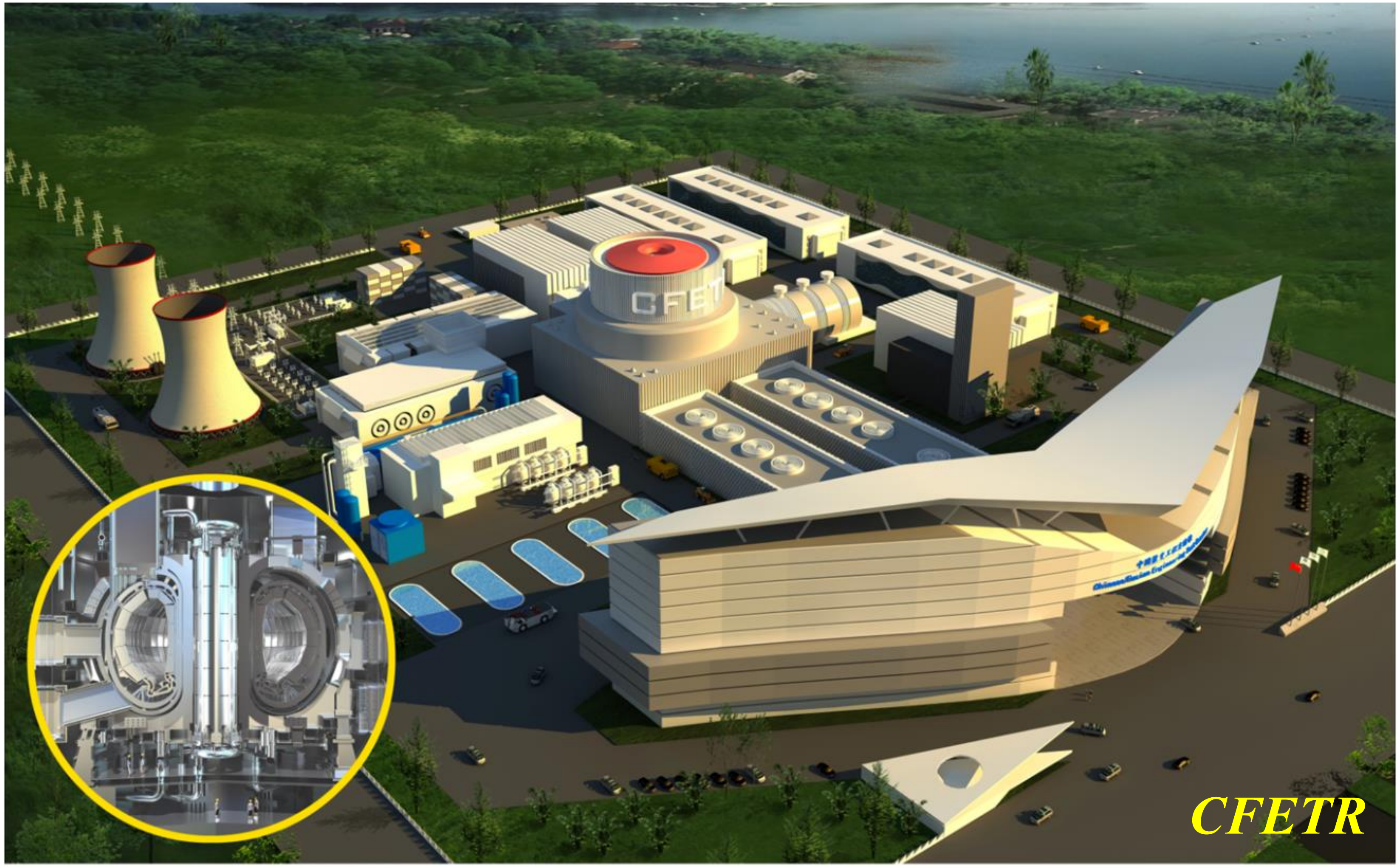
Simulation platform of neutron irradiation

Summary

Summary

- In order to achieve the nuclear fusion energy in 2050s, **a clear and phased roadmap** for the development of fusion reactor materials in China is produced, **including the modelling and simulation of fusion materials.**

- We have developed ***NINUM3***, a multi-scale modelling platform of materials under neutron irradiation, and ***Phase II for larger dose of fusion neutrons*** is under design and construction.



Fusion will be ready when society needs it, maybe even a short time before that

—— Lev Artsimovich, one of the founders of the tokamak