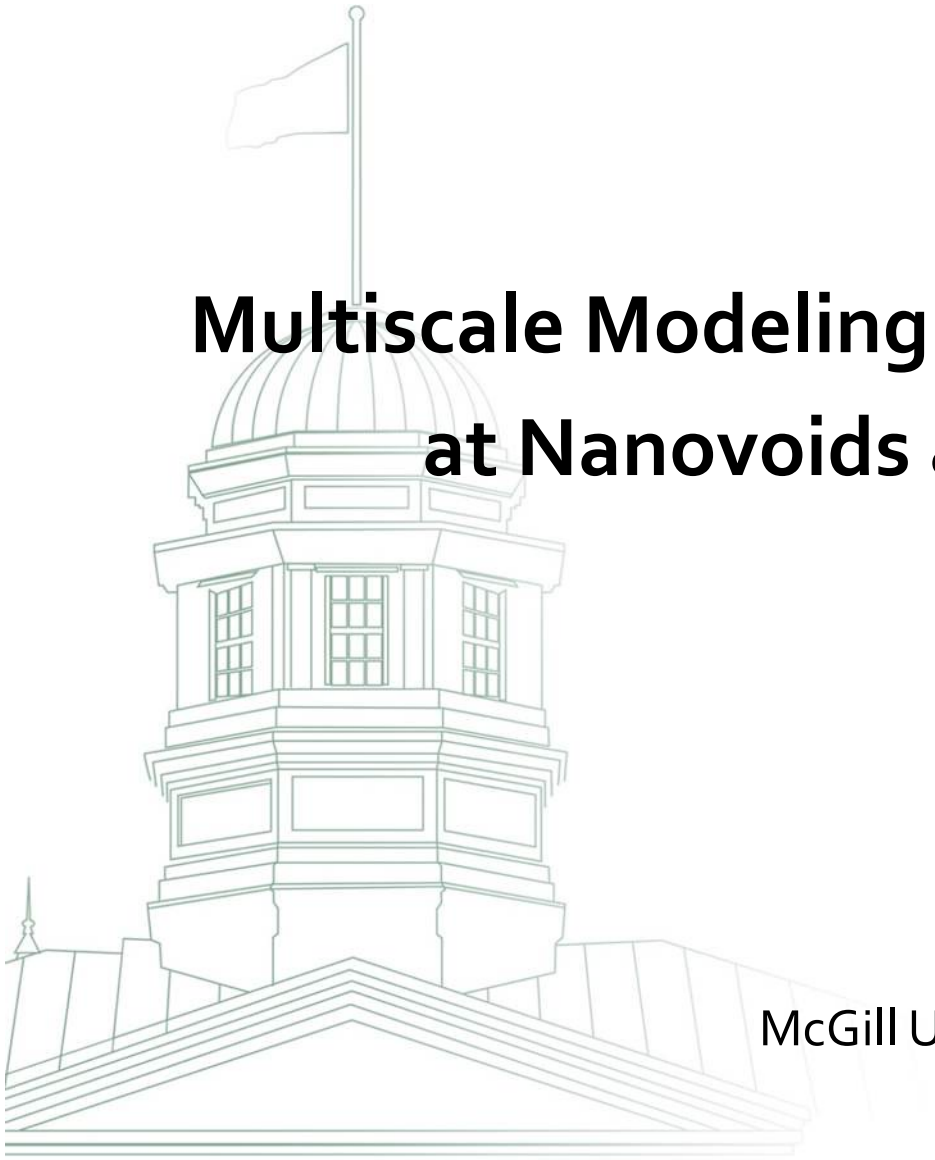


Multiscale Modeling of Hydrogen Trapping and Clustering at Nanovoids and Dislocations in BCC Metals

Jun Song

Materials Engineering

McGill University, Montréal, Quebec, Canada

Introduction

Why hydrogen matters

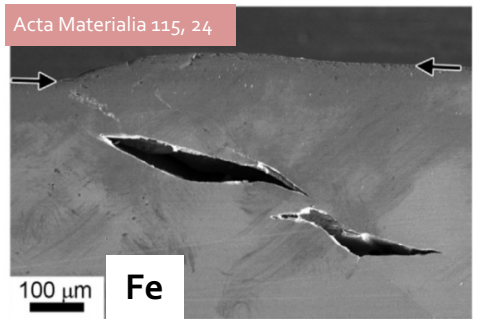
High H chemical potential

- Acid environments
- Pressurized H_2 storage
- Nuclear fusion reactor

Structural failures in metals

- Embrittlement
- Porosity/swelling
- Bubble/blister formation

H interact with ***defects*** in metals



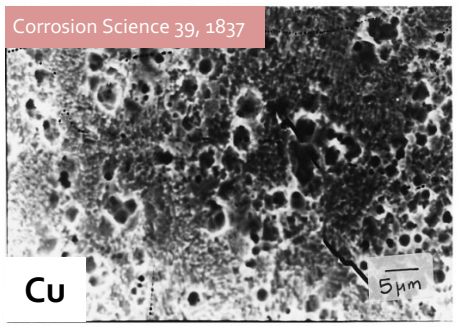
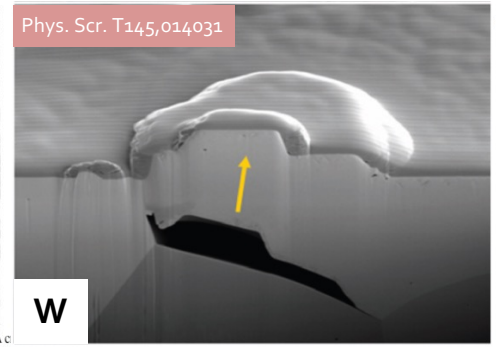
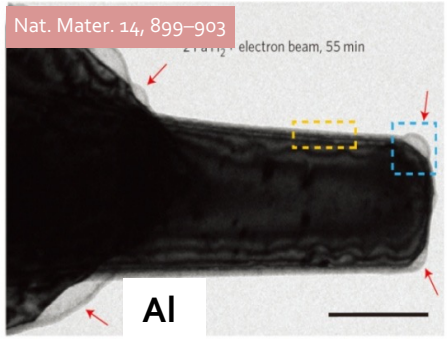


Fig. 7. Hydrogen-induced blistering on the surface of α-brass specimen charged at 85 mA c
for 24 hours.

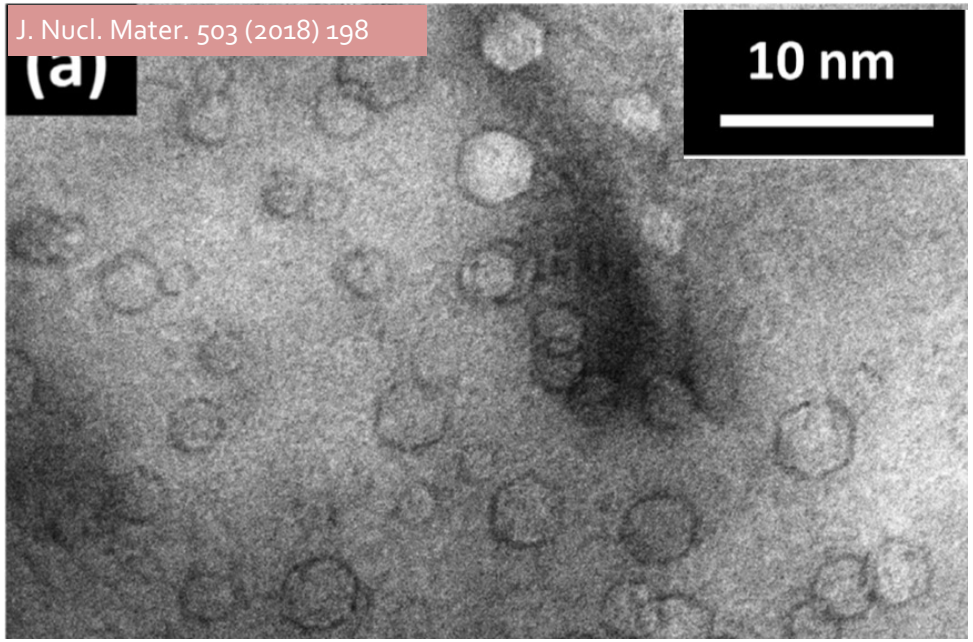




Introduction

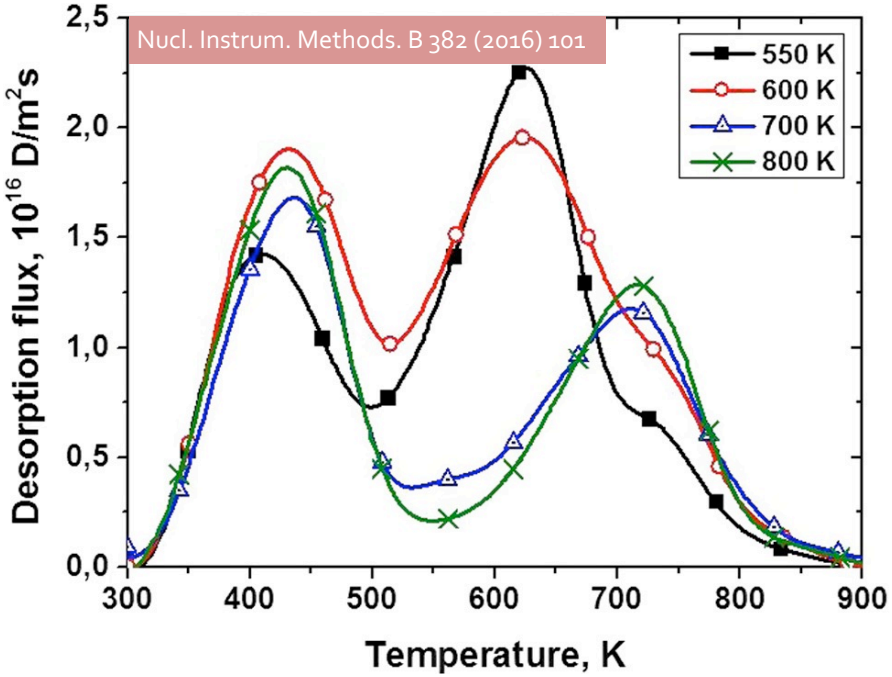
However, H-defect interactions at nanoscale remain *challenging*…

SEM/TEM



- To get atomic scale resolution
- To do *in situ* observations under irradiation

Thermal desorption spectrum



- To quantify contributions from different defects

Outline :

➢ H-nanovoid

- ❖ Structures and energies of nanovoids
- ❖ Hydrogen trapping in nanovoids

➢ H-dislocation

- ❖ H clustering at dislocations
- ❖ H stabilized junction and loop formation

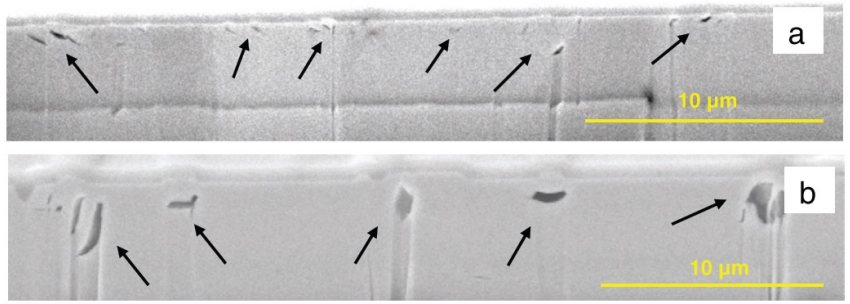
H-wall reaction in fusion reactor

Plasma facing materials

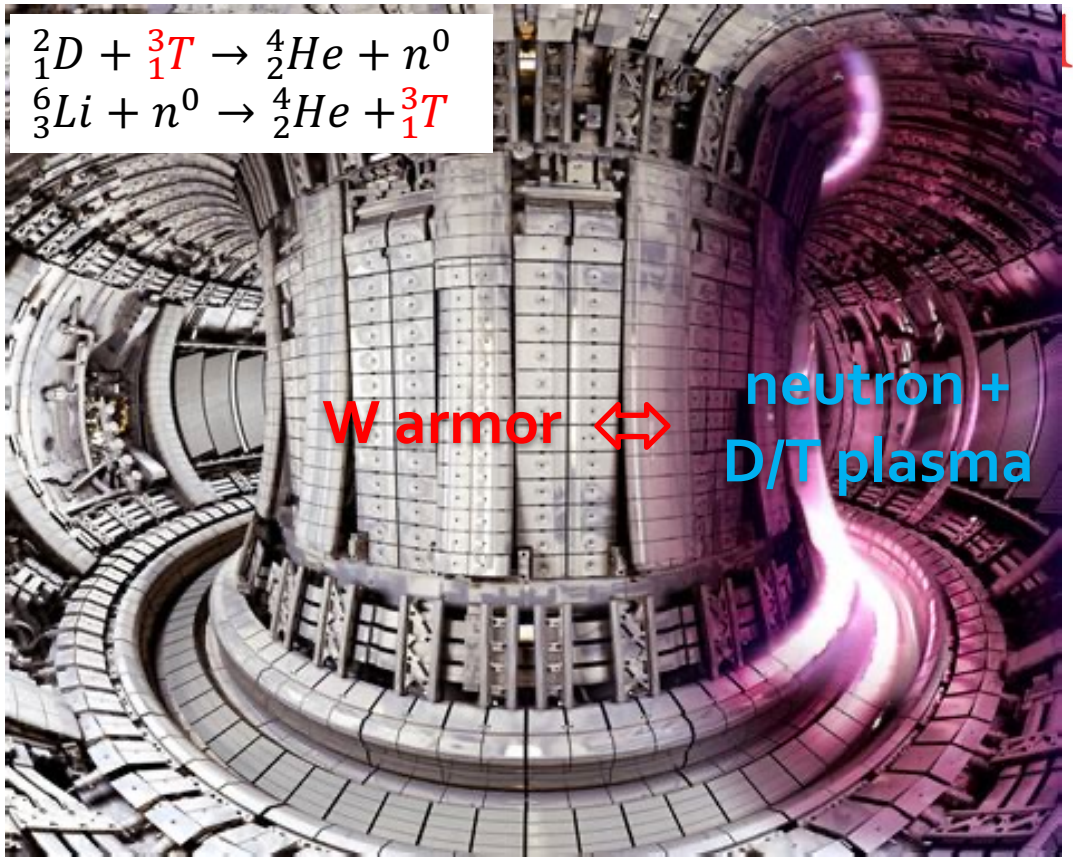
Neutron irradiation + D/T plasma

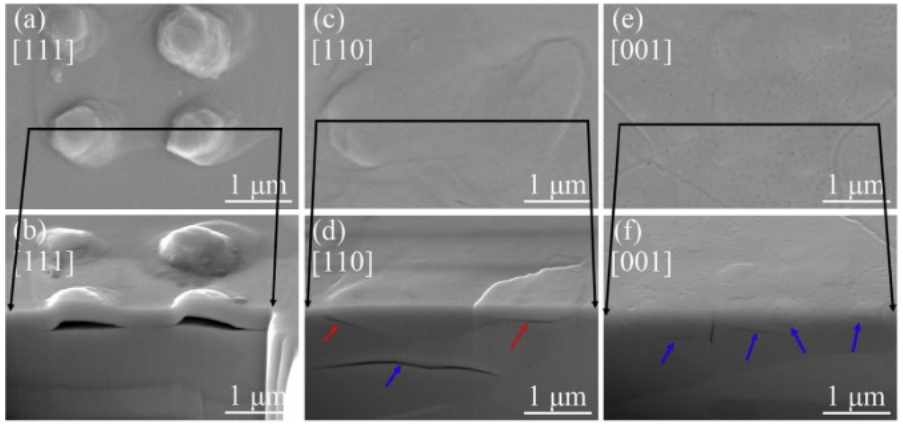
Nanovoids + D/T influx

Bubbling/blistering, D/T retention



$$^{2}_{1}D + ^{3}_{1}T \rightarrow ^{4}_{2}He + n^{0}$$
$$^{6}_{3}Li + n^{0} \rightarrow ^{4}_{2}He + ^{3}_{1}T$$





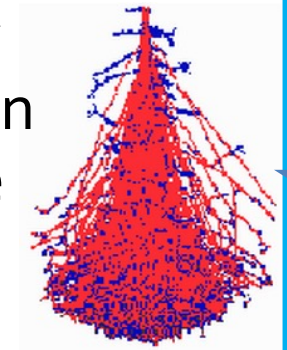
[1] Zayachuk, Y., et al. "Combined effects of crystallography, heat treatment and surface polishing on blistering in tungsten exposed to high-flux deuterium plasma." *Nuclear Fusion* 56.8 (2016): 086007.
[2] Jia, Y. Z., et al. "Mechanism for orientation dependence of blisters on W surface exposed to D plasma at low temperature." *Journal of Nuclear Materials* 477 (2016): 165-171.

