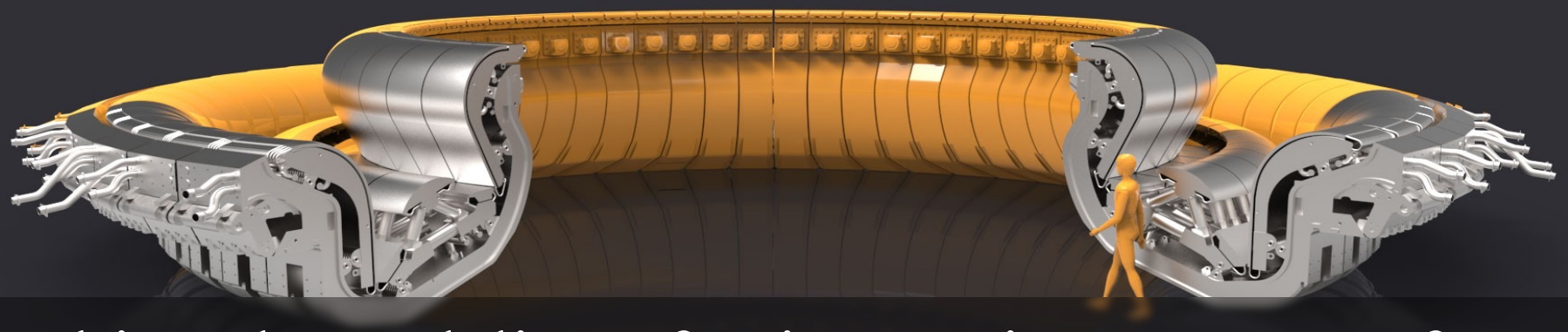


Multi-scale modeling of H interactions on W surfaces and W/Cu interlayers

Y. Silva-Solís[1], J. D. Cremé[1], J. Denis[1], E. A. Hodille[2] and Y. Ferro[1]

[1]Aix-Marseille University, CNRS, PIIM, F-13013 Marseille, France

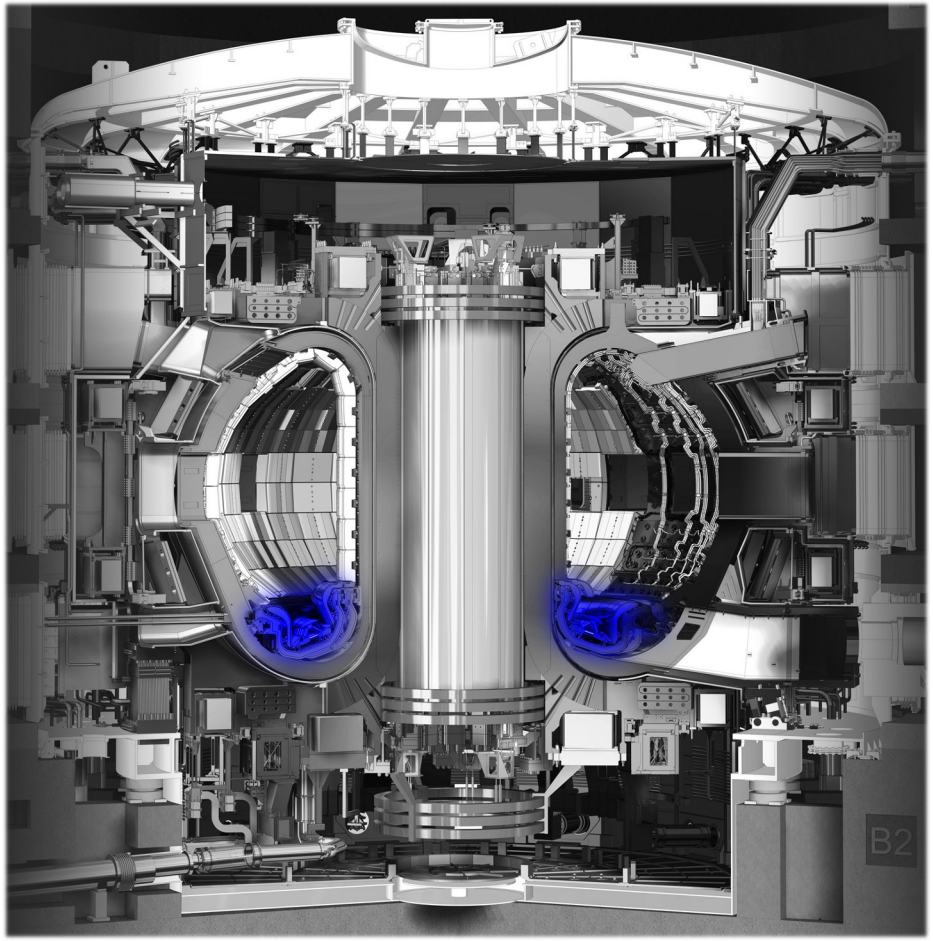
[2]CEA, IRFM, F-13108 Saint-Paul-lez-Durance, France

