Plasma Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices, IAEA, Vienna, November 26-28, 2013

Modeling and Simulation of Behaviors of Hydrogen, Helium and their Synergy in Irradiated Tungsten

Guang-Hong Lu

Beihang University

Tungsten: most promising PFM in future fusion devices

Why

- High melting point; high thermal conductivity; low sputtering

Extreme environment (3-fold irradiations)

- H/He plasma : low energy (0-100 eV), high flux (> 10^{24} $m^{-2}s^{-1}$)
- High heat flux: 10 MW/m^2 → several hundred MW/m^2
- Neutron : 14.2 MeV → radiation damage

Role

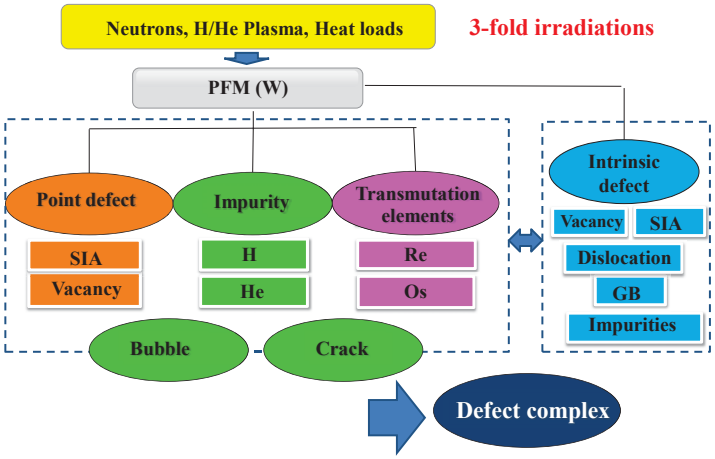
- Withstand H/He/heat flux

Requirement

- Structure integrity even at the high temperature

Defect formation, surface sputtering & erosion, blistering, cracking, degradation of mechanical properties

Irradiation-induced defects



H/He behaviors in irradiated W

- **The interaction of H/He and defects induced by irradiation coupled with intrinsic defects will be more complicated .**
- **How the H (and its isotopes) and He retention and blistering varies in W with irradiated defects is a key concern after deuterium-tritium reaction in the future fusion reactor.**
- **It is clear that to understand this requires a comprehensive knowledge from an atomic to a macroscopic point of view.**
- **Apart from the experiment, computer simulation at different scales will play an indispensable role on this aspect especially for simulation of the neutron irradiation.**

Hydrogen/helium interaction with defects in tungsten

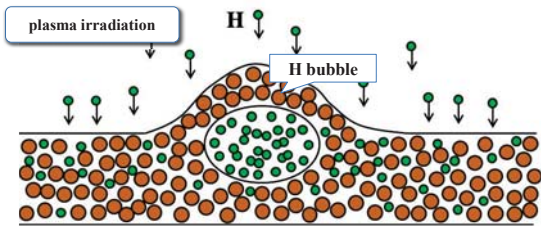
I Vacancy trapping mechanism for H bubble formation

II Strain-triggered cascading growth of H bubble

III Critical H concentration for formation and rapid growth of H bubble

Part *I*

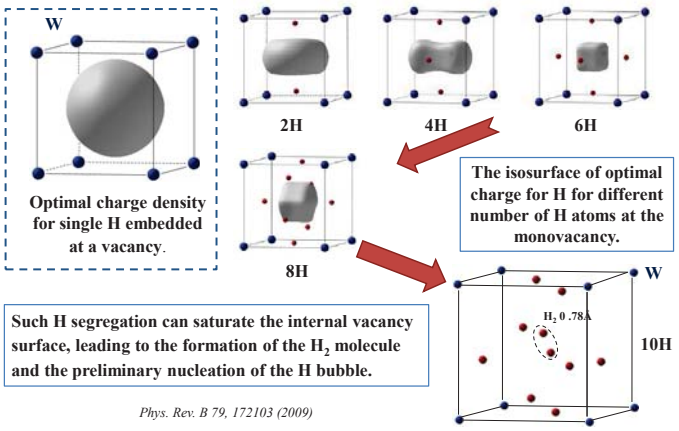
Mechanism for H bubble formation (nucleation) in W （First-principles method）



Process of H bubble formation

retention → nucleation → growth → blistering → Suppression of H bubble

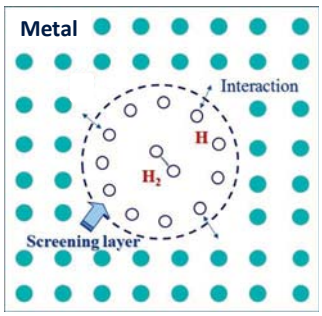
H occupation and accumulation in metals: optimal charge density



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.

