Decennial IAEA Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology, December 15-19, 2014

Behaviours of Hydrogen and Helium in tungsten: New Insights from Modelling & Simulation

Guang-Hong Lu

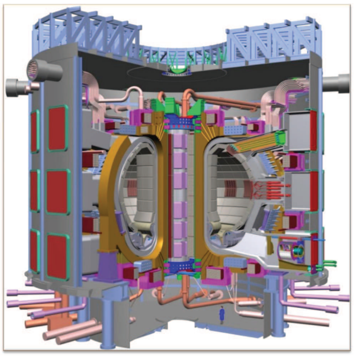
Beihang University
Beijing, China

Collaborators

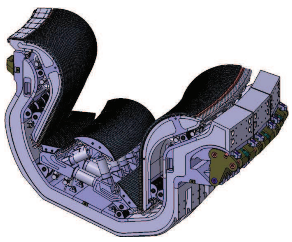
Fei Gao | Feng Liu | Hong-Bo Zhou | H.T. Lee | Wenqing Zhang

Guang-Nan Luo | Greg Temmeman | Y. Ueda | Yue-Lin Liu

Metallic materials for ITER & future fusion reactor



Full-W Divertor



Plasma facing materials: tungsten / molybdenum;
Structural materials: iron (RAFM) / vanadium

Body-centered cubic metal -based

The most promising metallic PFM: tungsten

Advantages

- High melting point; high thermal conductivity; low sputtering

Disadvantages

- High DBTT; recrystallization brittleness; high Z

Extreme 3-fold irradiations

- High heat flux: 10 MW/m^2 - several hundred MW/m^2
- H/He plasma: low energy (0 - 100 eV), high flux (> 10^{24} m^{-2}s^{-1})
- Neutron: 14.1 MeV → radiation damage

Role

- Withstand H/He/Heat flux

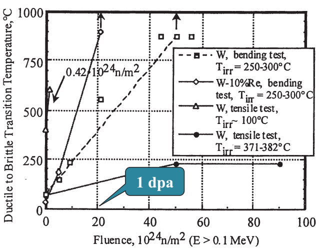
Neutron Irradiation

Neutron volumetric heating

- Neutron Wall Load: 1 - 5 MW/m^2

Property degradation

- hardening and increasing DBTT
- Swelling
- Degraded thermal conductivity



Influence of neutron irradiation on the DBTT

J.W. Davis, J. Nucl. Mater. 258-263 (1998) 308

Large Transmutation to Re and Os

	W	Re	Os	Ta
%	94	3.8	1.38	0.81

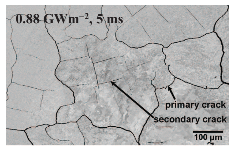
Full 5 years of DEMO conditions

Nucl. Fusion 51, 043005 (2011) .

High Heat Flux (HHF)

Steady state loads

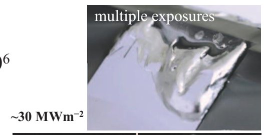
- 5-10 MW/m^2, $\triangle t$ = 450 s, n ~ 3000
  → recrystallization, embrittlement

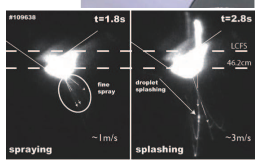


G. Pintsuk, Fusion Eng. Des. 82 (2007) 1720

Transients

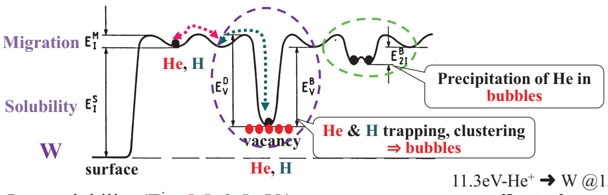
- ELMs: < 1GW/m^2, $\triangle t$ = 0.5 ms, n > 10^6
  thermal stress > yield stress
  → cracking, melting
- VDEs/disruption: up to 60 MJ/m^2
  temperature > melting point
  → melting





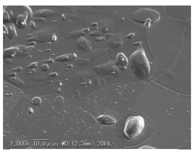
J.W. Coenen et al., J. Nucl. Mater. 415 (2011) S78