Multiscale Modeling

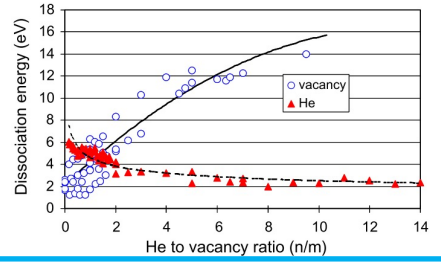
First-principles DFT + OKMC

- E.g., reproduction of He TDS in W

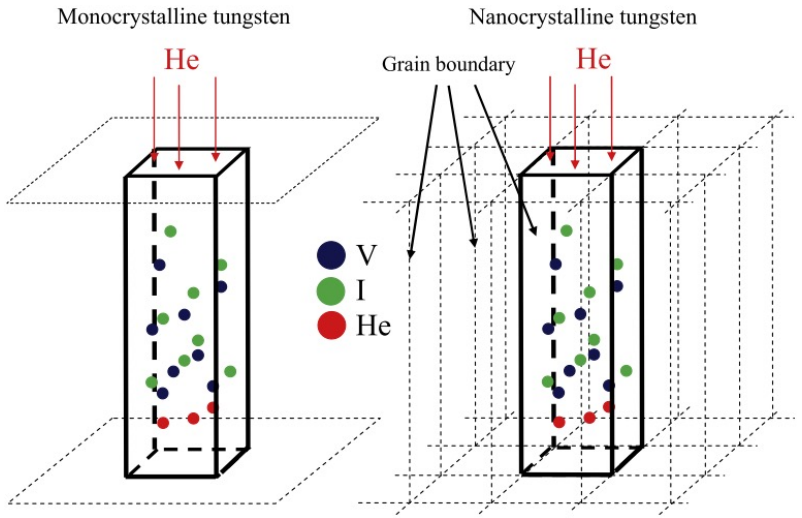
Primary irradiation damage (BCA) IM3D

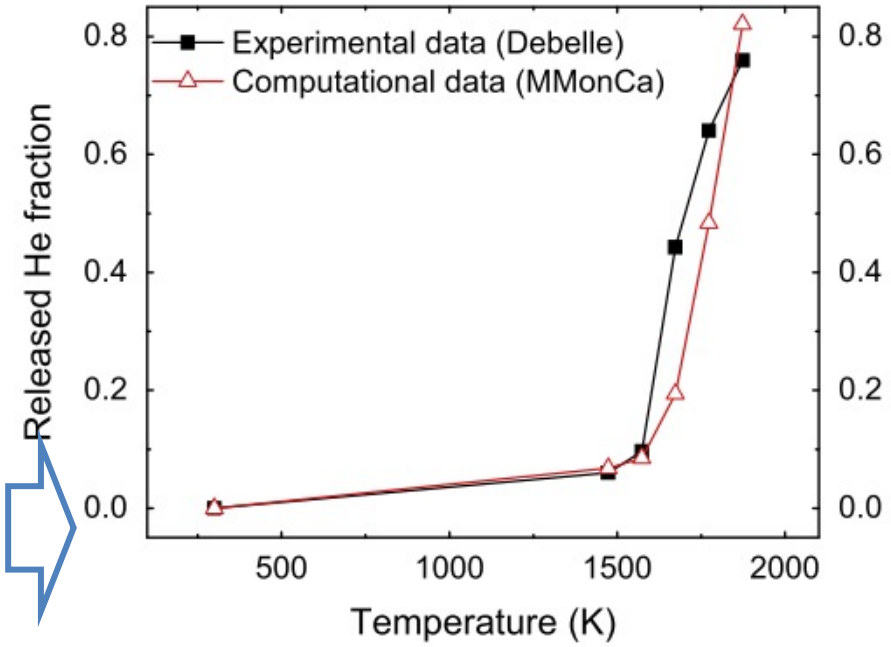


He-nanovoid interaction (DFT)



Long time evolution (OKMC)





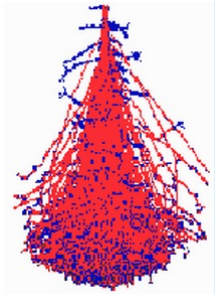
He-nanovoid interaction is the key

Valles, G., et al. "The influence of high grain boundary density on helium retention in tungsten." Journal of Nuclear Materials 457 (2015): 80-87.

H-Nanovoid Systems

Multiscale modelling for H

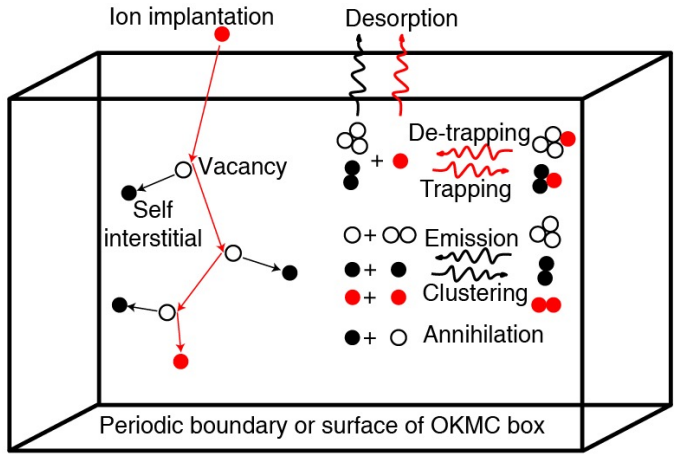
Primary irradiation damage (BCA)



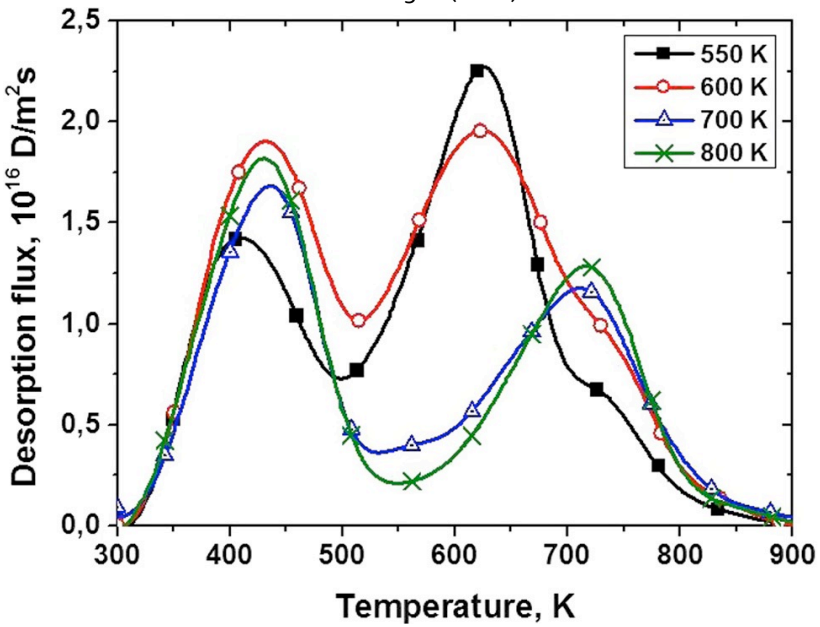
H-nanovoid interaction

?

Long time evolution (OKMC)



Nucl. Instrum. Methods. B 382 (2016) 101



H-nanovoid interaction is the key

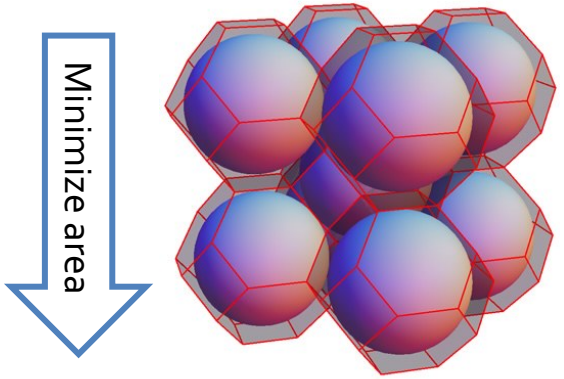
H-Nanovoid Systems

- ❖ **Structures and energies of nanovoids**
- ❖ **Hydrogen trapping in nanovoids**

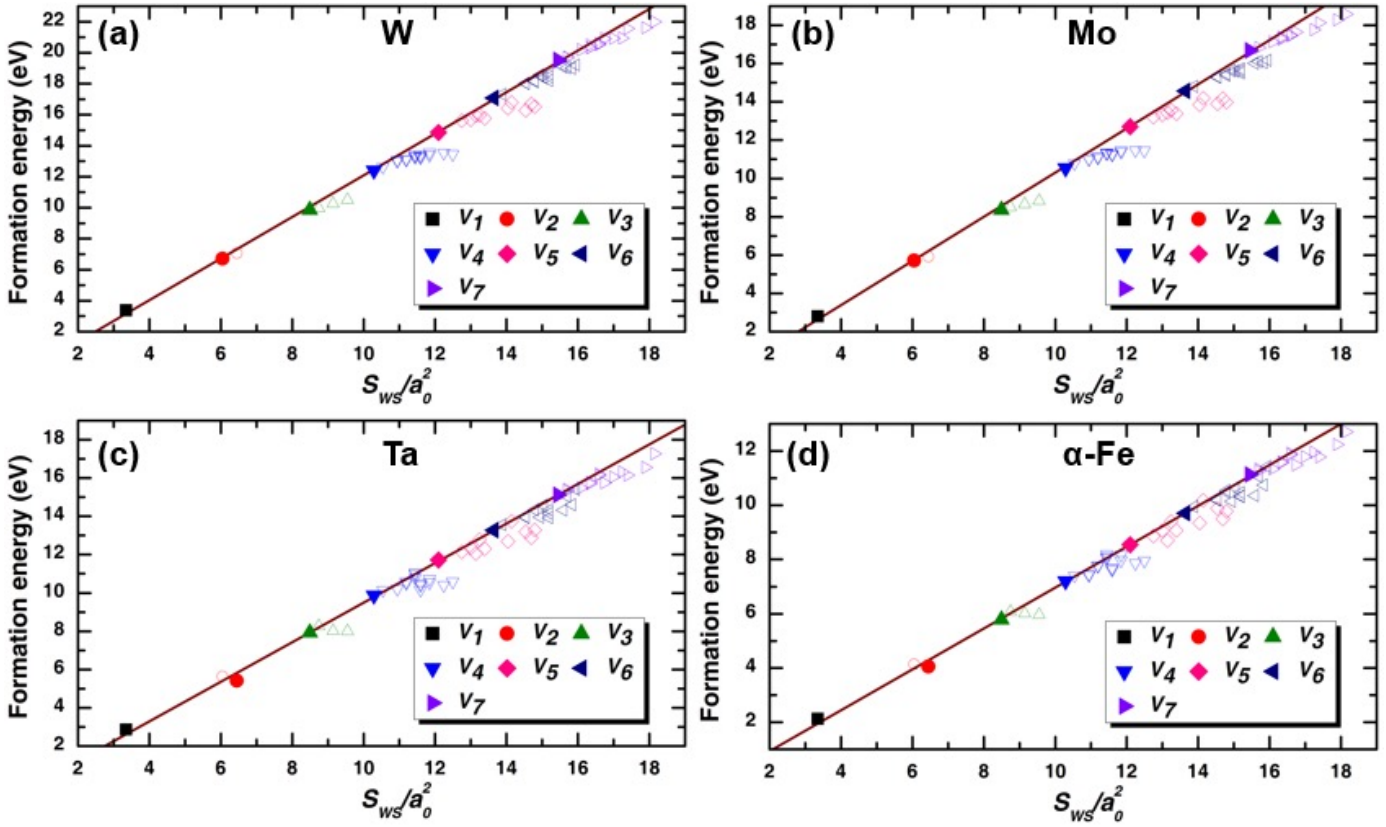
Structure search

- Nanovoid=cluster of vacancy Wigner-Seitz (WS) polyhedrons
- Compact structures (minimum WS area) have lowest energies

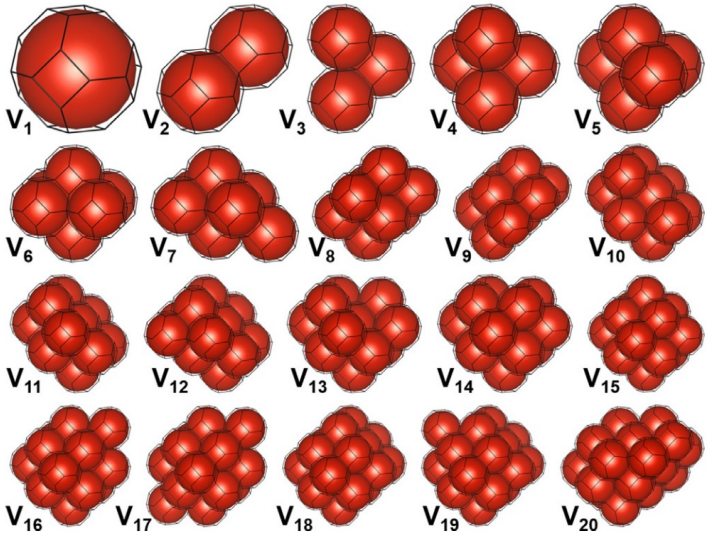
Wigner-Seitz polyhedrons of bcc vacancies



Brutal-force structure search for small nanovoids

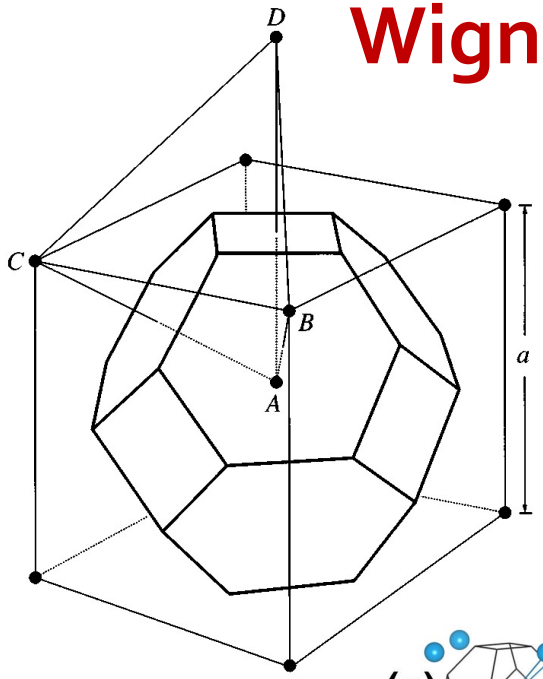


Predict stable structure for large nanovoids



J. Hou , Y. You, X. Kong, J. Song b , C.S. Liu . "Accurate prediction of vacancy cluster structures and energetics in bcc transition metals ." Acta Materialia 211 (2021) 116860

Wigner-Seitz (WS) Polyhedrons and Squares



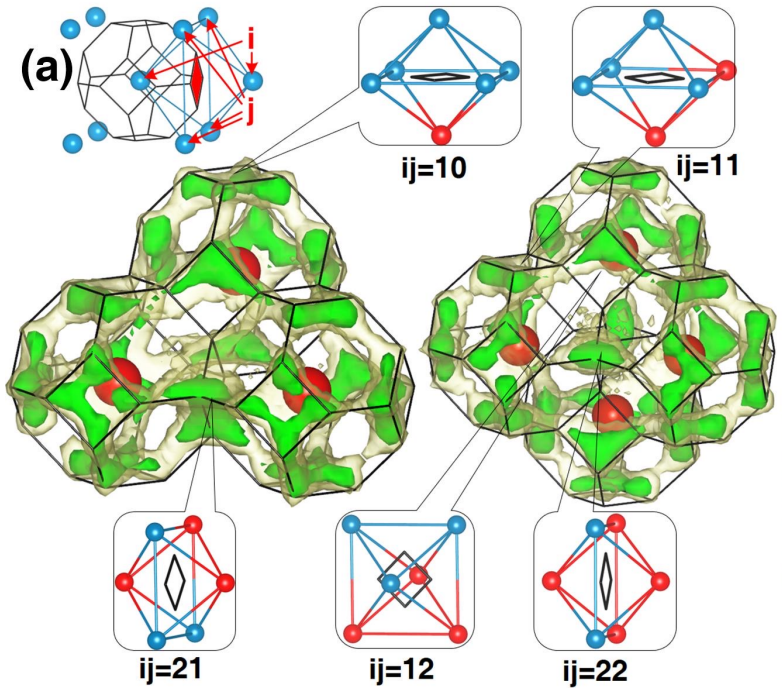


Table SI: Numbers of Wigner-Seitz squares on surfaces of V_1-V_8 nanovoids in BCC metals.

	ij=10	11	12	21	22	Sum
V_1	6					6
V_2	6	6				12
V_3	8	6	2	1		17
V_4	8	8	4		2	22
V_5	8	10	6		2	26
V_6	10	8	8		4	30
V_7	10	10	10		4	34
V_8	12	8	12		6	38

H-Nanovoid Systems

- ❖ **Structures and energies of nanovoids**
- ❖ **Hydrogen trapping in nanovoids**

Structure search

- Nanovoid=cluster of vacancy Wigner-Seitz (WS) polyhedrons
- Compact structures (minimum WS area) have lowest energies

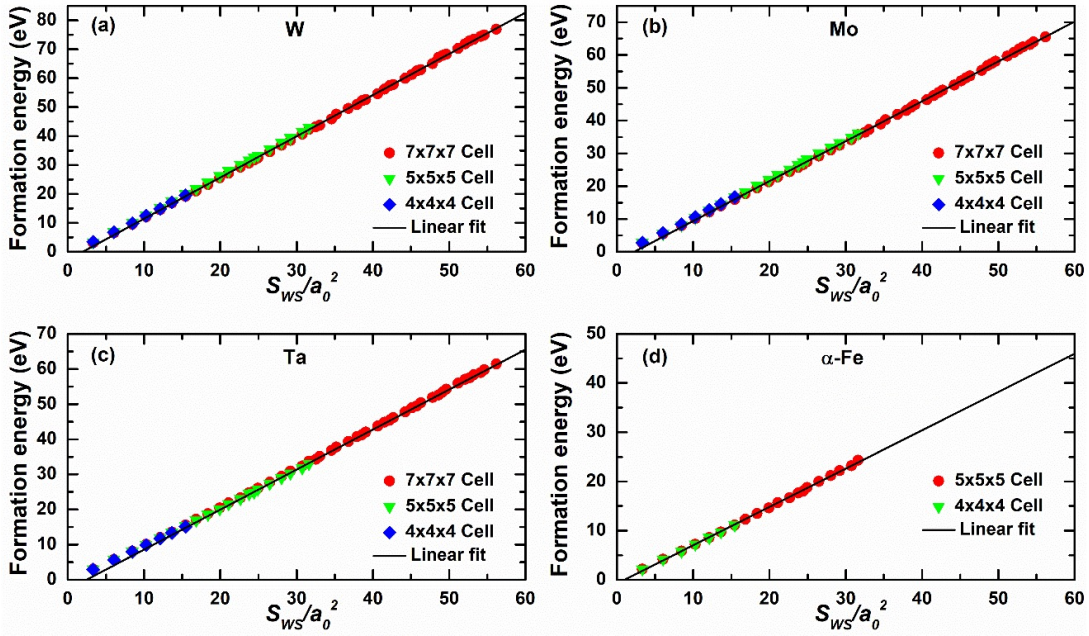
Energy pattern

- Formation energy varies linearly against WS area
- Parameter-free model for accurate binding energy prediction

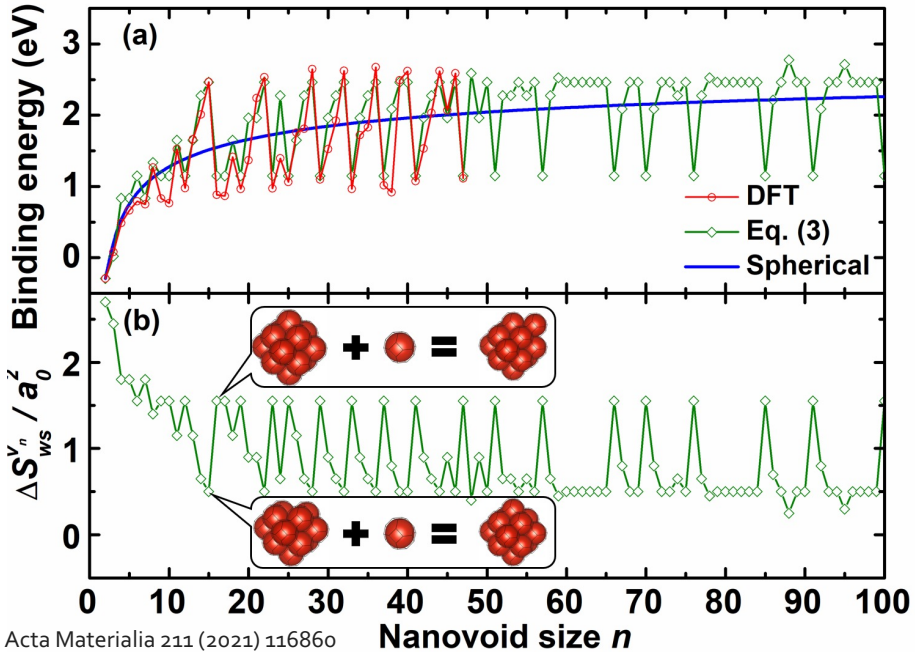
$$E_f^{V_n} = A + C \cdot S_{WS}^{V_n}$$

$$E_b^{V_n} = E_f^{V_1} + \left(E_b^{V_2} - E_f^{V_1}\right)\frac{\Delta S_{WS}^{V_n}}{\Delta S_{WS}^{V_2}} \quad \text{Eq. (3)}$$