Phys. Rev. B 79, 172103 (2009)

Vacancy-trapping mechanism of H in metals



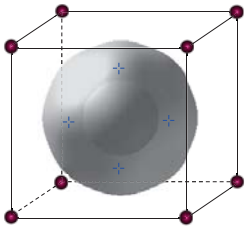
Vacancy or vacancy-like defects（GB, dislocation ）

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

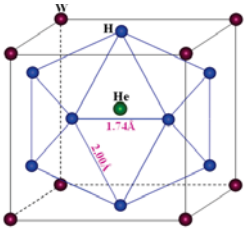
- **Enough space to provide an optimal charge density**

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.

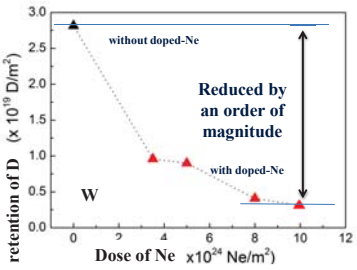


Atomic configuration of H at He-vacancy complex.

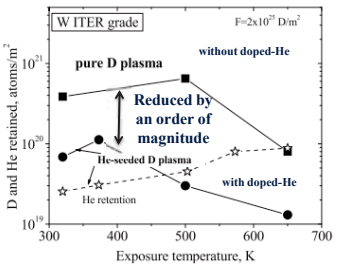
Inert gas elements cause a redistribution of charge density inside the vacancy to make it "not optimal" for the formation of H_2 molecule, which can be treated as a preliminary nucleation of the H bubbles.

Nucl. Fusion 50, 115010 (2010)

Suppressing H bubble formation by inert gas elements (Experiments)



Effect of Ne on D retention



Effect of He on D retention

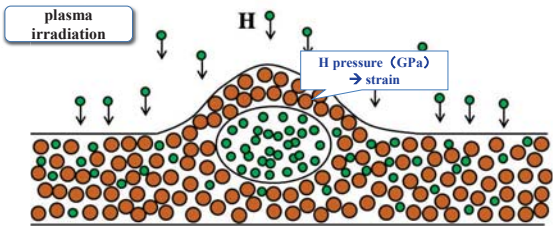
Long Cheng, G.-H. Lu, to be pubished

O.V. Ogorodnikova, J Appl Phys 109, 013309 (2011); M.J. Baldwin, Nucl Fusion 51, 103021 (2011)

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.

Part *II*

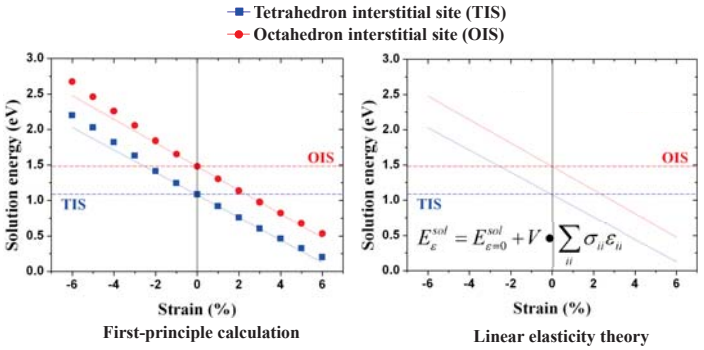
Strain-triggered cascading effect on H bubble growth （First-principles method）