Hydrogen/helium Plasma Irradiation



- Low solubility (E^i_s: 5.5, 3.5 eV)
- Fast interstitial migration (E^i_m: 0.24, 0.35 eV)
- Deep trapping in vacancy (4.7, 1.4 eV) & grain boundary, dislocation (defect)

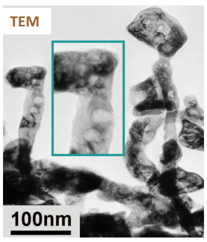
He & H agglomeration
→ bubble & blister
fuzz structure



38 eV-D$^+$→W @530K
10^{27} D/m^2

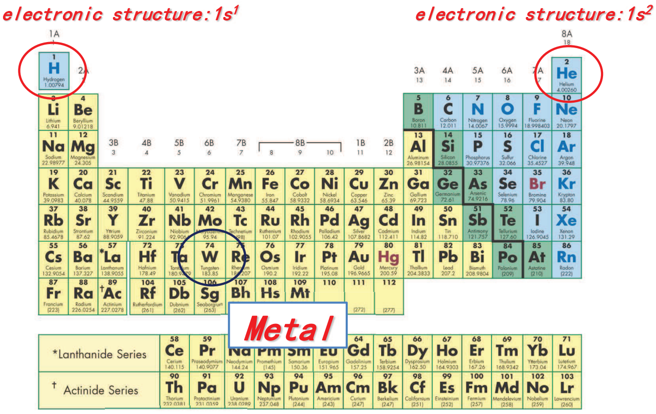
Alimov et al., Phys.Scr. 2009

11.3eV-He$^+$ → W @1250K,
3.5x10^{27}He$^+$/m^2



S. Kajita et al., Nucl. Fusion 47(2007) 1358.

electronic structure: 1s[1]　　*electronic structure: 1s[2]*



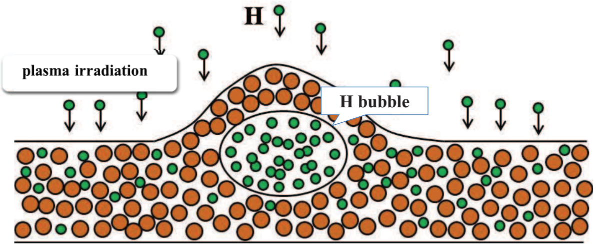
actinide metals

Do we fully understand H & He behaviors in metals?
(For plasma irradiation)

New insights: H & He behaviors in W

- **H bubble formation**
- **H bubble growth**
- **Critical H concentration for H bubble formation**
- **Stability of helium**
- **H-He synergistic effect**

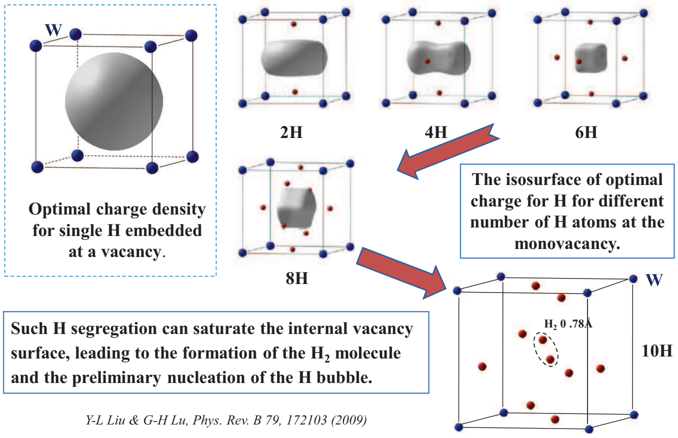
Mechanism for hydrogen bubble formation



Process of H bubble formation

retention → nucleation → growth → blistering → **Bubble control**

H occupation and accumulation in tungsten: optimal charge density (DFT)



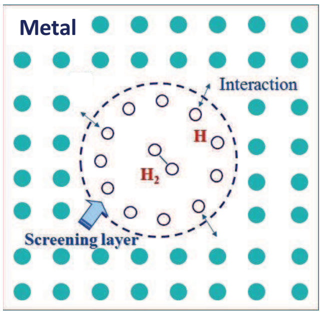
Optimal charge density for single H embedded at a vacancy.