Formation energy for V_1-V_{47}



Vacancy binding induced energy & area change



J. Hou , Y. You, X. Kong, J. Song b , C.S. Liu . "Accurate prediction of vacancy cluster structures and energetics in bcc transition metals ." Acta Materialia 211 (2021) 116860

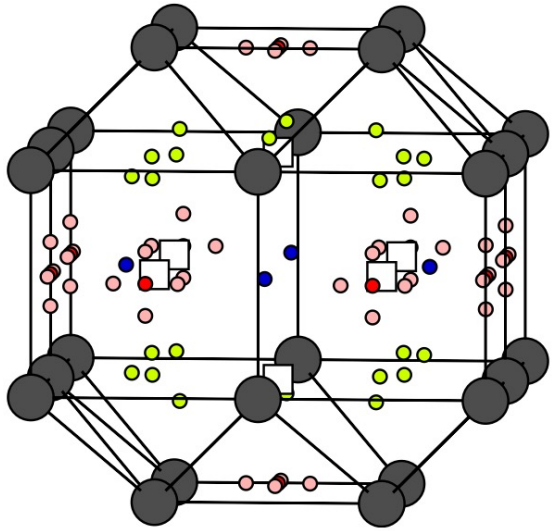
H-Nanovoid Systems

Hydrogen trapping in nanovoids

Atomistic characterization

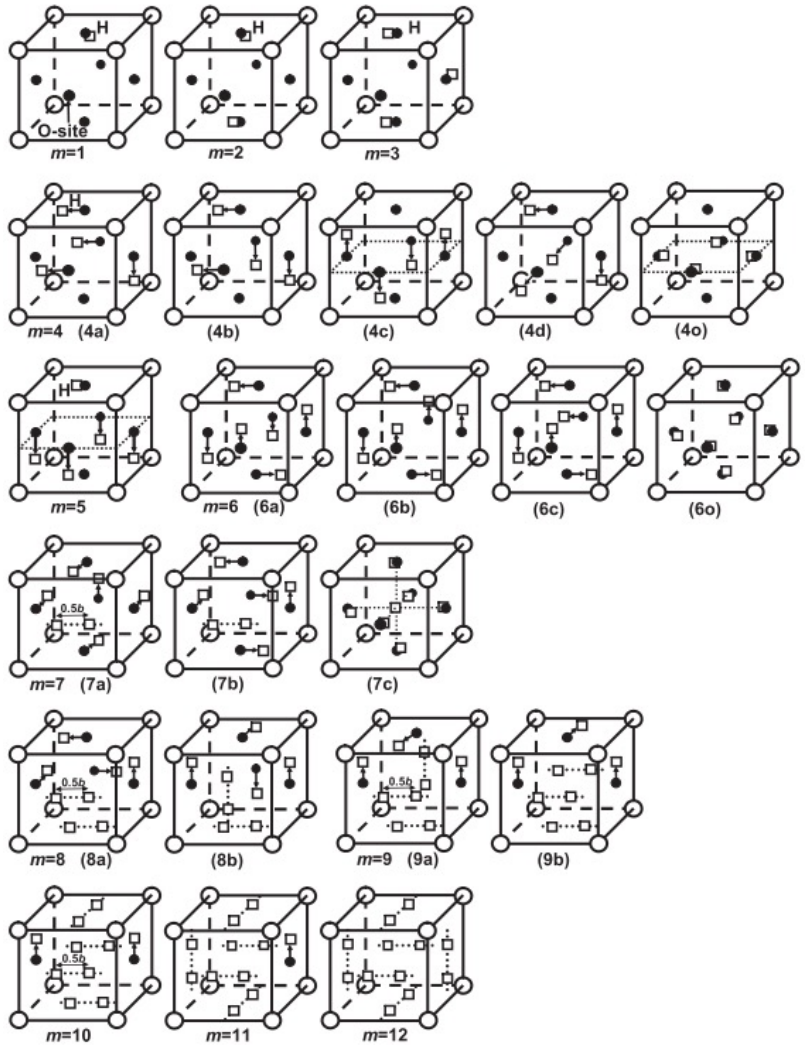
- **First-principles (DFT)**: *Brute-force*, mostly limited to very small voids (e.g., V_1)

J. Nucl. Mater. 476 (2016) 36



> 10^{22} possible structures for multiple H adsorption in V_6!

Ohsawa et al. PRB. 85 (2012) 094102



Possible structures of V_1H_m

H-Nanovoid Systems

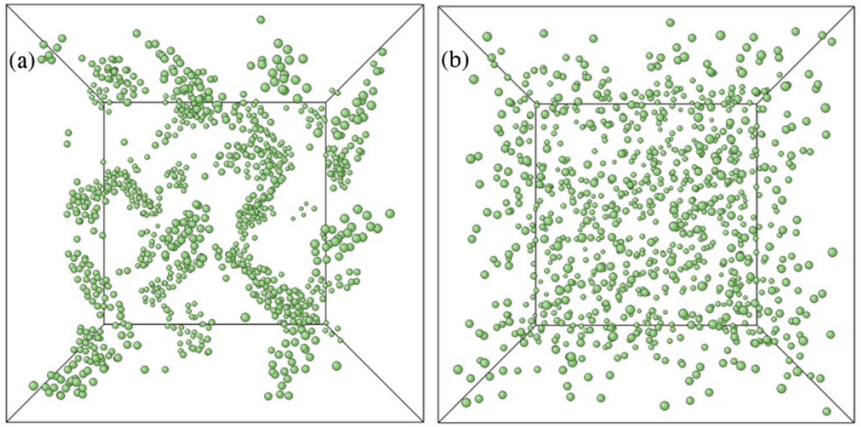
Hydrogen trapping in nanovoids

Atomistic characterization

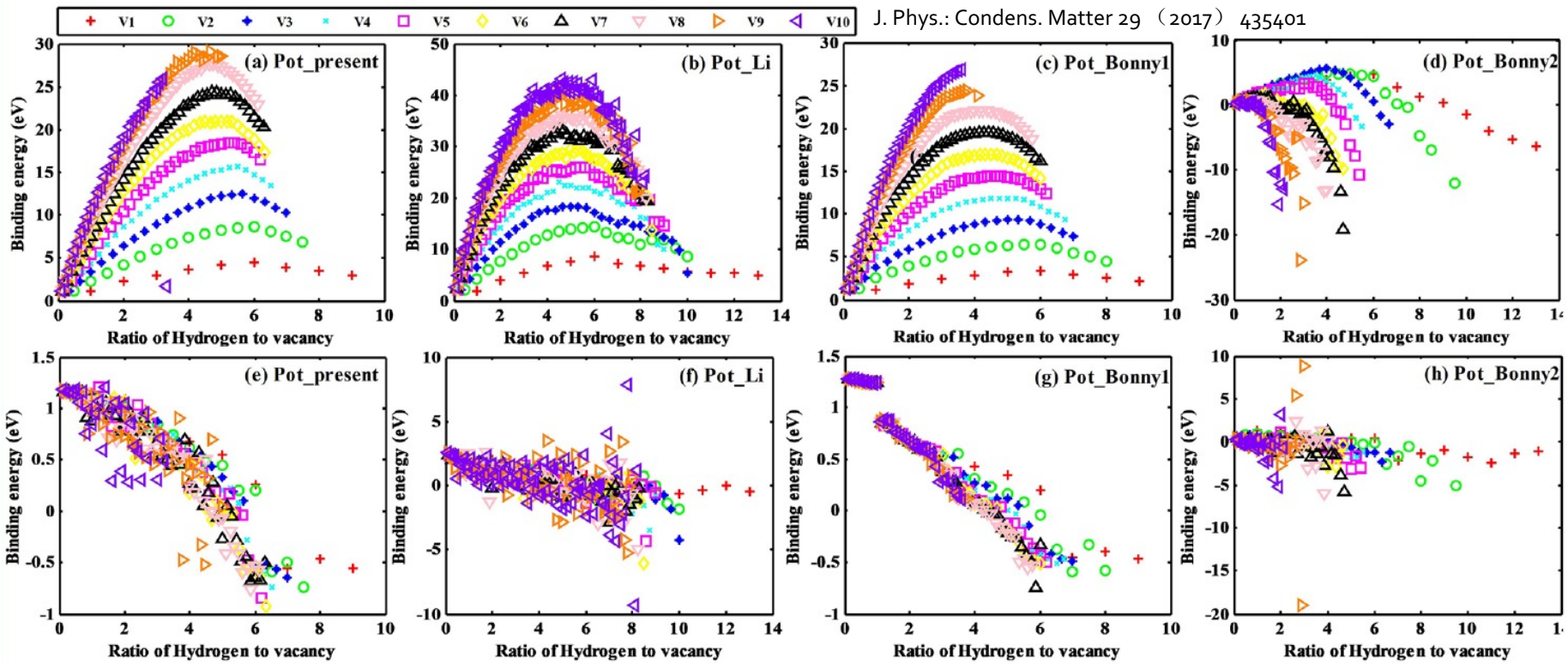
- Molecular statics/dynamics (MS/MD)

However, results highly interatomic ***potential dependent***!

J. Nucl. Mater., 463, 347-350



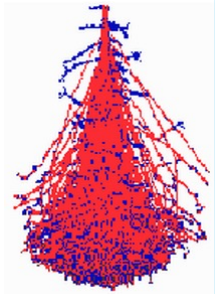
J. Phys.: Condens. Matter 29 （2017） 435401



H-Nanovoid Systems

Multiscale modelling for H

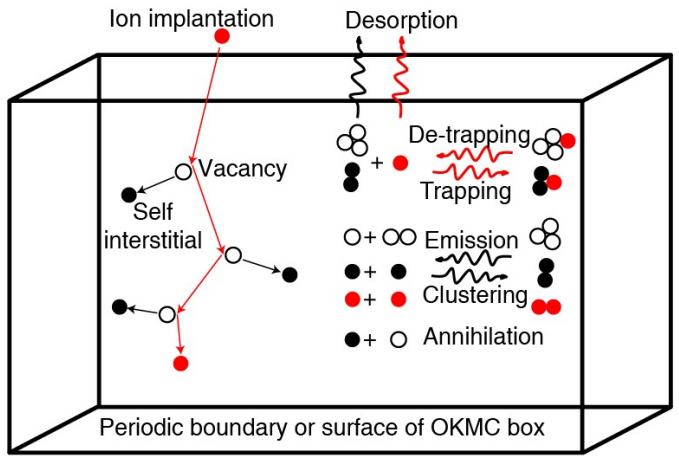
Primary irradiation damage (BCA)



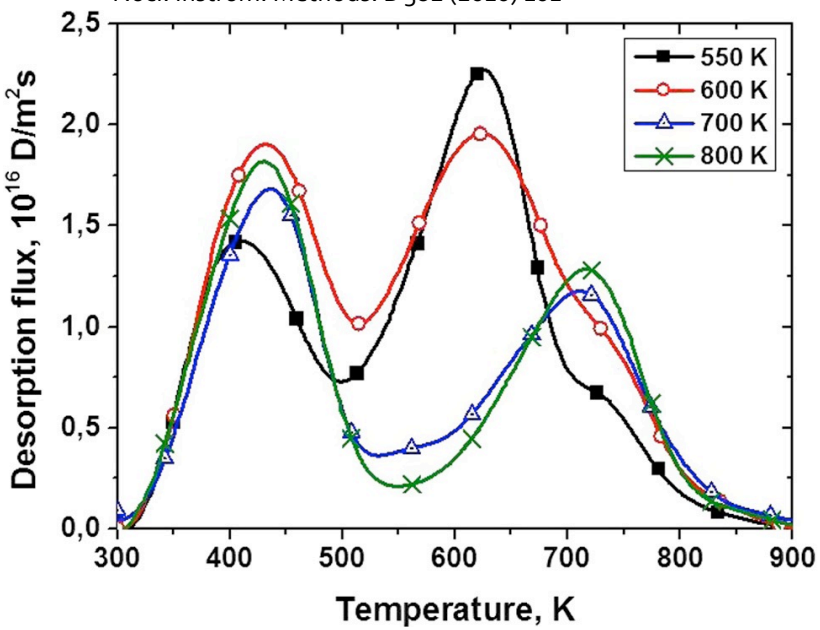
H-nanovoid interaction

?

Long time evolution (OKMC)



Nucl. Instrum. Methods. B 382 (2016) 101



Objective:

H-nanovoid interaction model

(sample system BCC tungsten)

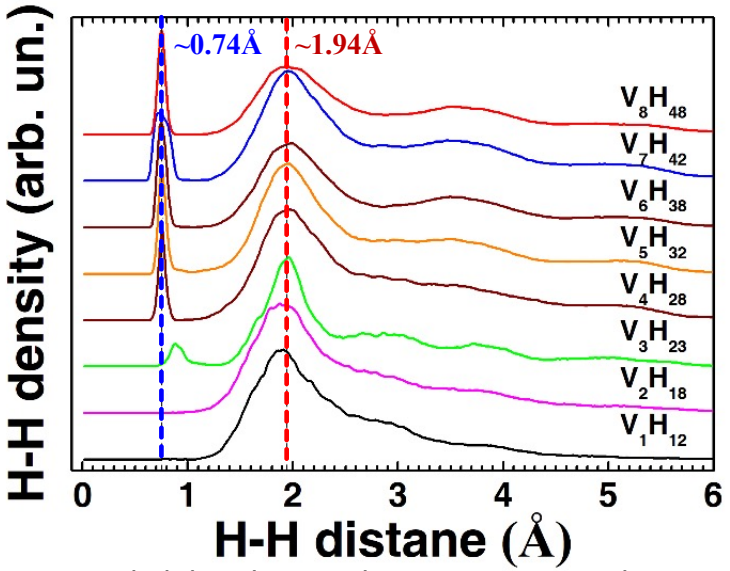
- H adsorption sites/sequence on inner surface of nanovoid
- Interaction between H adatoms
- H_2 molecule formation & ***predictive*** H bubble formation

H in Nanovoids

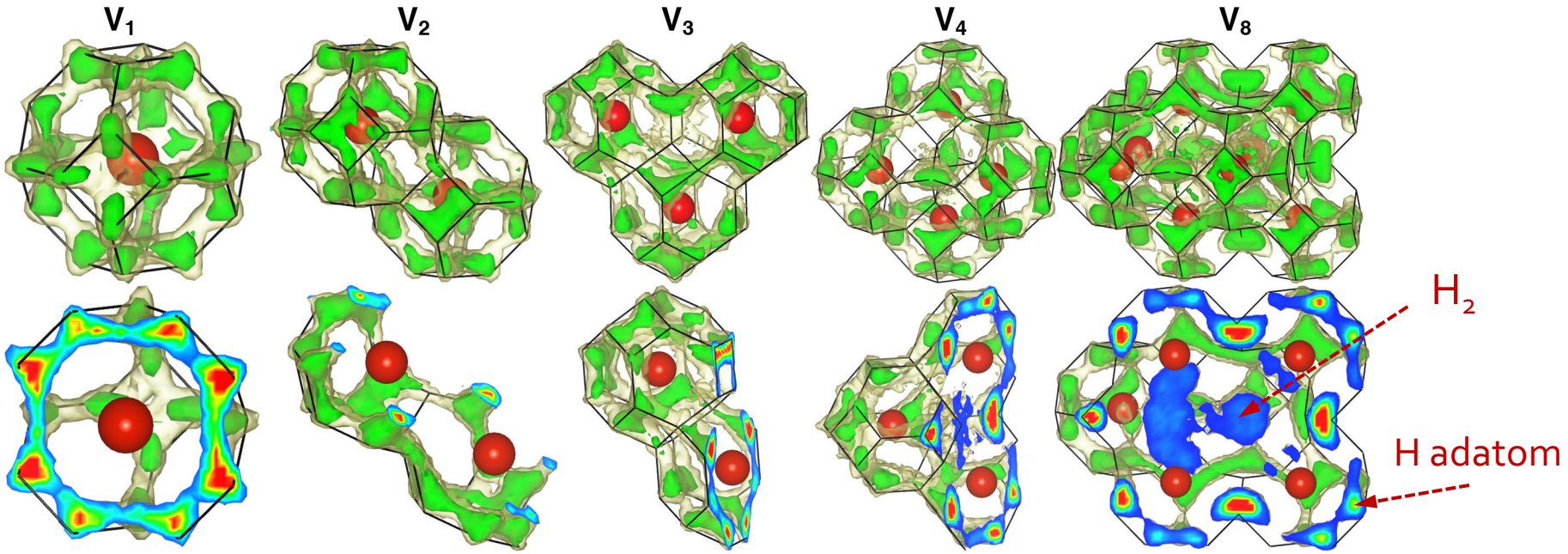
DFT & Ab-initio MD:

H ***spatial distribution*** in nanovoids in W

- H adatoms adsorb on Wigner-Seitz (WS) squares on nanovoid surfaces
- H_2 forms in nanovoid core ($V_{n\geq 3}$)



H-H radial distribution density in nanovoids at 600K

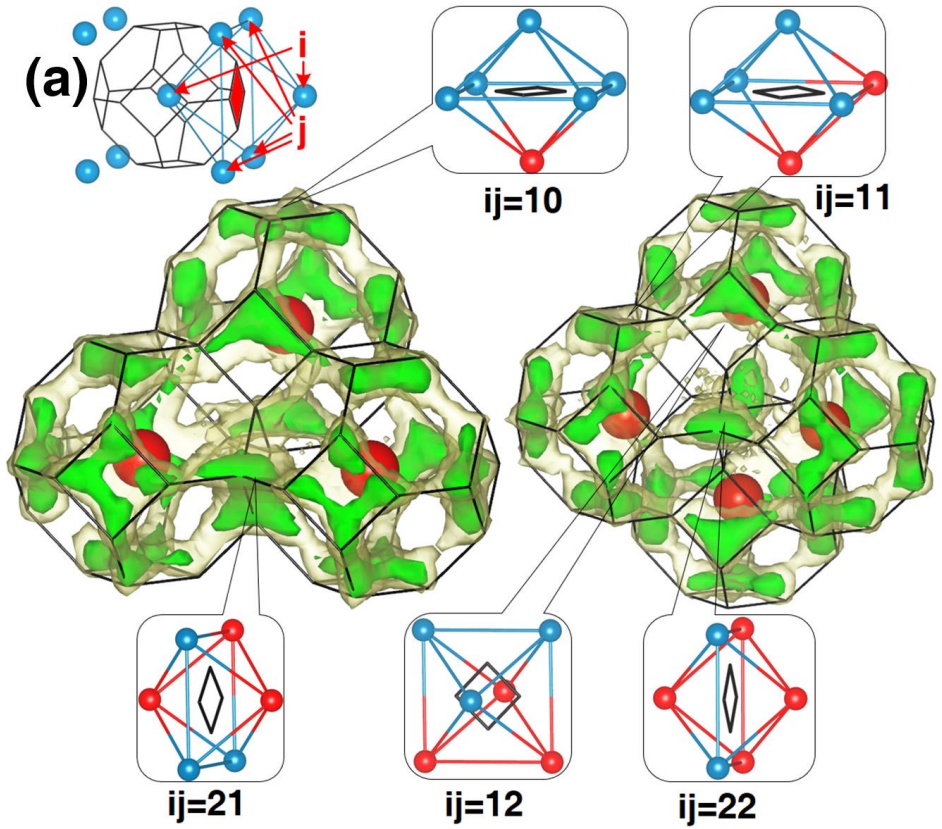


Probability density function in different nanovoids at 600K. ***Red spheres***: cores of constituting vacancies. ***Black lines***: edges of Wigner-Seitz cells.