Process of H bubble formation

retention → nucleation → growth → blistering → Suppression of H bubble

Dissolution of H in W under the isotropic strain



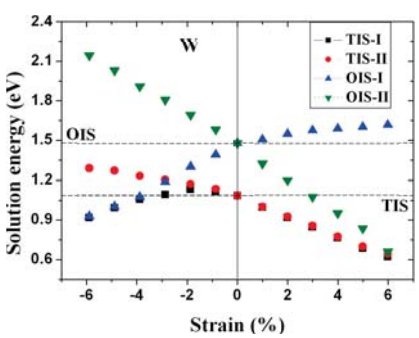
First-principle calculation

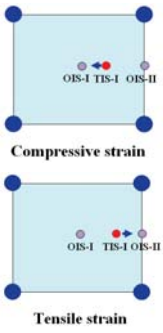
Linear elasticity theory

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

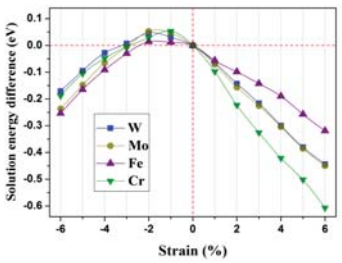


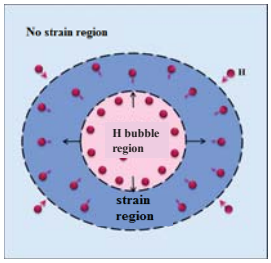


The solution energy of H "effectively" decreases with the increasing of both signs of anisotropic strain, due to the movement of H forced by strain.

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 → Enhancing H solubility → bubble growth → ……

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

W-H-He potentials for molecular dynamics simulations (X-C Li, G-H Lu, J Nucl Mater 2011, 2012)

- Modified W-H-He atomic potential
  - Bond-order potential (3-body)
- H/He behaviors in W
  - H_2 formation in W & Role of vacancy
  - H-induced vacancy formation
  - Temperature effects & dynamics

$$E = \sum_{i>j} f_{ij}^c(r_{ij})[V_{ij}^R - \frac{b_{ij}+b_{ji}}{2}V_{ij}^A(r_{ij})]$$

$$V^R(r) = \frac{D_0}{S-1}\exp[-\beta\sqrt{2S}(r-r_0)]$$

$$V^A(r) = \frac{SD_0}{S-1}\exp[-\beta\sqrt{2/S}(r-r_0)]$$

$$f^c(r) = \begin{cases} 1, & r \le \text{R - D} \\ \frac{1}{2} - \frac{1}{2}\sin(\frac{\pi}{2}(r-R)/D), & |R-r| \le D \\ 0, & r \ge R+D \end{cases}$$

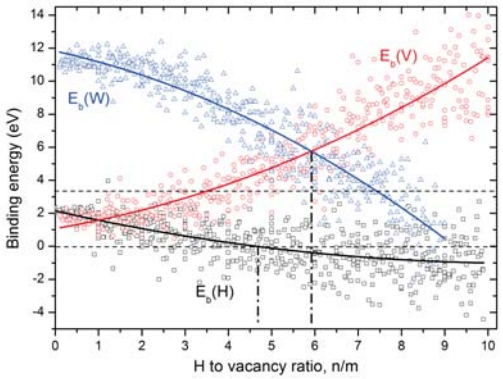
$$b_{ij} = (1+\chi_{ij})^{-1/2}$$

$$\chi_{ij} = \sum_{k(\neq i,j)} f_{ik}^c(r_{ik}) g_{ik}(\theta_{ijk}) \exp[\alpha_{ijk}(r_{ij}-r_{ik})]$$

$$g(\theta) = \gamma(1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h+\cos\theta)^2})$$

Growth of H/He bubble – molecular dynamics simulation

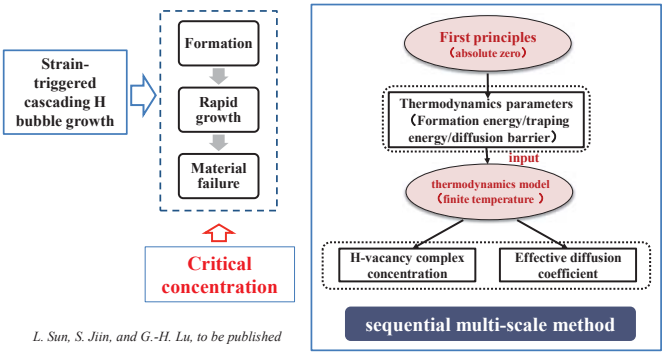
X-C Li, G-H Lu, to be published



Growth of H bubble: $V_m \rightarrow V_mH_n \rightarrow V_mH_n + V_x \rightarrow V_{m+x}H_n + H_x$

Part *III*

Critical H concentration for formation and rapid growth of H bubble



L. Sun, S. Jiin, and G.-H. Lu, to be published

Critical H concentration for H bubble formation

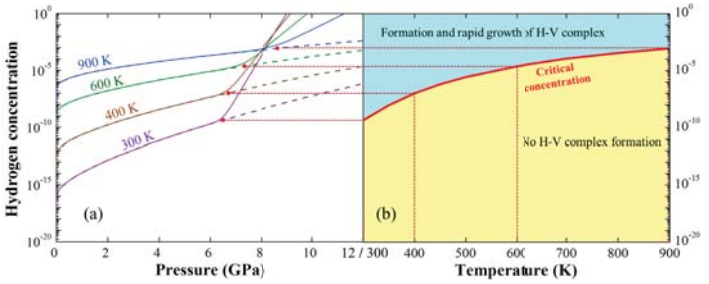
First principles + Thermodynamics model: Sequential multi-scale method