The isosurface of optimal charge for H for different number of H atoms at the monovacancy.

Such H segregation can saturate the internal vacancy surface, leading to the formation of the H_2 molecule and the preliminary nucleation of the H bubble.

Y-L Liu & G-H Lu, Phys. Rev. B 79, 172103 (2009)

Vacancy-trapping mechanism of H in metals



Vacancy or vacancy-like defects（GB, dislocation）

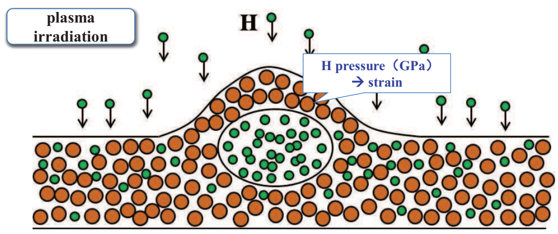
Phys. Rev. B 79, 172103 (2009); Nucl. Fusion 50, 025016 (2010); J. Nucl. Mater. 434, 395 (2013)

- **Enough space to provide an optimal charge density**

New insights: H & He behaviors in W

- **H bubble formation**
- **H bubble growth**
- **Critical H concentration for H bubble formation**
- **Stability of helium**
- **H-He synergistic effect**

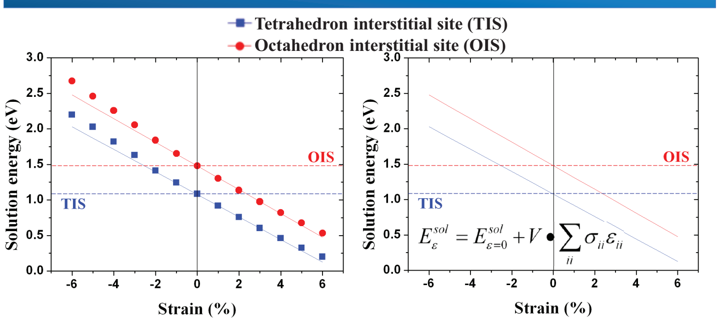
Hydrogen bubble growth: strain effect



Process of H bubble formation

retention → nucleation → growth → blistering → **Bubble control**

Dissolution of H in W under the isotropic strain



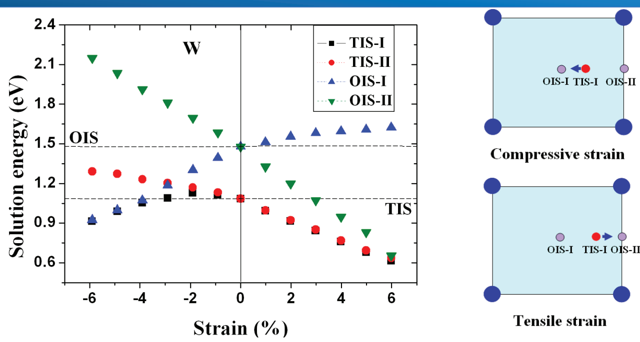
First-principle calculation

Linear elasticity theory

The H solution energy is a linear monotonic function of the triaxial strain.

Phys. Rev. Lett. 109, 135502 (2012); NIMB 269, 1731 (2011)

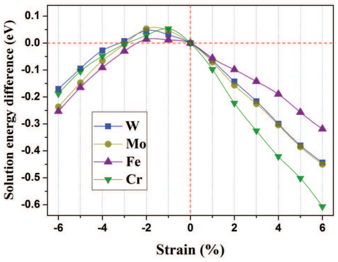
Dissolution of H in W under the anisotropic strain

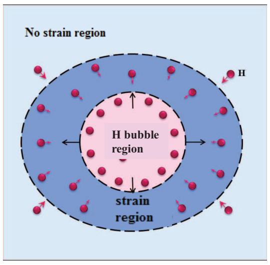


The solution energy of H “effectively” decreases with the increasing of both signs of anisotropic strain, due to the movement of H forced by strain.