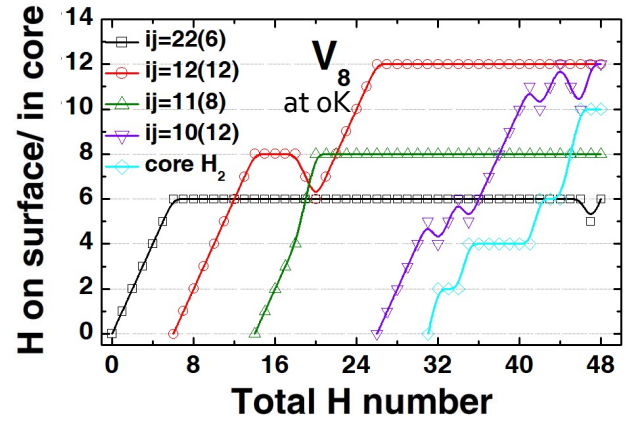
Adsorption sites and energies

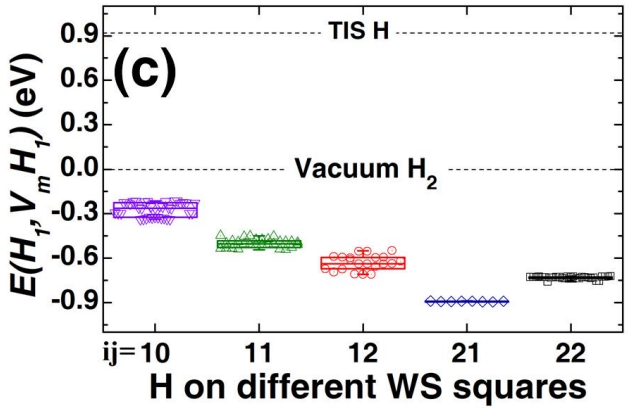
H adatoms on nanovoid surface (W)

- **5 (ij) types of WS squares** based on neighboring vacancy number
- **5 distinct H energy levels**, directly related to 5 types of WS squares
- H **sequentially occupy** WS squares with the lowest energy



E.g., V_3 and V_4 nanovoids during H adding at 600K





Trapping energy of a single H adatom on WS squares in V_1-V_8

$$E(H_k, V_m H_n) = E^{tot}(V_m H_n) - E^{tot}(V_m H_{n-k}) - \frac{k}{2} E^{tot}(H_2)$$

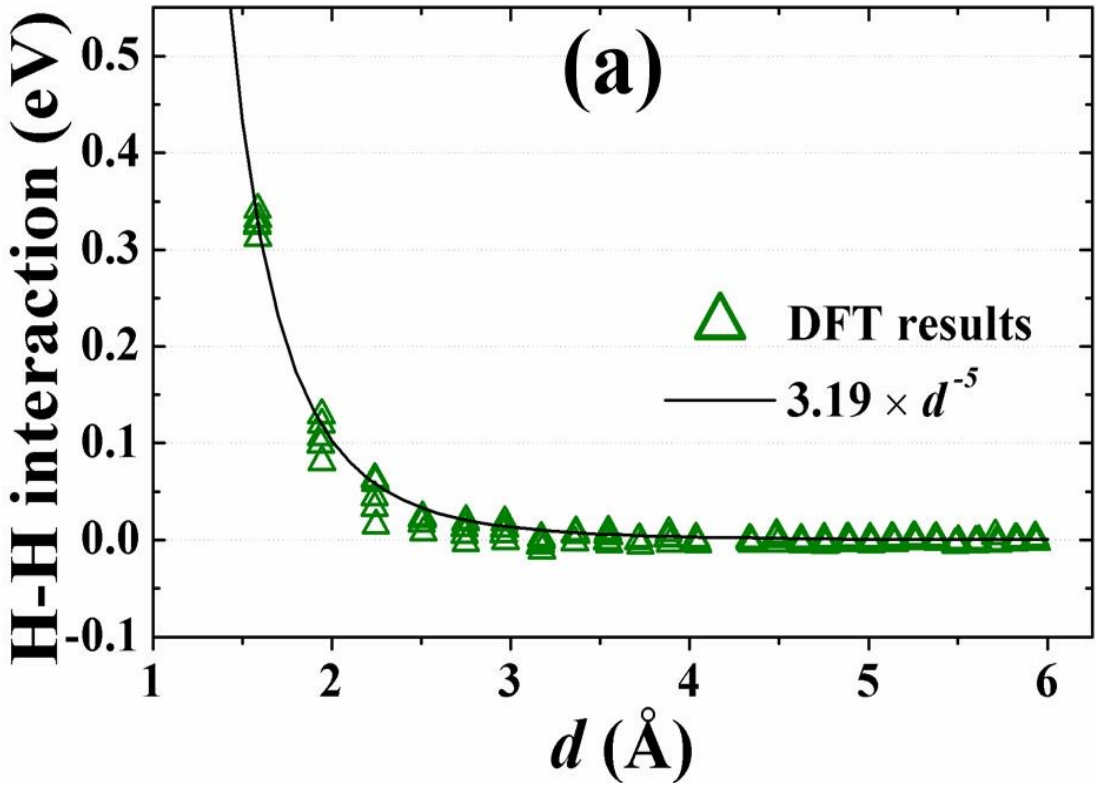
H-H Repulsion

However, **H-H repulsion** comes in as H saturates the nanovoid

First, ***pairwise*** H-H repulsion:

- Numerated ~1700 H-H structures in $V_{1\sim4}$ and V_8
- H-H are **mutually exclusive**, decay rapidly with distance
- Interaction energy is approximately a power function of d:

$$E^{int}(V_mH_2) = A_s d^{-5} \quad (A_s \sim 3.19\ \text{eV*Å}^5)$$



Multiple H Adsorption

However, **H-H repulsion** comes in as H saturates the nanovoid

A nanovoid with *multiple* H adatoms.

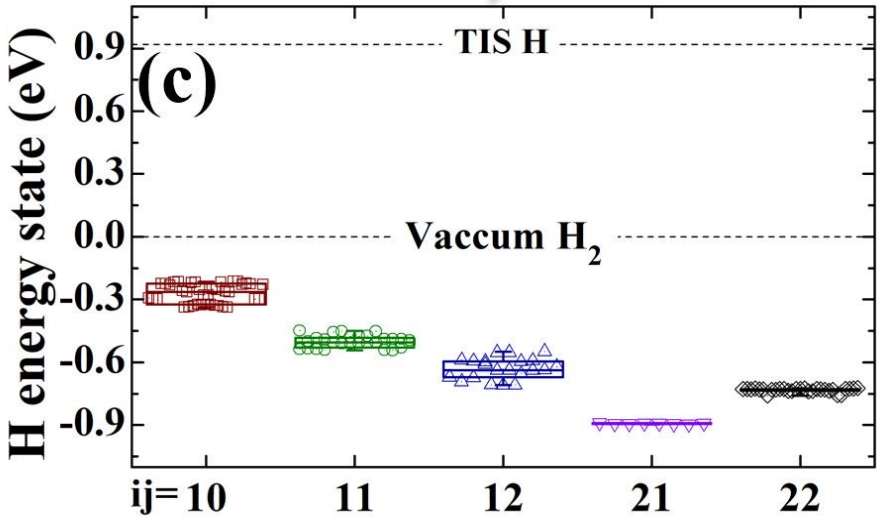
Total trapping energy $E(H_n, V_m H_n) = \sum_{k=1}^{n} E\left(H_1, V_m H_1^{S_k}\right) + E^{int}(V_m H_n)$.

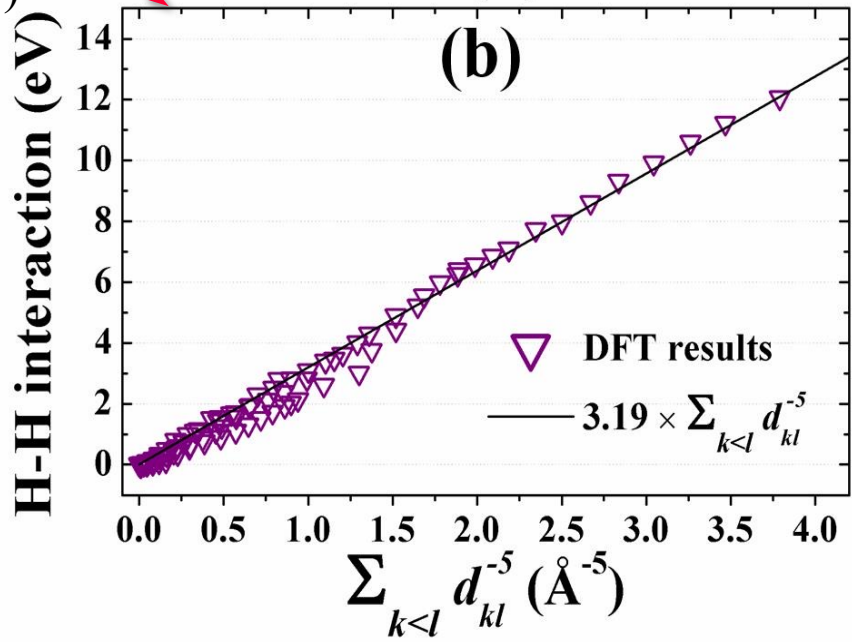
H-H interaction $E^{int}(V_m H_n)$ well approximated by simple summation of all pairwise H-H interaction terms!

$$E(H_n, V_m H_n) \cong \sum_{k=1}^{n} E_k^{ij} + A_s \sum_{k<l}^{n} d_{kl}^{-5}$$

$(A_s \sim 3.19\ \text{eV/Å}^5)$

Multiple H-H interaction





J. Hou et al. "*Predictive model of hydrogen trapping and bubbling in nanovoids in bcc metals*." Nature Materials 2019 (18), 833–839

.

Multiple H Adsorption

However, **H-H repulsion** comes in as H saturates the nanovoid

A nanovoid with *multiple* H adatoms.

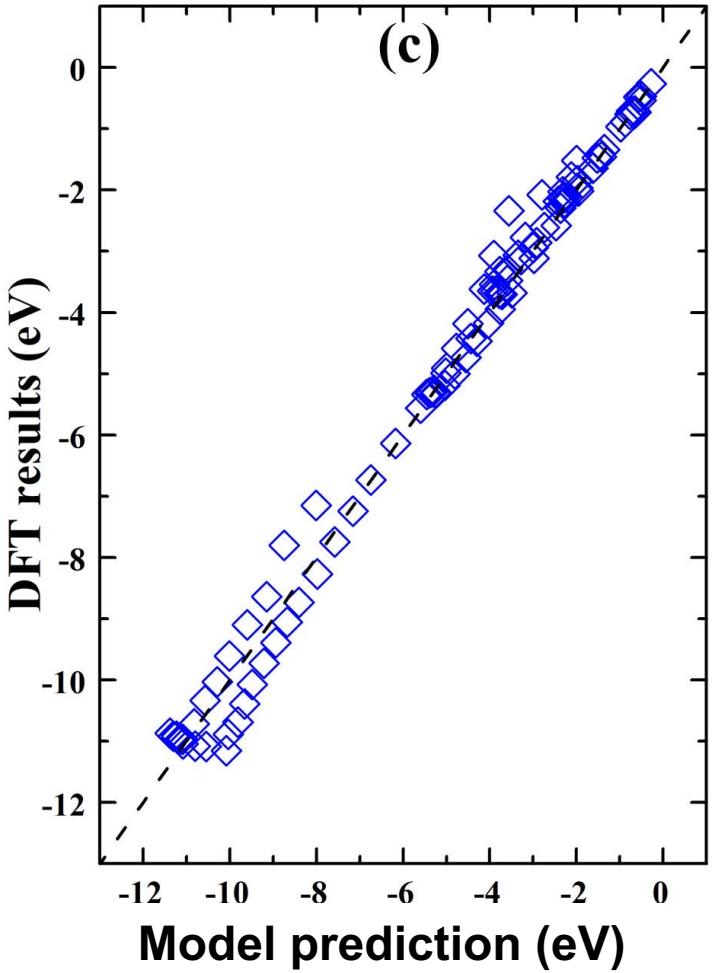
Total trapping energy

$$E(H_n, V_m H_n) \cong \sum_{k=1}^{n} E_k^{ij} + A_s \sum_{k<l}^{n} d_{kl}^{-5}$$

Prediction of trapping energetics of multiple H in a nanovoid achieved

However, configuration of H adatoms still necessary…

How about a more *general* nanovoid and *scale-up*?



Multiple H Adsorption

Simplification with approximations:

- *Sequential adsorption* of adatoms on WS squares
- *Maximization* of H-H distance → *uniform distribution*
- *Closed-pack* of H adatoms on nanovoid surface
- *Nearest-neighbor* H-H consideration ⇦ d^{-5} fast decay

Average NN H-H distance

$$d = \left(\frac{2a}{\sqrt{3}n}\right)^{0.5}$$, a is nanovoid surface area

Multiple H-H interaction

$$E(H_n, V_m H_n) \cong \sum_{k=1}^{n} E_k^{ij} + A_s \sum_{k<l}^{n} d_{kl}^{-5}$$

$$E^{int}(V_m H_n) \cong \frac{1}{2} A_s 6n \left(\frac{\sqrt{3}n}{2a}\right)^{2.5}$$

Trapping energy of the n^{th} H adatom in a V_mH_n cluster

$$E(H_1, V_m H_n) = E_n^{ij} + \frac{\partial E^{int}(V_m H_n)}{\partial n}$$

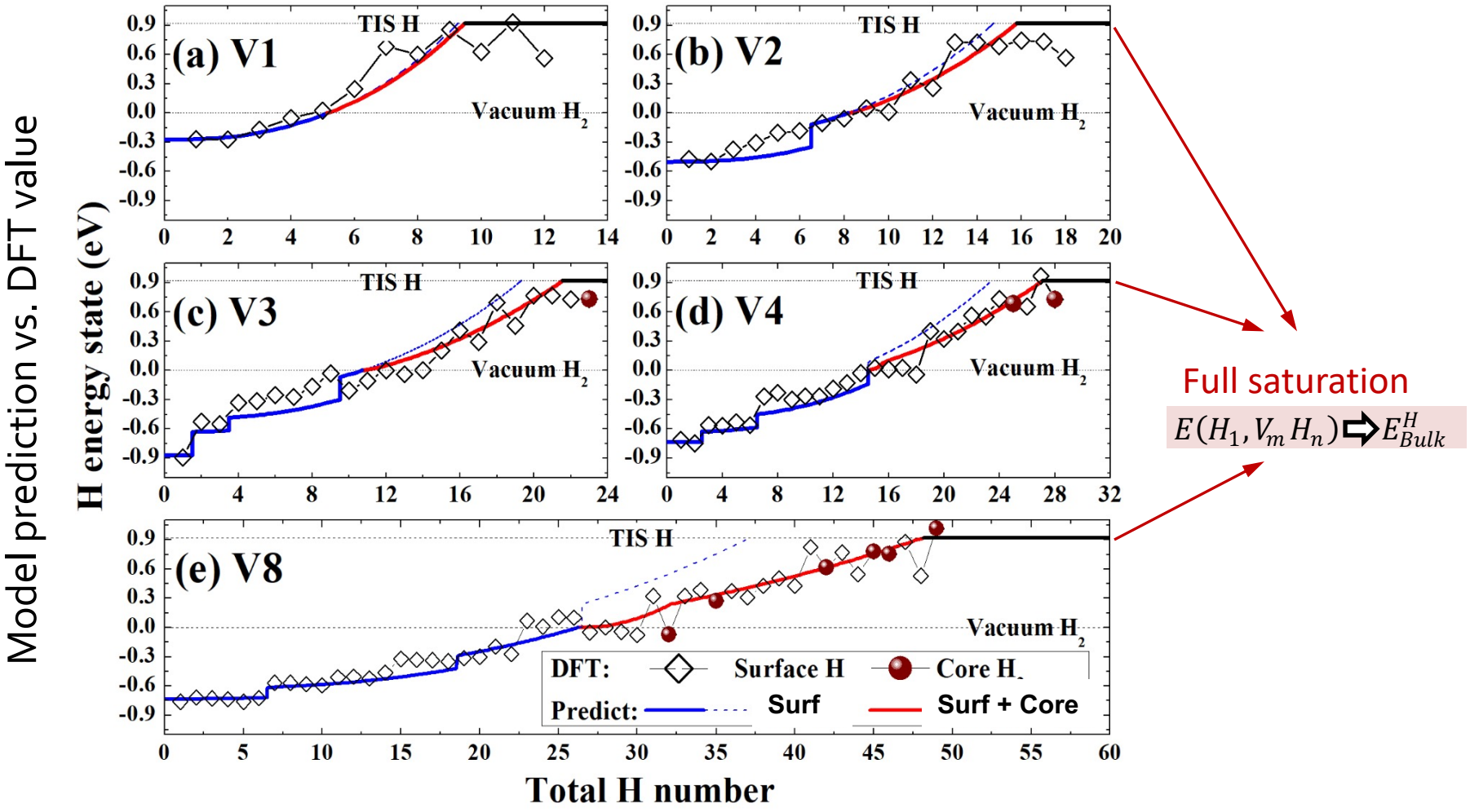
$$\cong E_n^{ij} + 7.3 A_s \left(\frac{n}{a}\right)^{2.5}$$