H-vacancy complex concentration

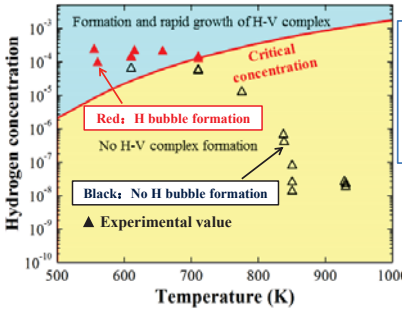
$$c_{H_v} = \sum_{n}^{n_{max}} n\Omega_0 \exp(-\frac{E_{H_nV}^{formation}}{k_B T})$$

Defect 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



The predicted H critical concentration for H bubble formation in W is consistent with experimental observations.

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

Predicted critical H concentration may serve as a criterion to evaluate the H-induced failure of PFMs in further fusion reactor

Hydrogen & helium in tungsten

- Intrinsic tungsten
- Vacancy
- Grain boundary
- Surface
- He-H interaction
- Impurity & alloying elements

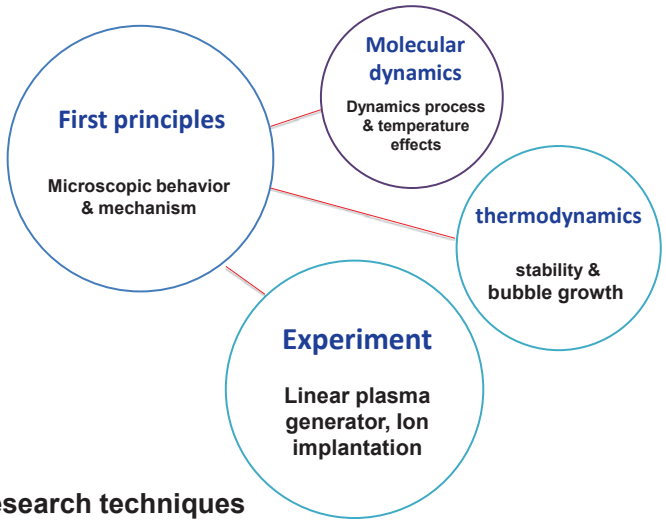
Modeling and simulation of hydrogen behavior in tungsten at different scales

Guang-Hong Lu and Hong-Bo Zhou
Department of Physics, Beihang University, Beijing 100191, China
Charlotte S. Becquart
Unité Matériaux et Transformations (UMET), UMR CNRS 8207, Université de Lille 1, ENSCL, F-59655 Villeneuve d'Ascq Cedex, France

Abstract:

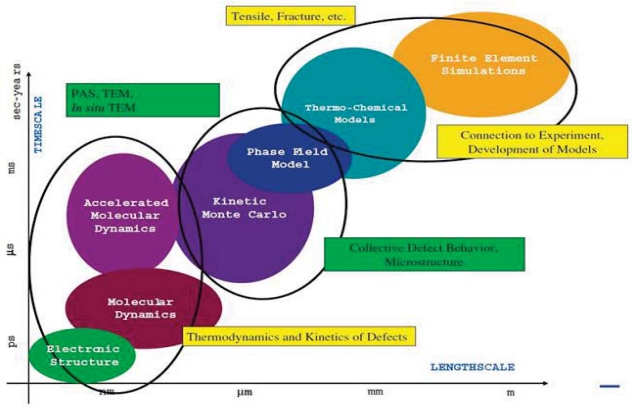
Tungsten (W) is considered to be one of the most promising plasma facing materials for next-step fusion energy systems. However, the retention and the blistering of hydrogen (H) isotopes in W remain to be a key issue that needs to be explored. Modeling and simulation are indispensable to understand the behavior of H isotopes including dissolution, diffusion, accumulation, and blistering, which can contribute directly to design, preparation, and application of W as a plasma facing material under a fusion environment. This paper reviews the recent findings regarding the behavior of H in W obtained via modeling and simulation at different scales.

Review paper



Research techniques

Hydrogen/helium & their synergy in irradiated tungsten



Thanks for your attention!