Phys. Rev. Lett. 109, 135502 (2012)

Strain-triggered cascading effect on H bubble growth





Enhancing effect of anisotropic strain on H dissolution is also applicable to other bcc metals.

H accumulation → Bubble formation → Anisotropic strain in W ↓

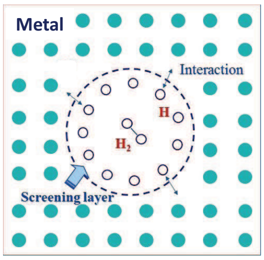
...... ← Bubble growth ← Enhancing H solubility

Phys. Rev. Lett. 109, 135502 (2012)

New insights: H & He behaviors in W

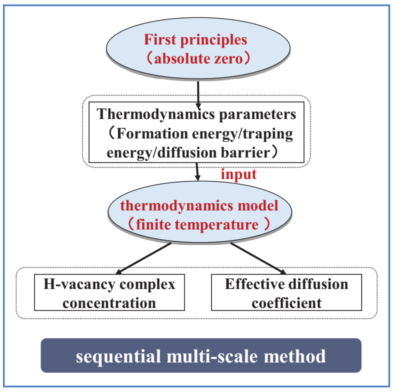
- H bubble formation
- H bubble growth
- Critical H concentration for H bubble formation
- Stability of helium
- H-He synergistic effect

Critical H concentration for formation and rapid growth of H bubble



Critical concentration

L. Sun, S. Jin, Wenqing Zhang, G.-H. Lu, Lee, Ueda, J Phys: Condens Matter (2014)



Critical H concentration for formation and rapid growth of H bubble

First principles + thermodynamics model ： sequential multi-scale method

H-vacancy complex concentration

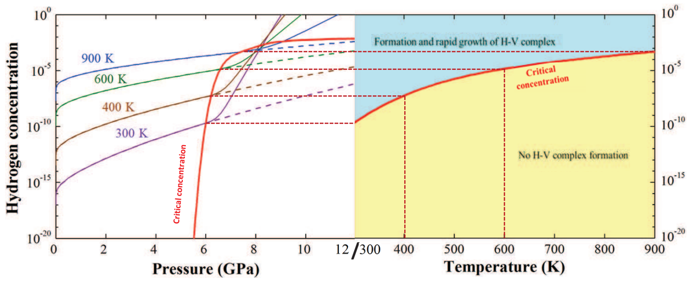
$$c_{H_v} = \sum_{n}^{n_{max}} n\Omega_0 \exp\left(-\frac{E^{formation}_{H_nV}}{k_BT}\right)$$

Formation energy

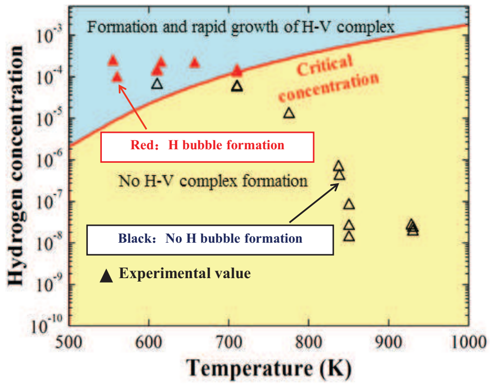
$$E^{formation}(X) = E_{tot}(X) - E_{tot}(bulk) - \sum_i n_i\mu_i$$

H chemical potential

$$\mu_H = \mu_H(T=0K) + \mu_H(T,p)$$



Critical H concentration for H bubble formation: Comparison with experiments



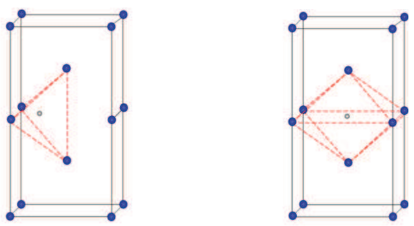
Experiments： Peng, Lee and Ueda, J Nucl Mater 438 (2013) S1063

New insights: H & He behaviors in W

- H bubble formation
- H bubble growth
- Critical H concentration for H bubble formation
- Stability of helium
- H-He synergistic effect

Effective volume of helium

Body-centered cubic system



（TIS） （OIS）

- volume： $V_{OIS} > V_{TIS}$ ➡ stability： $S_{OIS} > S_{TIS}$
- solution energy： $E_{OIS} > E_{TIS}$ ➡ stability： $S_{OIS} < S_{TIS}$?