Multiple H Adsorption

H adatom trapping energy state

$$E(H_1, V_m H_n) = E_n^{ij} + \frac{\partial E^{int}(V_m H_n)}{\partial n} \cong E_n^{ij} + 7.3 A_s \left(\frac{n}{a}\right)^{2.5}$$

(a is nanovoid surface area)



Full saturation

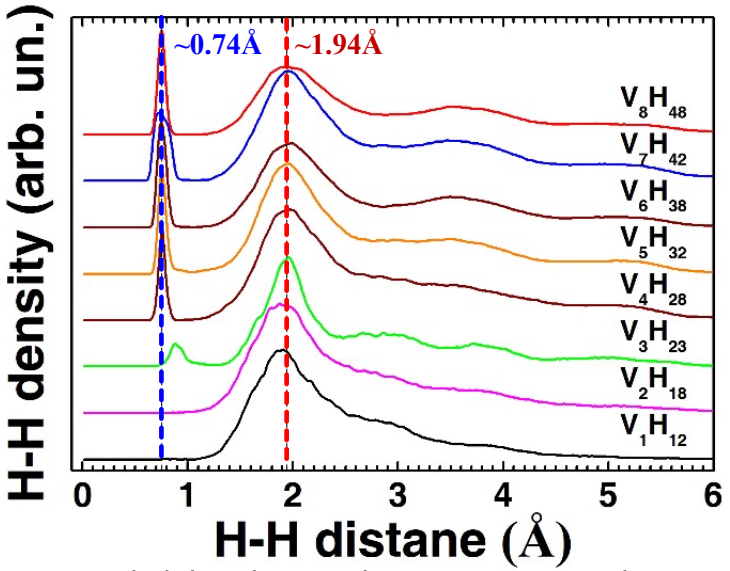
$E(H_1, V_m H_n) \Rightarrow E_{Bulk}^H$

H in Nanovoids

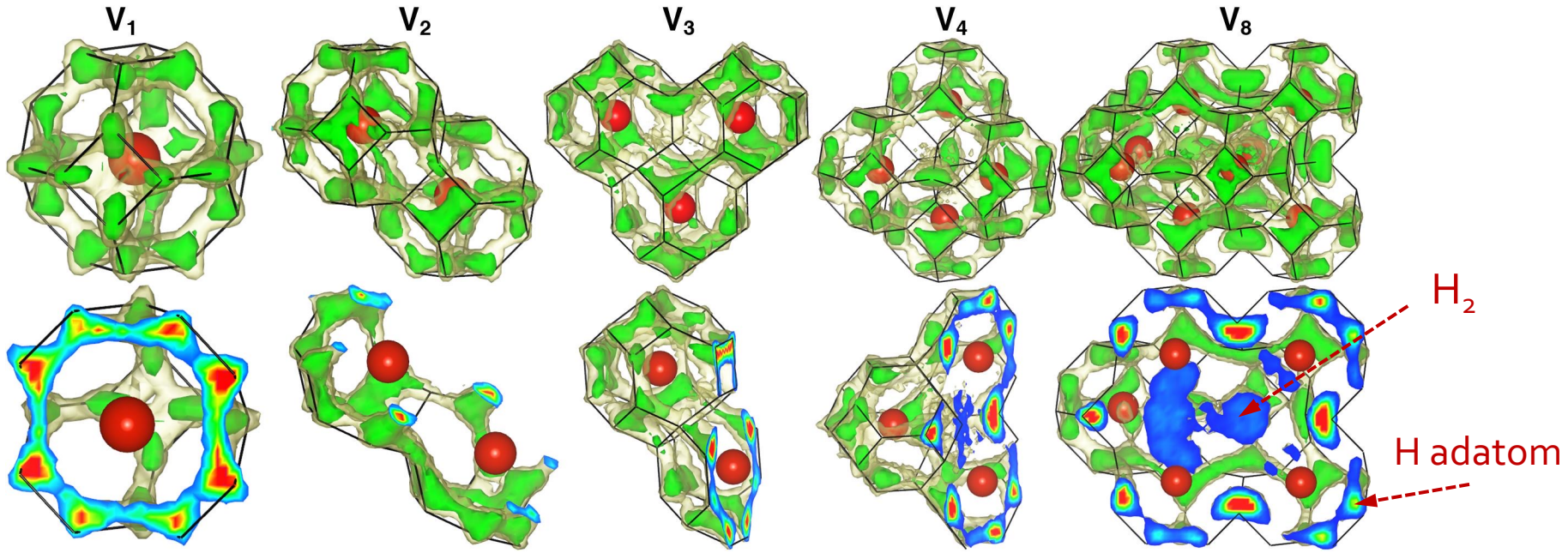
DFT & Ab-initio MD:

H ***spatial distribution*** in nanovoids in W

- H adatoms adsorb on Wigner-Seitz (WS) squares on nanovoid surfaces
- H_2 forms in nanovoid core ($V_{n\geq 3}$)



H-H radial distribution density in nanovoids at 600K



Probability density function in different nanovoids at 600K. ***Red spheres***: cores of constituting vacancies. ***Black lines***: edges of Wigner-Seitz cells.

H_2 Formation in Nanovoid Core

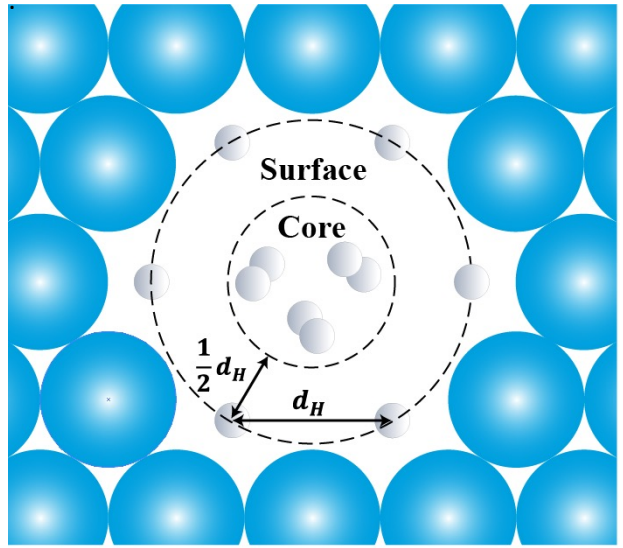
J. Hou et al., *Nature Materials* 2019 (18), 833–839

Approximation of a spherical nanovoid

- Equation of states (EOS) for H_2

$$p = A_c \left(\frac{n_c}{v}\right)^3$$

p: H_2 pressure
n_c: 2× # of H_2 molecule
v: core volume
A_c: constant, ~ 8.01 eV/Å^5



- Energy state of a H atom
  - If in core H_2 molecule

$$E(H_1, V_m H_n) = \int_0^p \left(\frac{\partial v}{\partial n}\right)_P dP = \frac{3}{2} A_c \left(\frac{n}{v}\right)^2,$$

  - If on surface as an adatom

$$E(H_1, V_m H_n) = E_n^{ij} + \frac{\partial E^{int}(V_m H_n)}{\partial n}$$
$$\cong E_n^{ij} + 7.3 A_s \left(\frac{n}{a}\right)^{2.5}$$

In equilibrium
(n_c in H_2 and n_s as adatoms):

$$E(H_1, V_m H_n) = \frac{3}{2} A_c \left(\frac{n_c}{v}\right)^2$$
$$= E_{n_s}^{ij} + 7.3 A_s \left(\frac{n_s}{a}\right)^{2.5}$$

n_c and n_s fully determined

Meanwhile…

$$\mu_{core}^H = \mu_B^H = E_{Bulk}^H + k_B T \ln\left(\frac{C_H}{1 - C_H}\right) \Rightarrow p = \frac{1}{\sqrt{A_c}} \left[\frac{2}{3}\left(E_{Bulk}^H + k_B T \ln\left(\frac{C_H}{1 - C_H}\right)\right)\right]^{\frac{3}{2}},$$

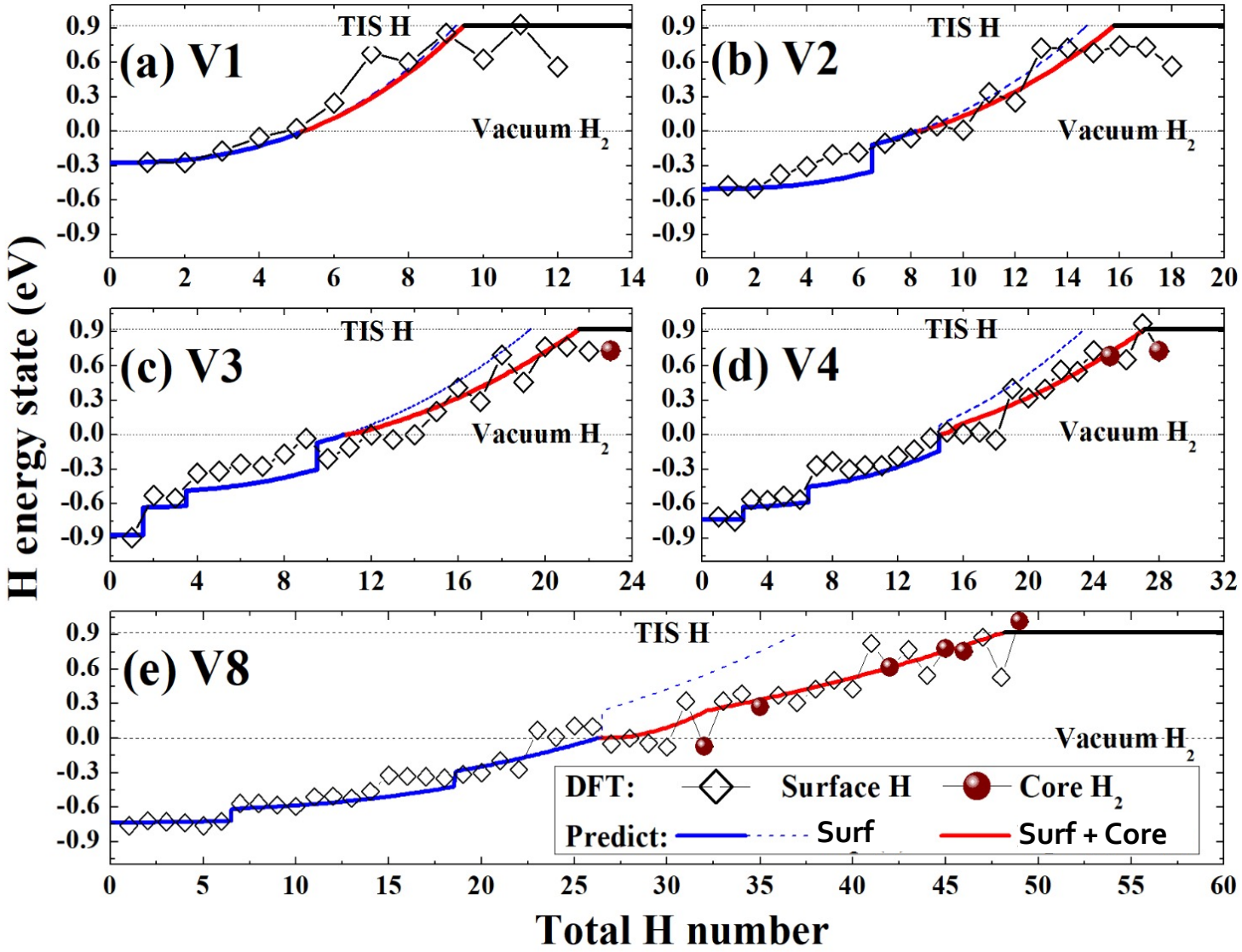
Full Prediction of H in Nanovoid

Surface H: $E(H_1, V_m H_{n_s}) \approx E_{n_s}^{ij} + 7.3A_s\left(\frac{n_s}{a}\right)^{2.5}$

Core H_2 : $E(H_1, V_m H_{n_c}) = \frac{3}{2}A_c\left(\frac{n_c}{v}\right)^2$

Together:

$$E(H_1, V_m H_n) = \frac{3}{2}A_c\left(\frac{n_c}{v}\right)^2 = E_{n_s}^{ij} + 7.3A_s\left(\frac{n_s}{a}\right)^{2.5}$$



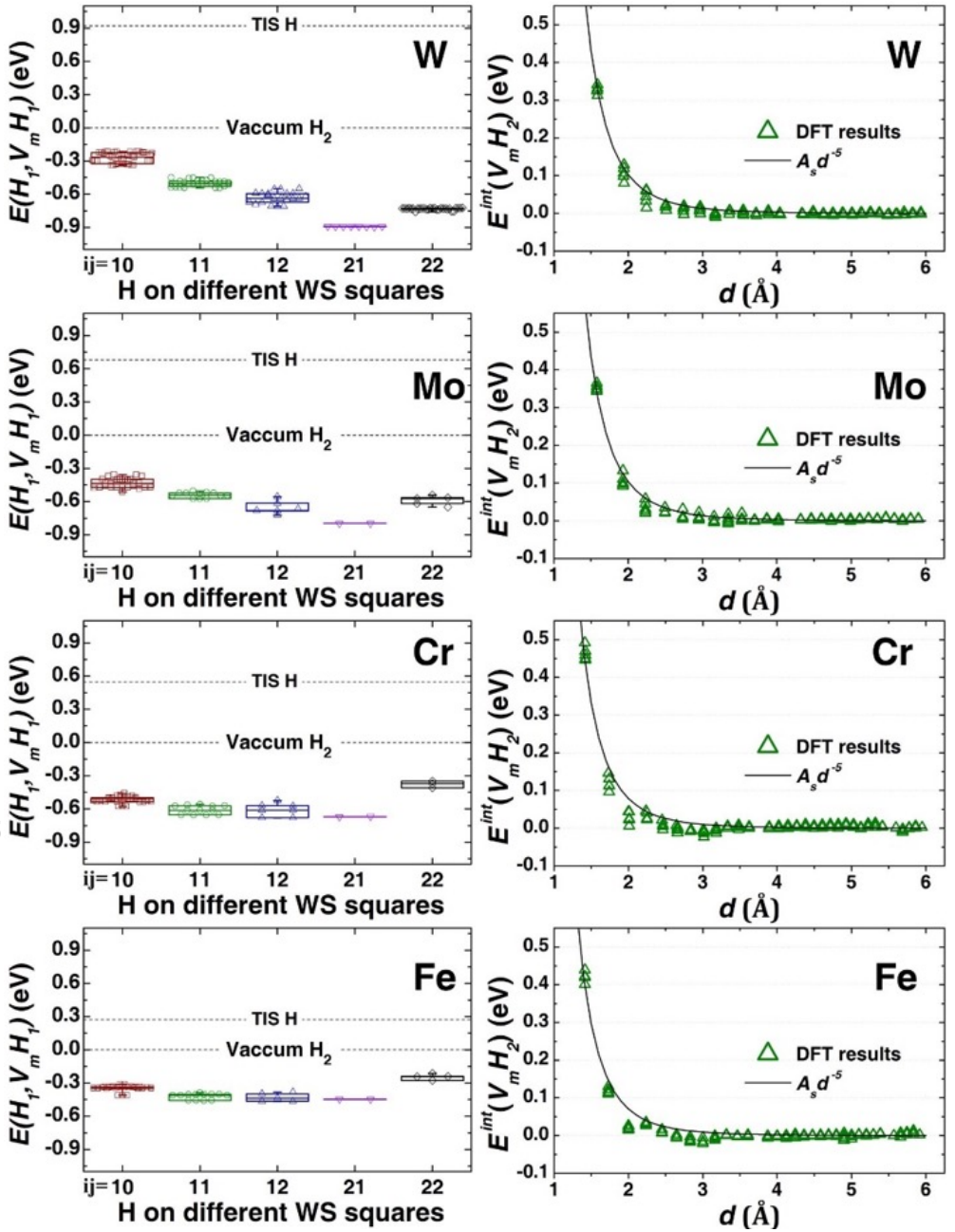
Generality of the Model

BCC systems of Mo, Cr, Fe

- Adsorption on WS squres, with 5 energy levels
- d^{-5} pairwise H-H repulsion
- EOS of H_2 is not material dependent

$$E(H_1, V_m H_n) = \frac{3}{2} A_c \left(\frac{n_c}{v}\right)^2 = E_{n_s}^{ij} + 7.3 A_s \left(\frac{n_s}{a}\right)^{2.5}$$

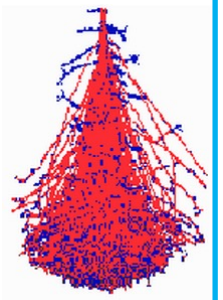
Model applicable to other BCC metals



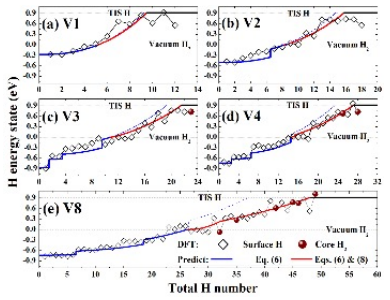
Application of the Model

Multiscale modelling
versus
TDS experiments

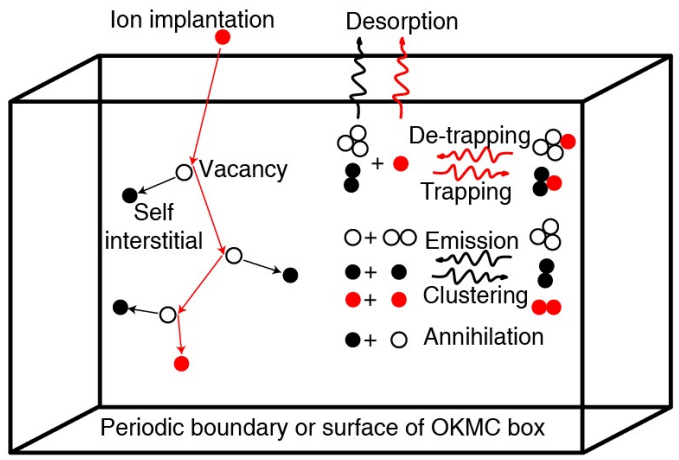
Primary irradiation damage (BCA)