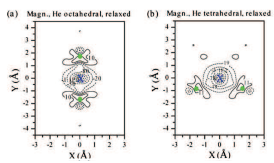
Several factors affecting the stability of helium in metals

TABLE II. Magnetic moment μ of He defect and its neighboring Fe atoms separated from He by the distance r.

	He	1st Fe		2nd Fe	
	μ (μ_B)	r (Å)	μ (μ_B)	r (Å)	μ (μ_B)
octa, unrelaxed	0.012	1.41	1.67	1.99	2.17
octa, relaxed	0.015	1.66	2.01	2.09	2.24
tetra, unrelaxed	0.007	1.58	1.99	2.54	2.17
tetra, relaxed	0.012	1.76	2.15	2.57	2.21
sub, unrelaxed	0.000	2.45	2.25	2.83	2.08
sub, relaxed	0.000	2.47	2.29	2.85	2.11

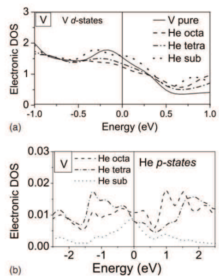
Magnetism, He in Fe

Phys. Rev. Lett. 94, 046403 (2005)



Bonding properties

Phys. Rev. B 80, 054104 (2009)



Hybridization

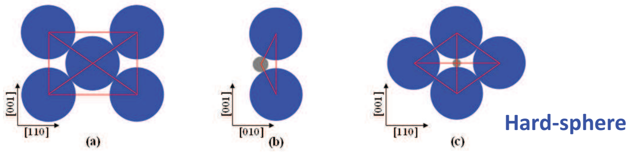
Phys. Rev. B 78, 134103 (2008)

Close-shell structure of He ?

Lattice model：a qualitative description of the effective helium volume

Interstitial helium volume based on different models

Lattice model	V_{TIS} (a^3)	V_{OIS} (a^3)	V_{TIS}/V_{OIS}
Point-lattice	1/12	1/3	0.25
Voronoi	25.68%	25.11%	1.02
Hard-sphere	0.84%	0.13%	6.46

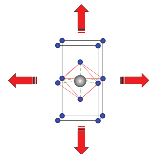


Bulk TIS OIS

The accuracy of the effective helium volume calculation depends on the employed lattice model. Hard-sphere model gives a precise description of the effective helium volume compared with other lattice models.

Euro Phys Lett 96, 66001 (2011)

Stress tensor：A quantitative indicator of effective helium volume in metals



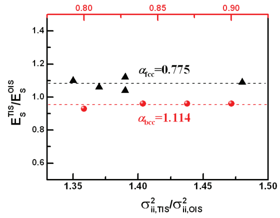
The He-induced stress

the He-induced stress (in Gpa) in bcc metals

		W	Mo	Fe	Cr	V
σ_{TIS}	XX=ZZ	-1.97	-1.79	-2.54	-2.29	-1.31
	YY	-1.87	-1.76	-2.61	-2.59	-1.79
σ_{OIS}	XX=YY	-1.58	-1.48	-2.38	-1.98	-1.59
	ZZ	-2.89	-2.55	-3.24	-3.44	-1.81

$$E_s \sim \sigma_{ii}^2 / B$$

$$\frac{E_s^{TIS}}{E_s^{OIS}} = \alpha \cdot \frac{\sigma_{ii,TIS}^2}{\sigma_{ii,OIS}^2}$$



- Stress tensor could be used to indicate the effective helium volume in metals, thus has an influence on the solution of helium.
- The stability of helium in metals depends on the effective volume.