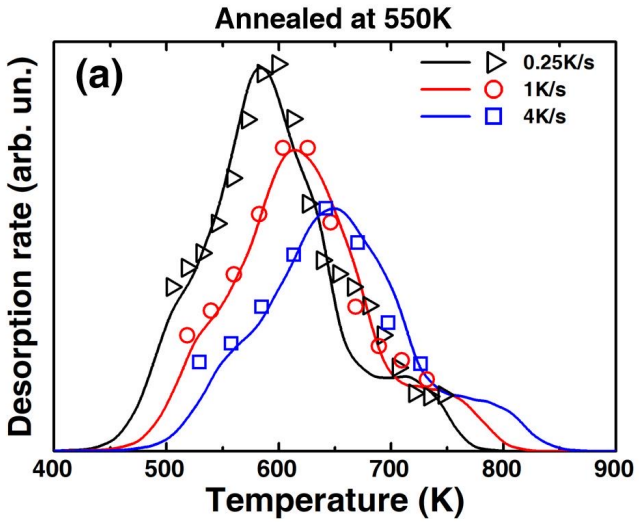
H-nanovoid model



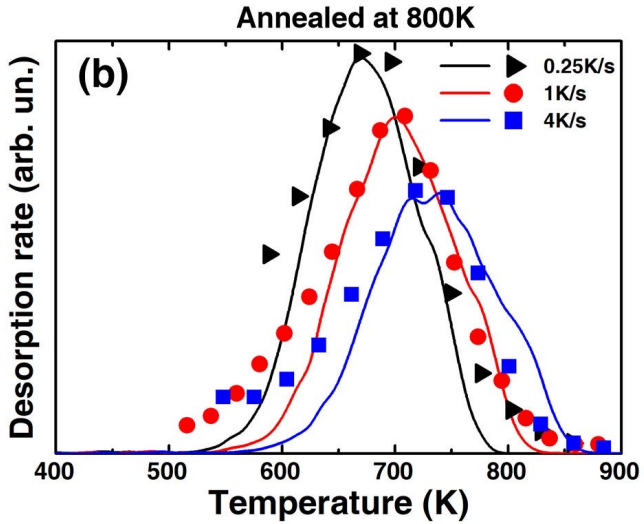
Long time evolution (OKMC)



Nucl. Instrum. Methods. B 382 (2016) 101



J. Nucl. Mater. 477 (2016) 292-297



Lines: multiscale predictions
Dots: experimental data

Application of the Model

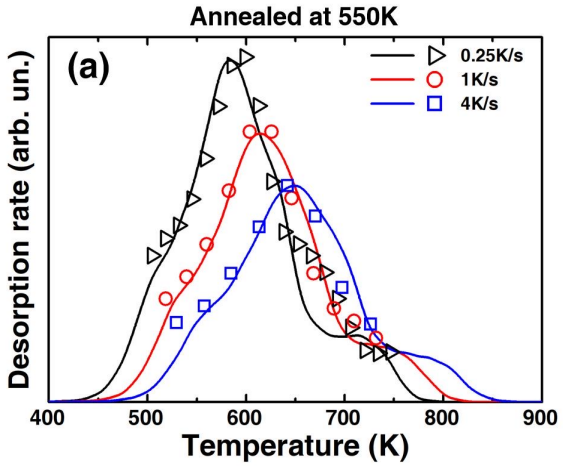
Multiscale modelling
versus
TDS experiments

550 K annealing

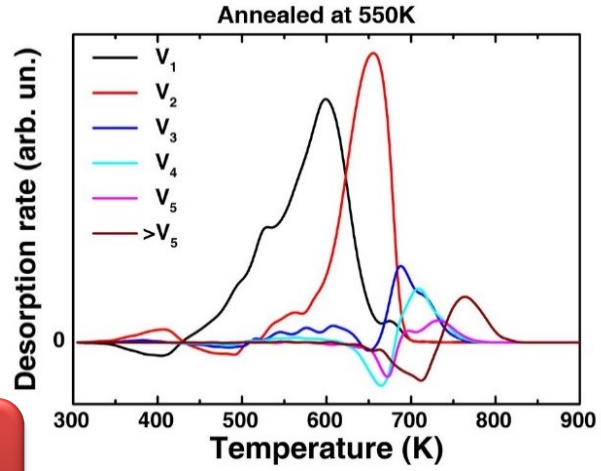
10 keV D^+ irradiation

0.67 eV D^+ irradiation

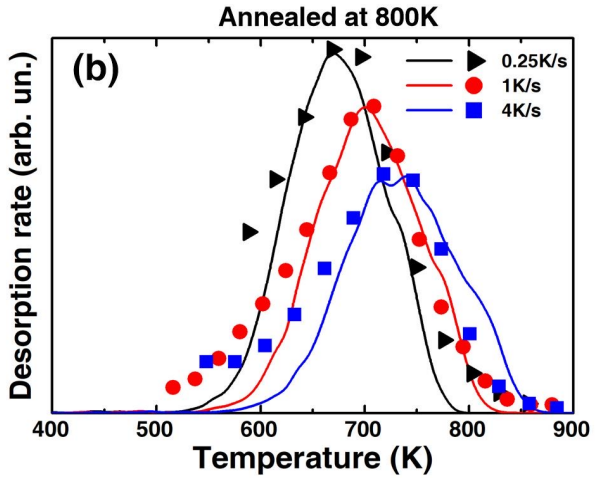
800 K annealing

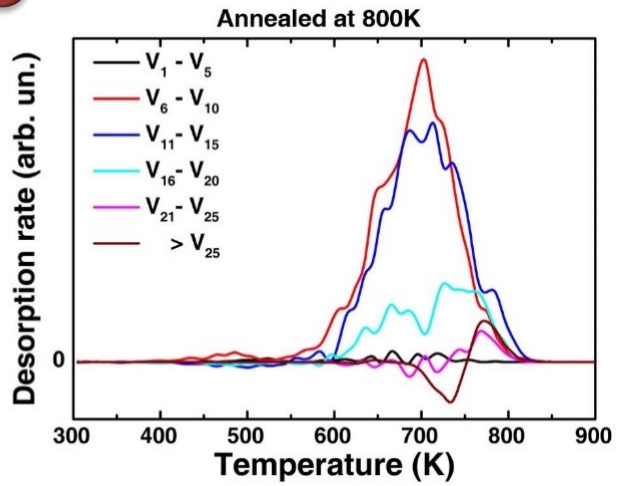


desorption mostly from V_1/V_2



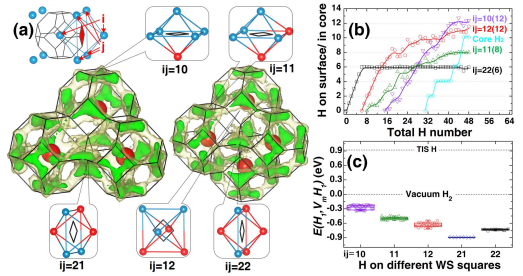
Desorption mostly from V clusters

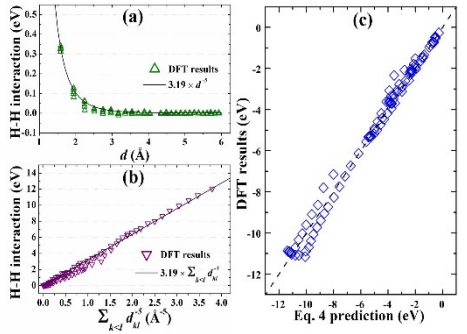


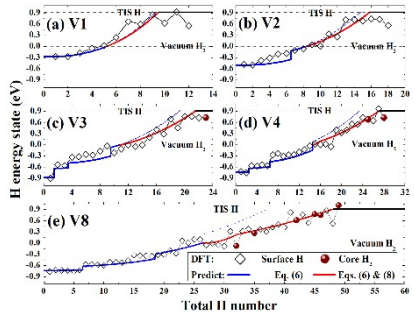


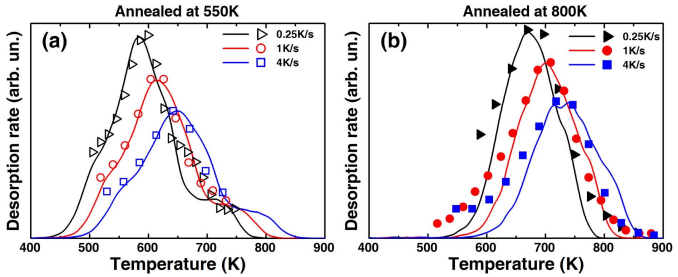
Part I: Summary

- H adatoms adsorption on Wigner-Seitz (WS) squares on nanovoid surface, with 5 distinct energy levels
- H adatoms are mutually exclusive, with d^{-5} repulsion energy (pairwise)
- Combining EOS of H_2, built a predictive model for H trapping and bubble formation in nanovoids
- Multiscale simulations based on the model reproduced related TDS experiments









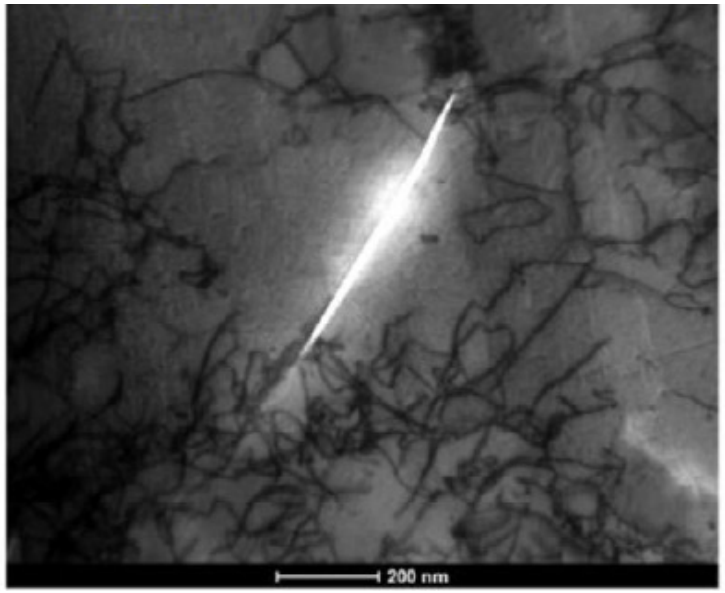
Outline :

- H-nanovoid
  - Structures and energies of nanovoids
  - Hydrogen trapping in nanovoids

- **H-dislocation**
  - **H clustering at dislocations**
  - **H stabilized junction and loop formation**

H Blister Formation w/o Irradiation

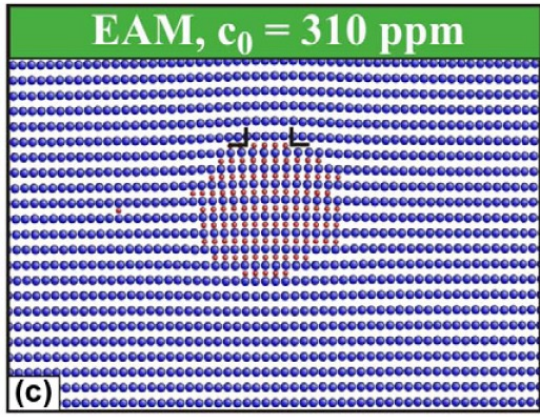
H induced crack shaped blister



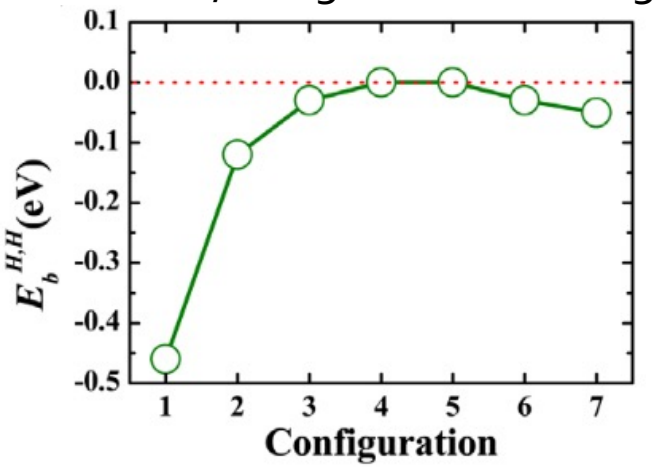
- No irradiation, ~~nanovoid~~
- Intra-granular blister, ~~GB~~
- Purified W, ~~second phase~~

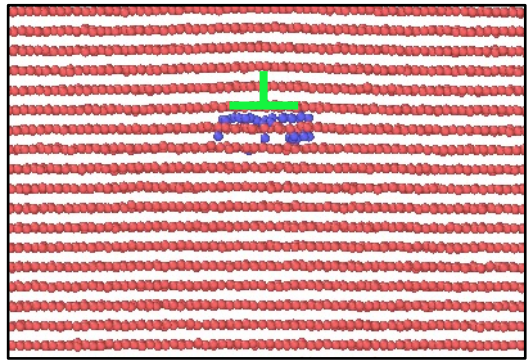
How does H blister nucleate?

FCC Ni, H-H attraction cause notable H clustering at dislocation



Weak H-H attraction in BCC metals, marginal H clustering





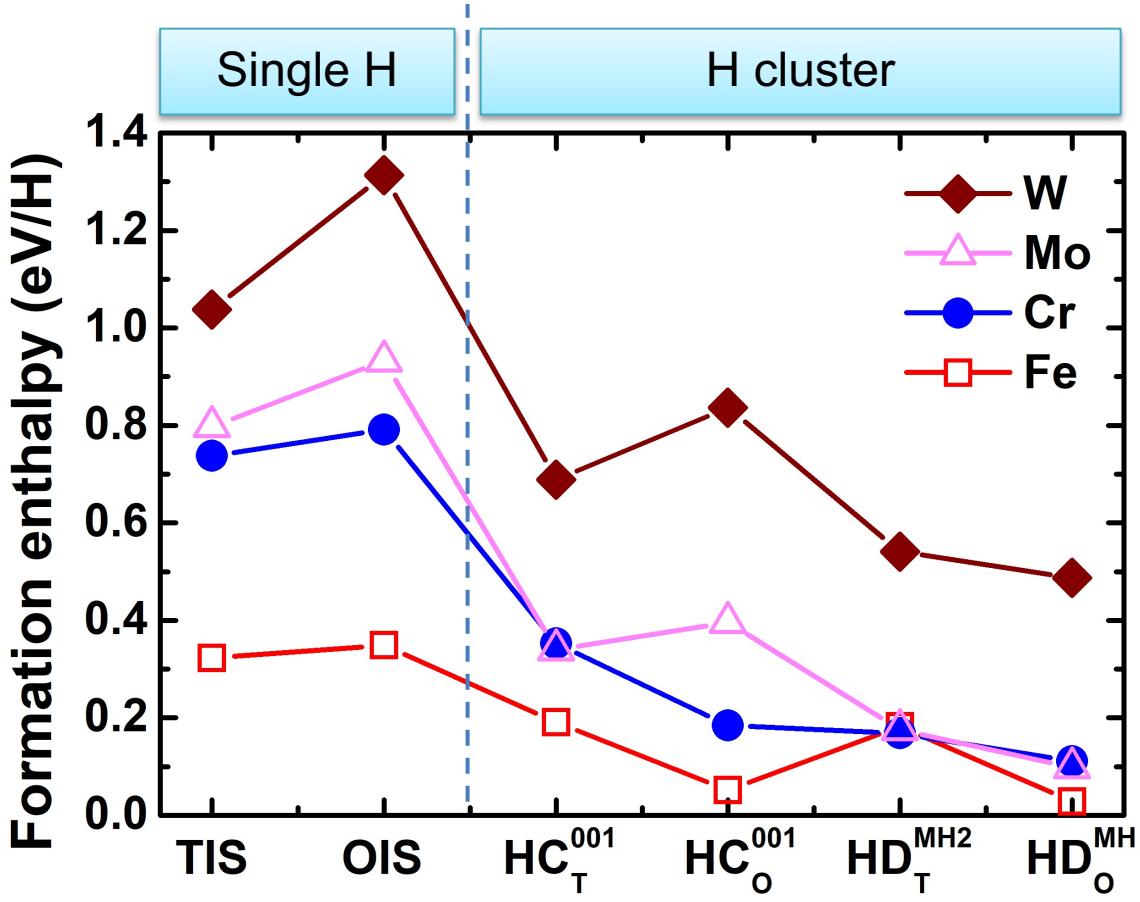
E.g., {110}<111>/2 edge dislocation in Fe

Chen, W. Q., et al. "Nucleation mechanism of intra-granular blisters in tungsten exposed to hydrogen plasma." *Scripta Materialia* 187 (2020): 243-249.
Von Pezold, et al.. "H-enhanced local plasticity at dilute bulk H concentrations: The role of H–H interactions and the formation of local hydrides." *Acta Materialia* 59.8 (2011): 2969-2980.
Kong, Xiang-Shan, et al. "First-principles calculations of transition metal solute interactions with hydrogen in tungsten." *Nuclear Fusion* 56.2 (2015): 026004.

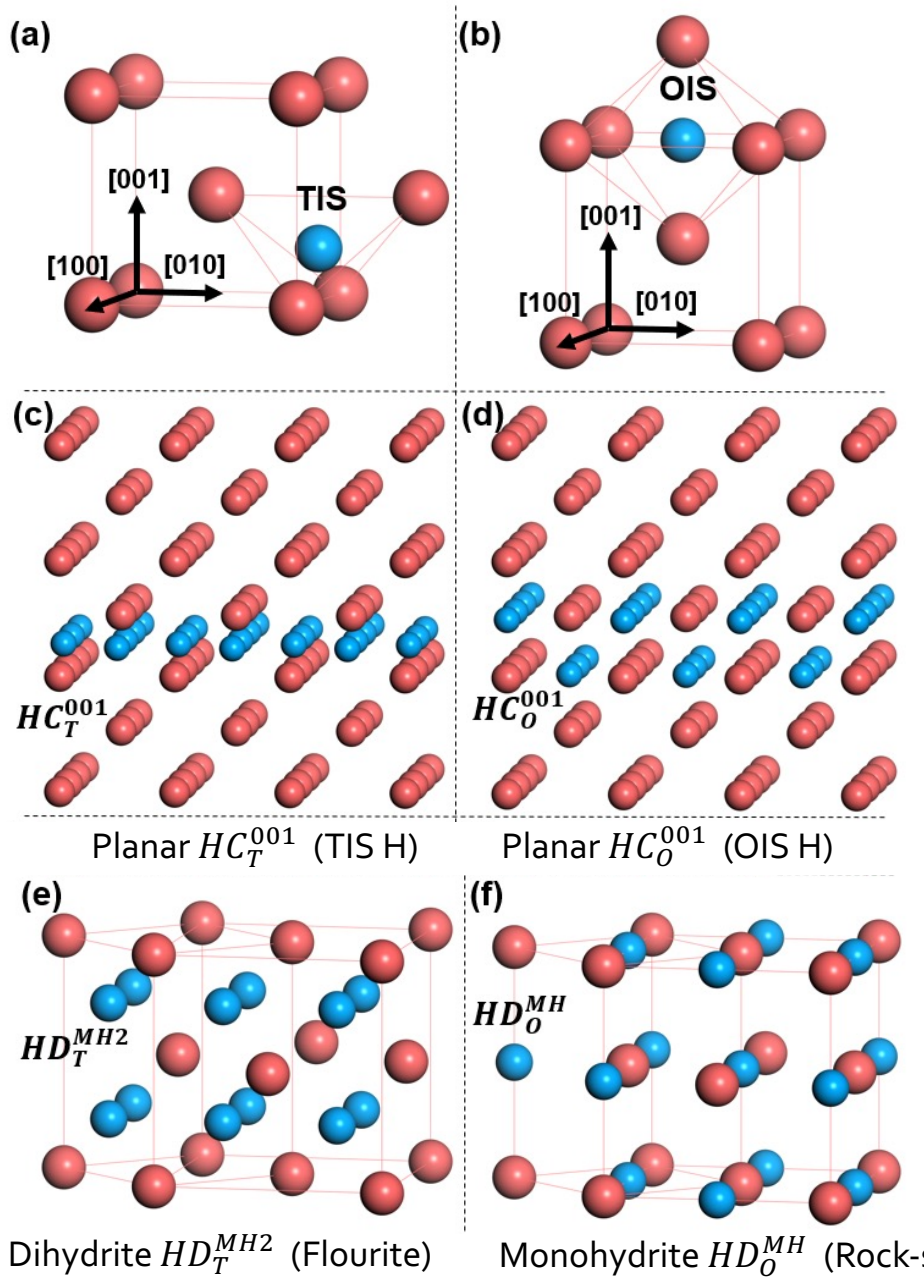
Long-range Elastic Attraction

However,

- For large H clusters, long-range **elastic attraction** exists.