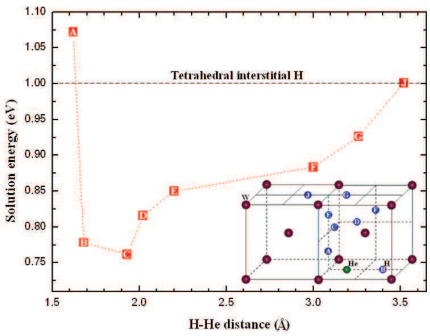
Euro Phys Lett 96, 66001 (2011)

New insights: H & He behaviors in W

- H bubble formation
- H bubble growth
- Critical H concentration for H bubble formation
- Stability of helium
- H-He synergistic effect

Synergistic behaviors of H & He in intrinsic W

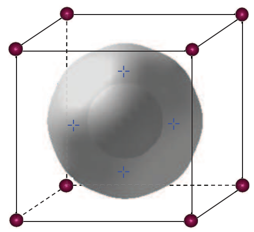
H. B. Zhou & G-H Lu, *Nucl. Fusion* (2010)



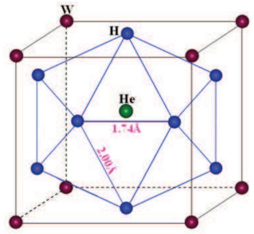
- Solution energy of H：0.76 eV, 0.23eV lower than that of TIS in W without He.
- H-He binding energy in intrinsic W: 0.23 eV; **attractive interaction**

Suppressing H bubble via inert gas elements

- **Inert gas element（He/Ne/Ar）: closed shell electronic structure**



Optimal charge isosurface for a single H embedded at He-vacancy complex.

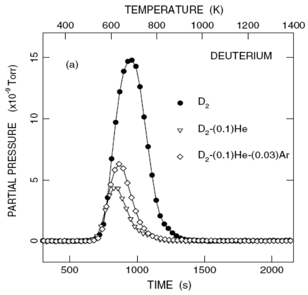


Atomic configuration of H at He-vacancy complex.

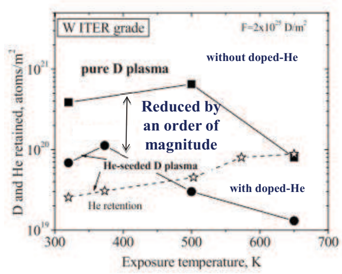
Inert gas elements cause a redistribution of charge density inside the vacancy to make it "not optimal" for the formation of H_2 molecule, which can be treated as a preliminary nucleation of the H bubbles.

H-B Zhou & G-H Lu, Nucl. Fusion 50, 115010 (2010)

Reduced retention of D by He in experiments



M.J. Baldwin, Nucl Fusion 51, 103021 (2011)



O.V. Ogorodnikova, J Appl Phys 109, 013309 (2011)

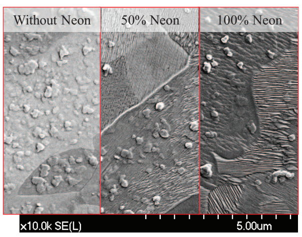
Effect of He on D retention

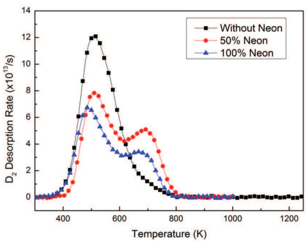
Helium is the product of fusion reaction, and thus the H bubble may be able to be suppressed by controlling the content of He in fusion process.

Effect of Ne Irradiation on D Retention in W

Experiment Set-up

- Sequential exposure of W to Ne and D plasma.
- T_{surf} (~250 °C) and D Fluence (1×10^{26} D) were fixed.
- Ratio of Ne to D is 0, 50% and 100%.





- Ripple structure on W surface evolved with increasing neon fluence;
- Ripple co-existed with D-induced blistering;
- D desorption at 700K : visible after neon irradiation;
- Total D retention reduced by a factor of 1.6 in maximum.