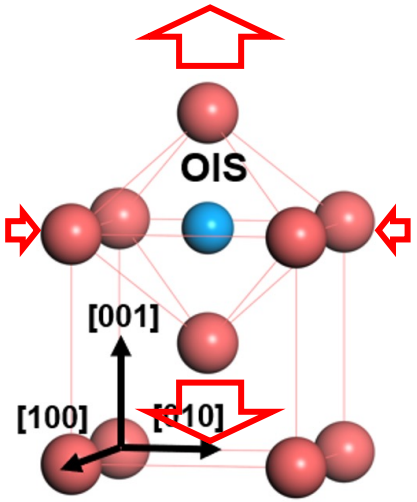
Jie Hou et al 2018 *Nucl. Fusion* 58 096021



High Anisotropy

Highly anisotropic volume tensor

<00l> tension preference

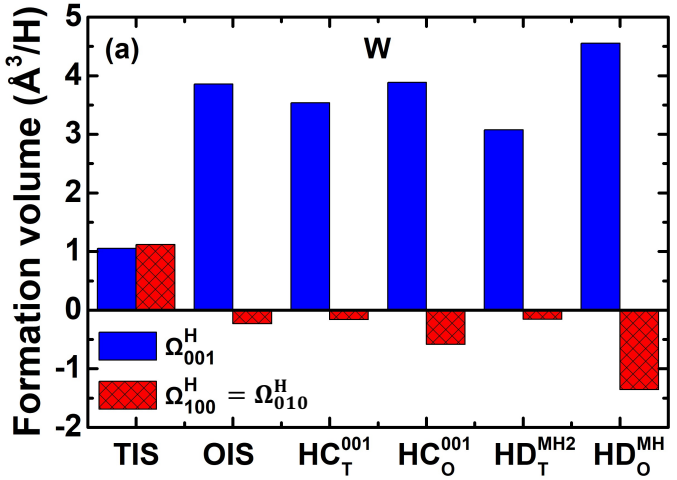


H volume tensor

$$\tilde{\Omega}^H = \begin{bmatrix} \Omega_{100} & 0 & 0 \\ 0 & \Omega_{010} & 0 \\ 0 & 0 & \Omega_{001} \end{bmatrix}$$

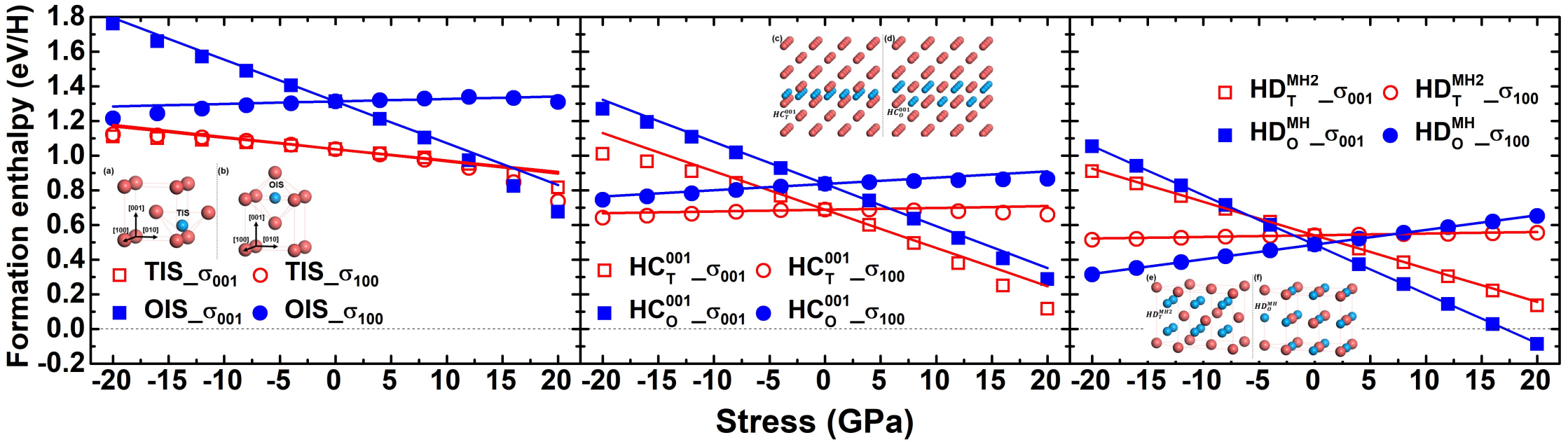
With $\Omega_{001} \gg \Omega_{100}$

Jie Hou, et al. *Acta Materialia* 201 (2020) 23–35



Linear elastic theory prediction: $H_f^H(\tilde{\boldsymbol{\sigma}}^{ext}) = H_f^H(0) - \tilde{\boldsymbol{\sigma}}^{ext} : \tilde{\boldsymbol{\Omega}}^H(0)$

Lines: linear elastic prediction **Dots**: DFT

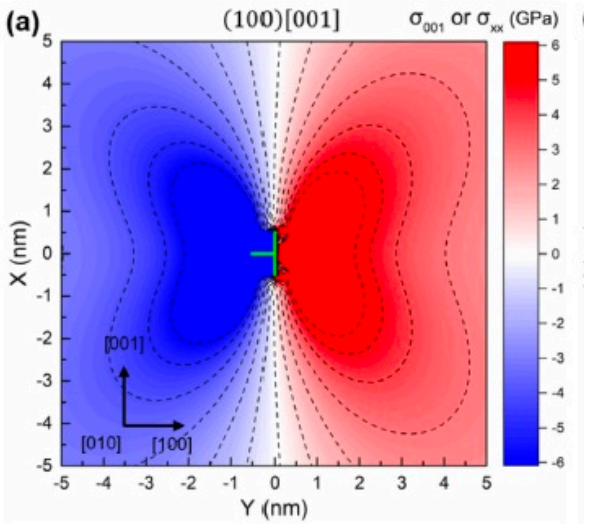


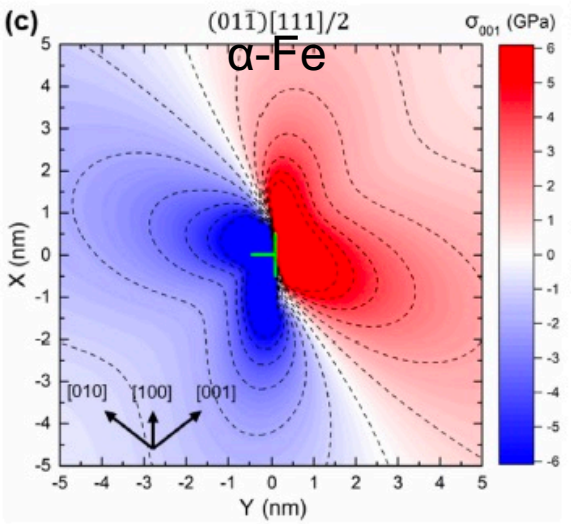
High Anisotropy

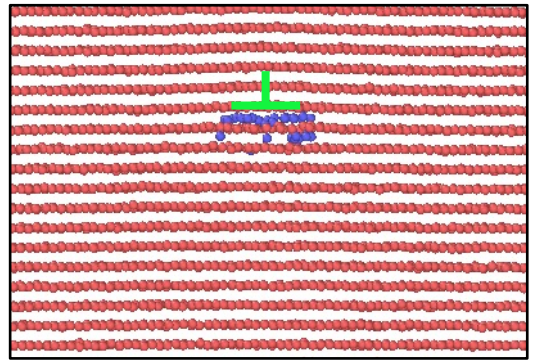
Highly anisotropic volume tensor

<001> tension preference

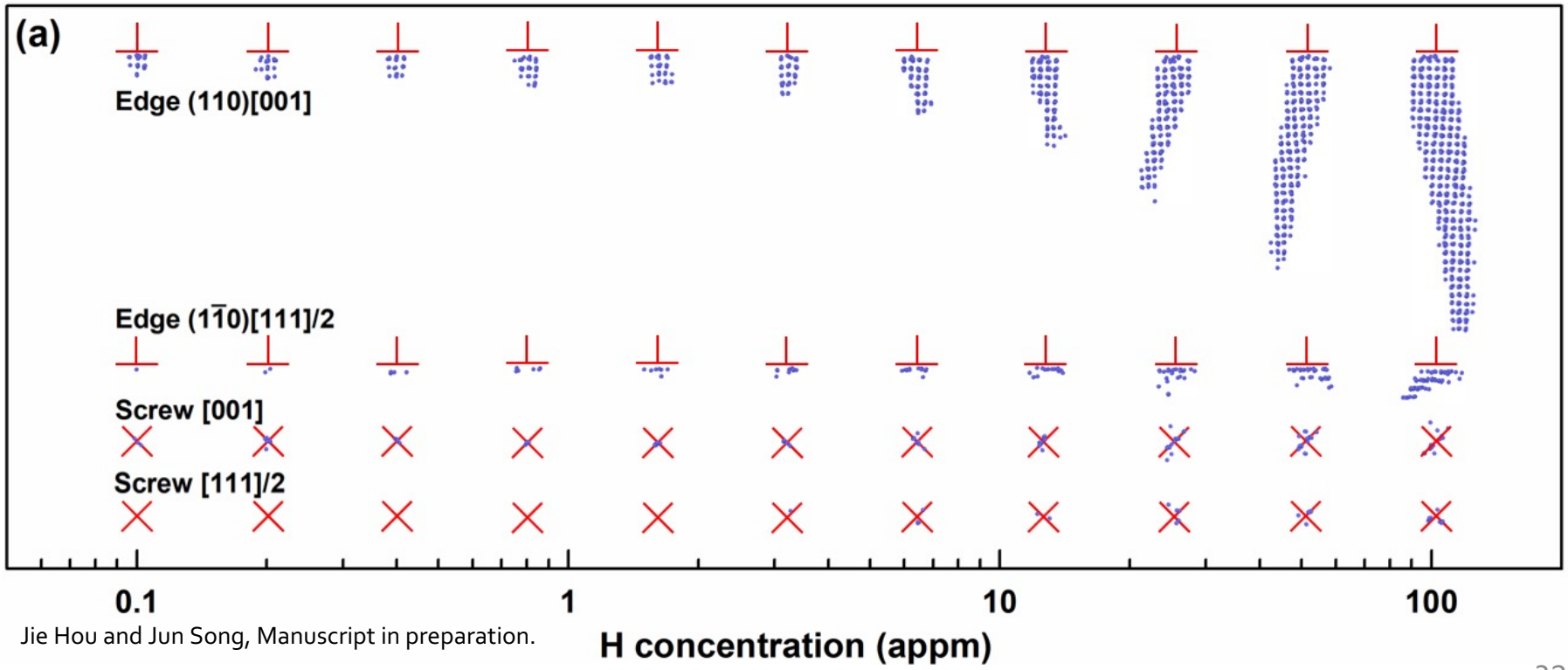
Facilitate H clustering at <001> edge







E.g., {110}<111>/2 edge dislocation in Fe



Jie Hou and Jun Song, Manuscript in preparation.

Highly anisotropic volume tensor

<001> tension preference

Facilitate H clustering at <001> edge

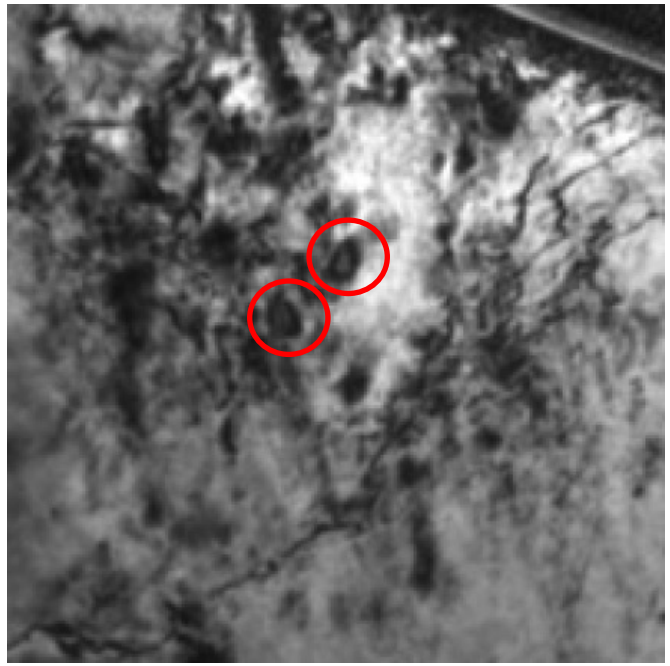
Reduce line energy of <001> edge

promote

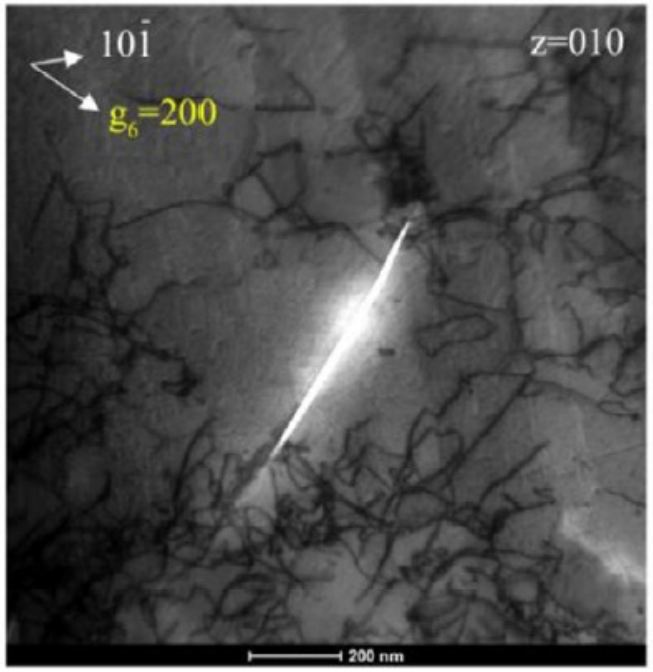
<001> junction formation

<001> dislocation loop formation

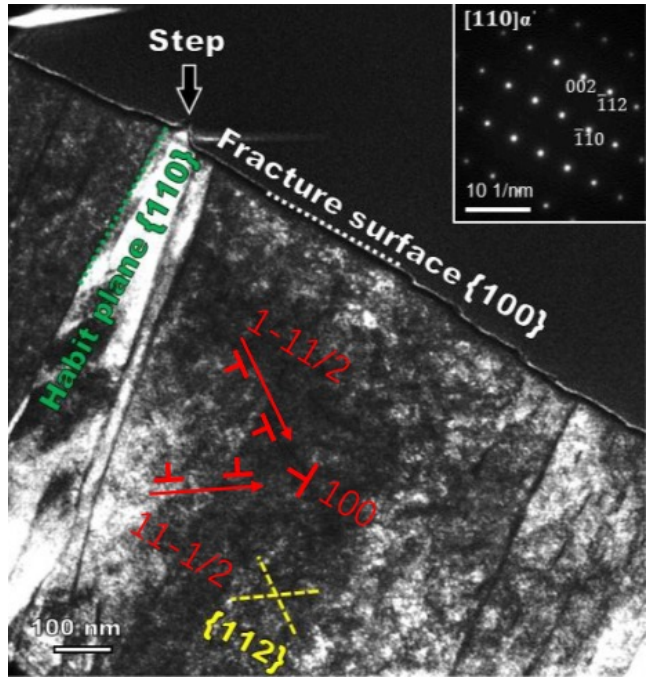
<001> dislocation loop formation in FeAl during H charging and deformation



<001> blister from dense dislocation network in W under H charging



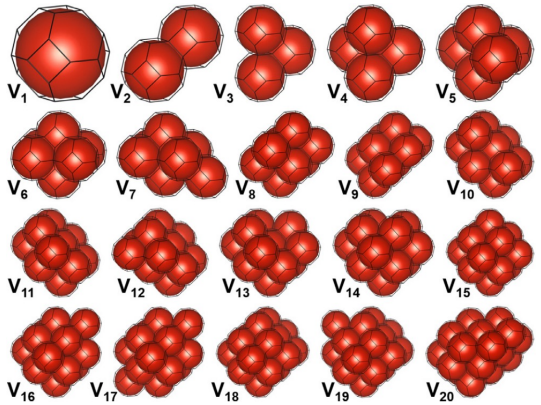
Martensite show {001} HE fracture, with intersecting dislocation bands beneath fracture surface

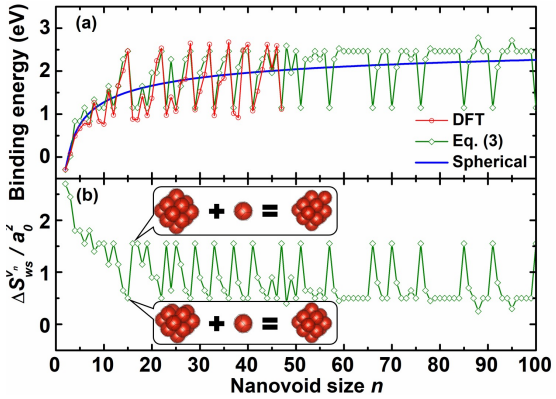


[1] D. Yun, T. Hajilou, D. Wan, N. Kheradmand, and A. Barnoush. "In-situ micro-cantilever bending test in environmental scanning electron microscope: Real time observation of hydrogen enhanced cracking." Scripta Materialia 127 (2017): 19-23.
[2] Chen, W. Q., X. Y. Wang, K. L. Li, Y. N. Wang, T. W. Morgan, B. Xu, Y. L. Chiu, and W. Liu. "Nucleation mechanism of intra-granular blisters in tungsten exposed to hydrogen plasma." *Scripta Materialia* 187 (2020): 243-249.
[3] Cho, L., et al. "Characteristics and Mechanisms of Hydrogen-Induced Quasi-Cleavage Fracture of Lath Martensitic Steel." *Acta Materialia*: 116635.