IOP Publishing | International Atomic Energy Agency Nuclear Fusion

Nucl. Fusion 54 (2014) 086001 (21pp) doi:10.1088/0029-5515/54/8/086001

Special Topic

A review of modelling and simulation of hydrogen behaviour in tungsten at different scales

Guang-Hong Lu[1], Hong-Bo Zhou[1] and Charlotte S. Becquart[2]

[1] Department of Physics, Beihang University, Beijing 100191, People's Republic of China
[2] Unité Matériaux et Transformations (UMET), UMR CNRS 8207, Université de Lille 1, ENSCL, F-59655 Villeneuve d'Ascq Cedex, France

E-mail: LGH@buaa.edu.cn (G.-H. Lu)

Received 9 September 2013, revised 11 February 2014
Accepted for publication 13 February 2014
Published 24 July 2014

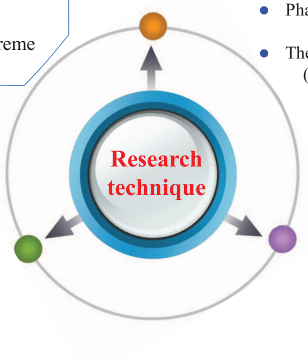
Abstract

Tungsten (W) is considered to be one of the most promising plasma-facing materials (PFMs) for next-step fusion energy systems. However, as a PFM, W will be subjected to extremely high fluxes of low-energy hydrogen (H) isotopes, leading to retention of H isotopes and blistering in W, which will degrade the thermal and mechanical properties of W. Modelling and simulation are indispensable to understand the behaviour of H isotopes including dissolution, diffusion, accumulation and bubble formation, which can contribute directly to the design, preparation and application of W as a PFM under a fusion environment. This paper reviews the recent findings regarding the behaviour of H in W obtained via modelling and simulation at different scales.

Keywords: tungsten, hydrogen, modelling and simulation, fusion

Techniques to investigate material properties under extreme fusion conditions

Fusion-related material tests
- Limited Tokamaks
- Coupled parameters
- Material tests under extreme conditions

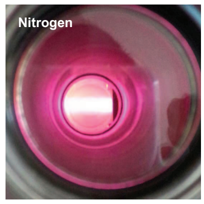


Computational Simulation
- First principles (electronic scale)
- Molecule dynamics (atomic scale)
- Phase Field (mesoscale)
- Thermodynamics (continuous scale)

Tokamak Experiments
- Tokamak (EAST-MAPES)

Experimental Simulation
- Linear device
- Ion beam
- Electron beam
- Neutron source

Linear plasma generator: STEP



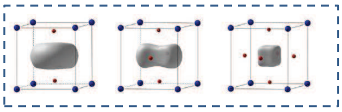
Ion energy: 0-100 eV
Ion flux: 10^{22} $m^{-2}s^{-1}$

Summary

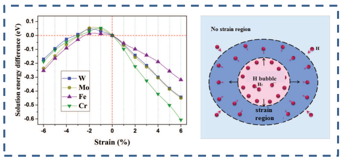
H & He behavior in W: new insights
- **Key issue to solve material problem for fusion reactor**
- **More complicated than expected**
- **Needs more exploration.**

Lattice model	V_{TIS} (a^3)	V_{OIS} (a^3)	V_{TIS}/ V_{OIS}
Point-lattice	1/12	1/3	0.25
Voronoi	25.68%	25.11%	1.02
Hard-sphere	0.84%	0.13%	6.46

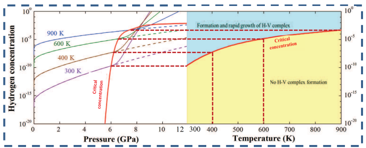
Effective helium volume in metals: a stress tensor indicator
(first principles) (Euro Phys Lett 2011)



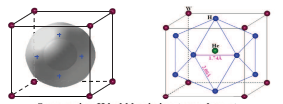
H occupation and accumulation in metals: optimal charge density
(first principles & molecular dynamics)
(Phys Rev B 2009,2013; J Nucl Mater 2011,2013; AIP Advances 2014)



H bubble growth: strain-triggered cascading effect
(first principles & sequential multi-scale method) (Phys Rev Lett 2012)



H bubble formation: critical concentration for rapid growth
(Sequential multi-scale method : first principles & thermodynamics model)
(J Phys Condens Matt 2014)



Suppressing H bubble via inert gas elements
(first principles & Uniform electron gas model)
(H-B Zhou & G-H Lu, Nucl. Fusion 50, 115010 (2010))