Predictive model for nanovoid structure and energetics

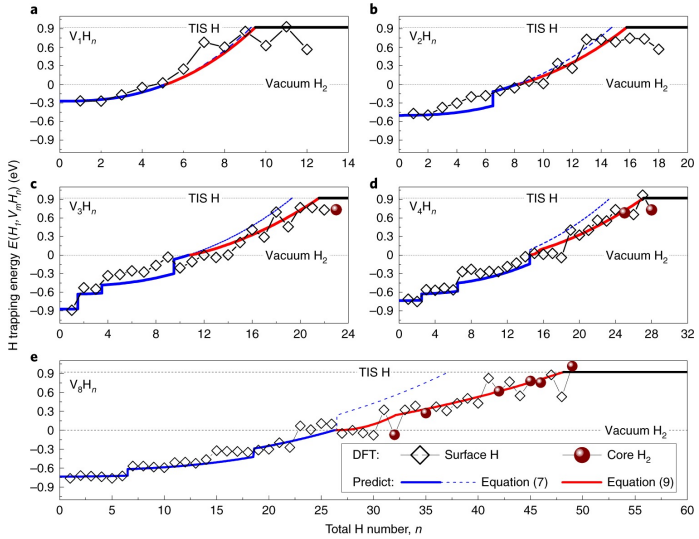
$$E_b^{Vn} = E_f^{V1} + \left(E_b^{V2} - E_f^{V1}\right)\frac{\Delta S_{WS}^{Vn}}{\Delta S_{WS}^{V2}}$$

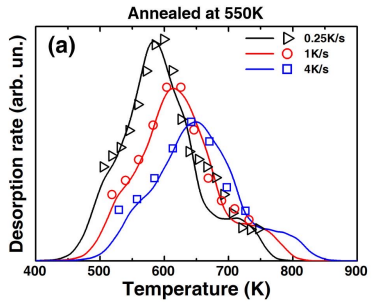


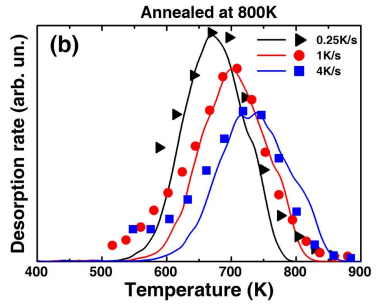


Predictive model for H trapping and bubble formation in nanovoids,

$$E(V_mH_n) = \frac{3}{2}A_c\left(\frac{n_c}{v}\right)^2 = E_{n_s}^{WS} + 7.3A_s\left(\frac{n_s}{a}\right)^{2.5}$$

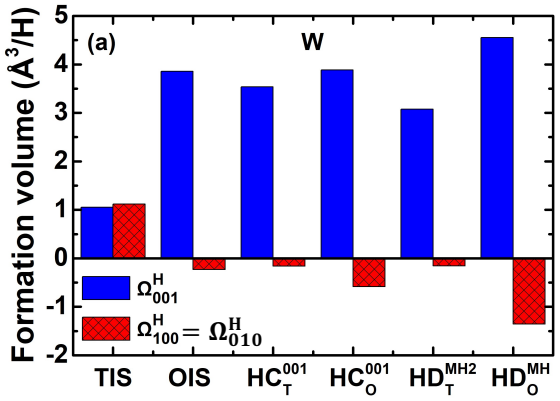






Strong stress anisotropy of H clustering, enable <001> junction/loop formation

$$H_f^H(\tilde{\boldsymbol{\sigma}}^{\boldsymbol{ext}}) = H_f^H(0) - \tilde{\boldsymbol{\sigma}}^{\boldsymbol{ext}} : \tilde{\boldsymbol{\Omega}}^{\boldsymbol{H}}(0)$$



Other Relevant Topics

H-nanovoid

H-dislocation

..?..

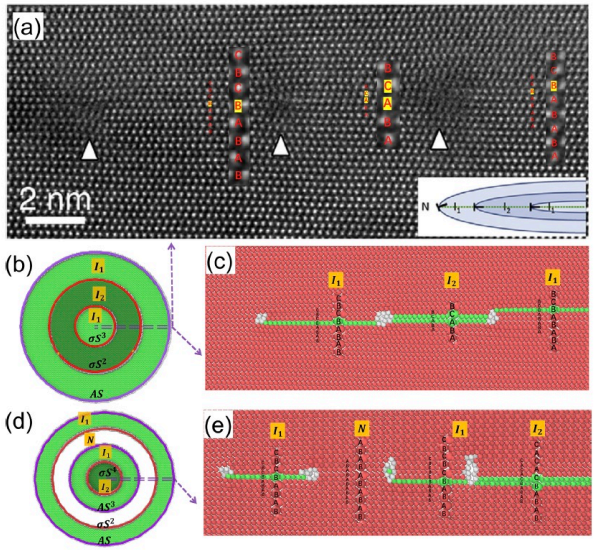
Complex events involving secondary defects or defect ensembles

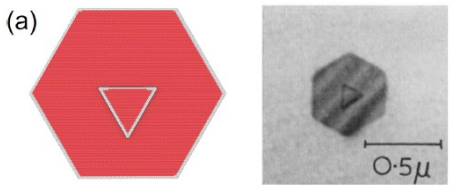
H-induced damages

Evolution (***unfaulting***) of dislocation loops

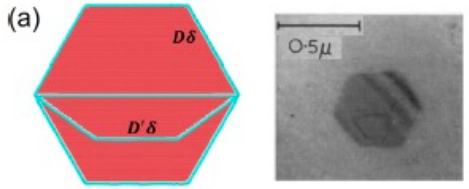
1. Developed a ***general*** and ***flexible*** approach for constructing configurations of ***arbitrary shaped*** dislocation loops & faults

C. Chen, J. Zhang and J. Song Acta Materialia 208 (2021) 116745
C. Chen and J. Song, International Journal of Plasticity 152 (2022) 103231

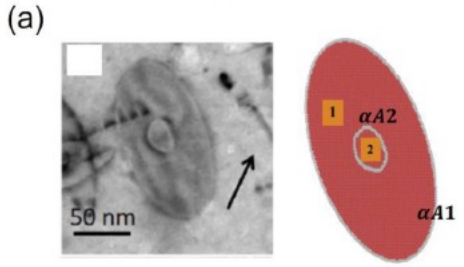


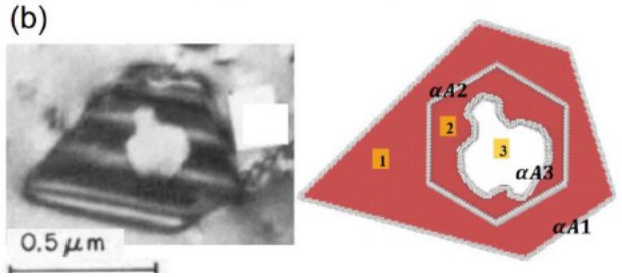


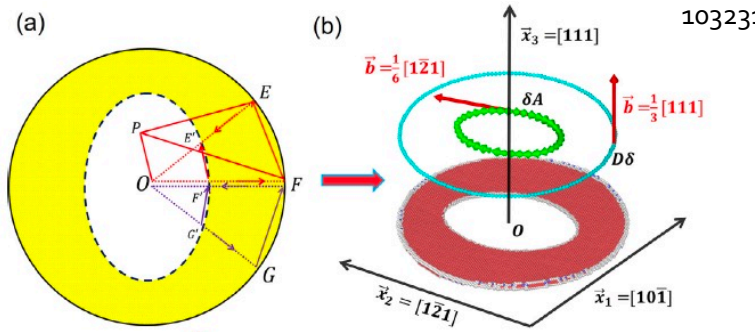
Double-layer loop

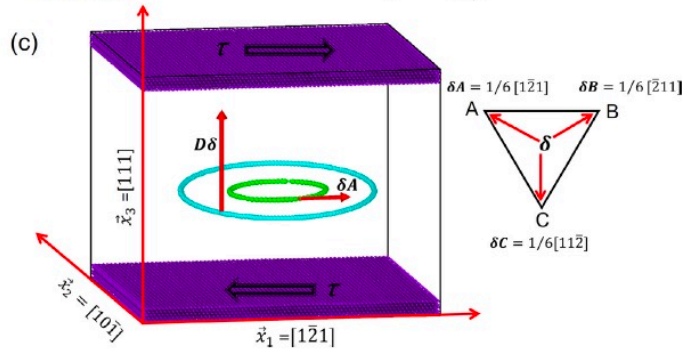


Triple-layer loop









Other Relevant Topics

H-nanovoid

H-dislocation

→ .. ? .. →

Complex events involving secondary defects or defect ensembles

H-induced damages

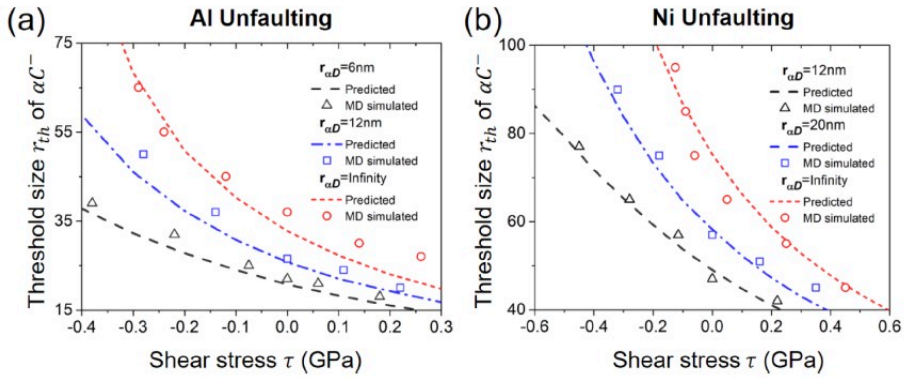
Evolution (***unfaulting***) of dislocation loops

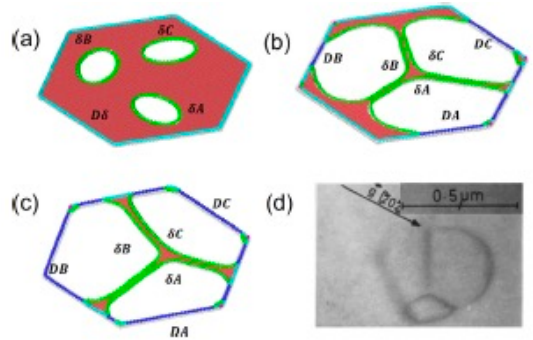
2. Reproduce experimental morphologies and developed a continuum model for ***quantitatively prediction of threshold unfaulting conditions***

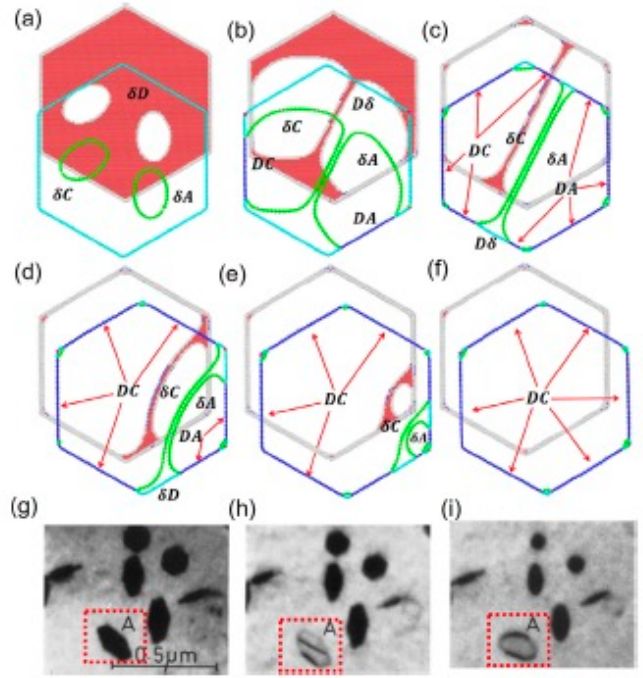
C. Chen, J. Zhang and J. Song Acta Materialia 208 (2021) 116745
C. Chen and J. Song, International Journal of Plasticity 152 (2022) 103231

$$E_{tot}(\epsilon, r, \sigma) = \left(E^{\alpha C^-} + E_{int}^{\alpha D^+}\right) - E_{ext} - E_{SF} \qquad \frac{dE_{tot}(\epsilon, r, \sigma)}{dr} = 0$$

$$E_{int}^{\alpha D^+} = -\frac{G}{8\pi}\oint_{\alpha C^-}\oint_{\alpha D^+} \partial_k\partial_k R_a b_i^{\alpha C^-} b_j^{\alpha D^+} dx_i^{\alpha C^-} dx_j^{\alpha D^+} - \frac{G}{4\pi(1-\nu)}\oint_{\alpha C^-}\oint_{\alpha D^+} \partial_i\partial_j R_a b_i^{\alpha C^-} b_j^{\alpha D^+} dx_k^{\alpha C^-} dx_k^{\alpha D^+}$$
$$\frac{G}{4\pi(1-\nu)}\left[\oint_{\alpha C^-}\oint_{\alpha D^+} \partial_k\partial_k R_a b_i^{\alpha C^-} b_i^{\alpha D^+} dx_j^{\alpha C^-} dx_j^{\alpha D^+} - \nu\oint_{\alpha C^-}\oint_{\alpha D^+} \partial_k\partial_k R_a b_i^{\alpha C^-} b_j^{\alpha D^+} dx_j^{\alpha C^-} dx_i^{\alpha D^+}\right]$$







Other Relevant Topics

H-nanovoid

H-dislocation

→ .. ? .. →

Complex events involving secondary defects or defect ensembles

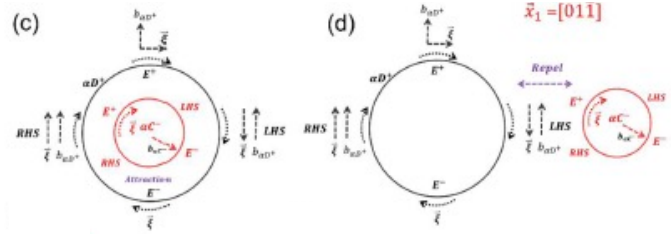
H-induced damages

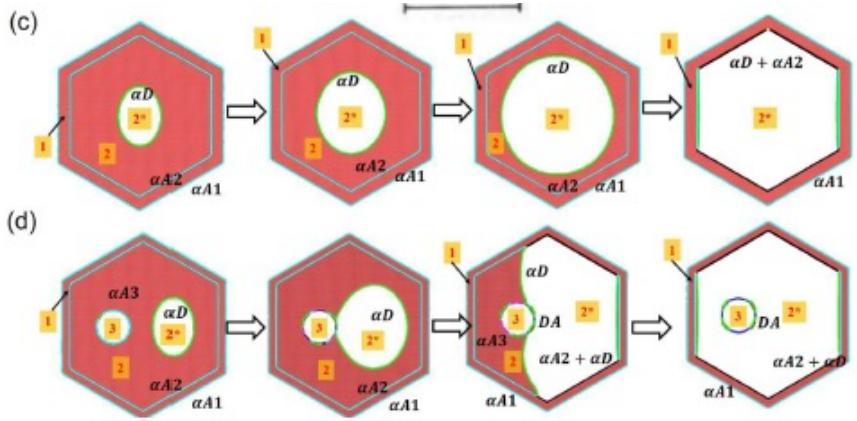
↓

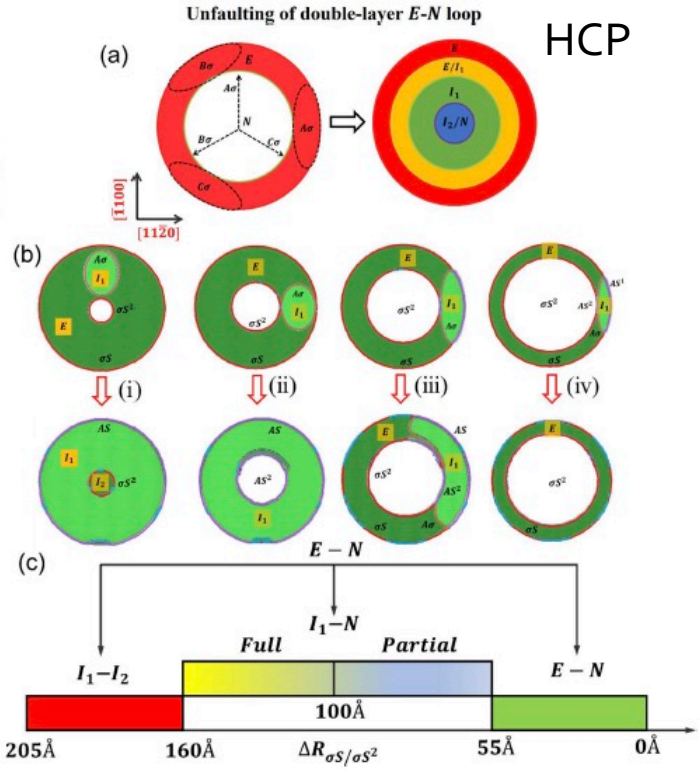
Evolution (***unfaulting***) of dislocation loops

C. Chen, J. Zhang and J. Song Acta Materialia 208 (2021) 116745
C. Chen and J. Song, International Journal of Plasticity 152 (2022) 103231

3. Identify ***unfaulting mechanisms*** and ***pathways*** and clarify associated ***dislocation reactions***







Acknowledgement & Others

Dr. Jie Hou
Materials Engineering, McGill University

Prof. Xiang-Shan Kong
Materials Science and Engineering, Shandong University

Prof. Cheng Chen
School of Aeronautics, Northwestern Polytechnical University

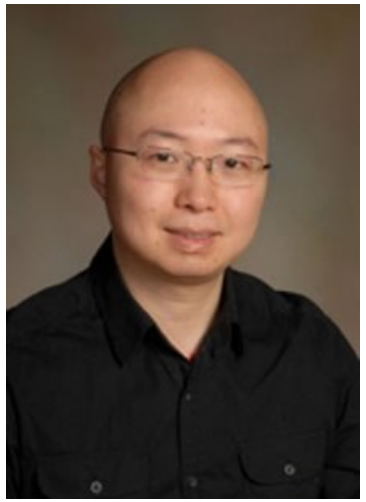
NSERC CRSNG

compute • calcul CANADA

Acknowledgement

McGill Hydrogen Embrittlement Facilities (MHEF) https://mhef.lab.mcgill.ca/

Co-directed by Prof. Stephen Yue, Prof. Jun Song, Dr. Salim Brahimi


Research directions:

i. Multicale HE studies involving experiments, DFT/atomistic and FEA simulations
ii. Susceptibility of fastener and pipeline materials to HE
iii. Coating processes and embrittlement
iv. Susceptibility of aerospace materials and coating processes

Thank You
Questions?