Outline

1. Introduction.
2. Methodology.
3. Surface, sub-surface and bulk phenomenon.
4. Interface: W/Cu in the PFUs.
5. Conclusions.

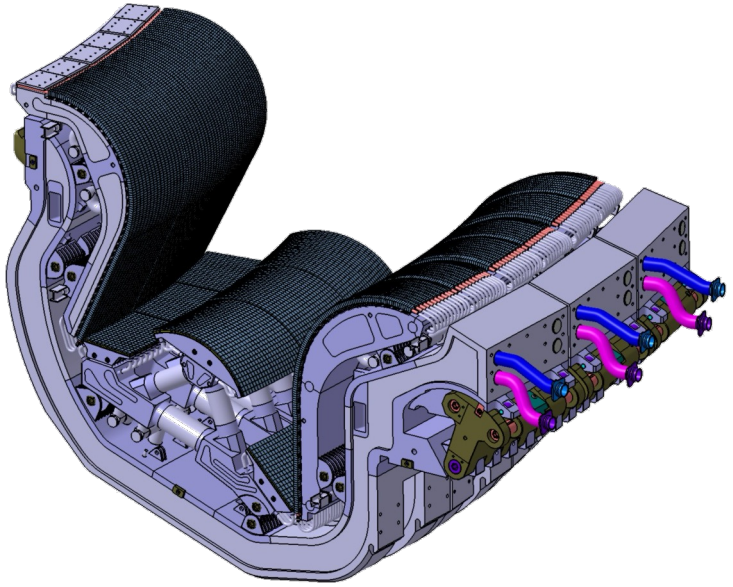
What are we interested in?

ITER tokamak



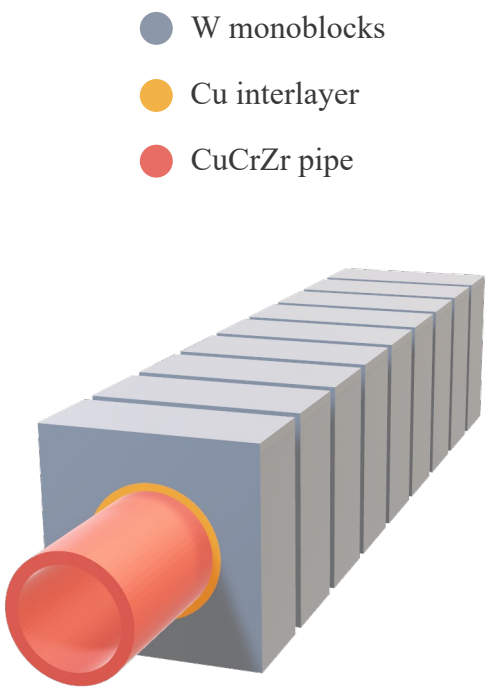
Plasma-material interaction

ITER-like divertor



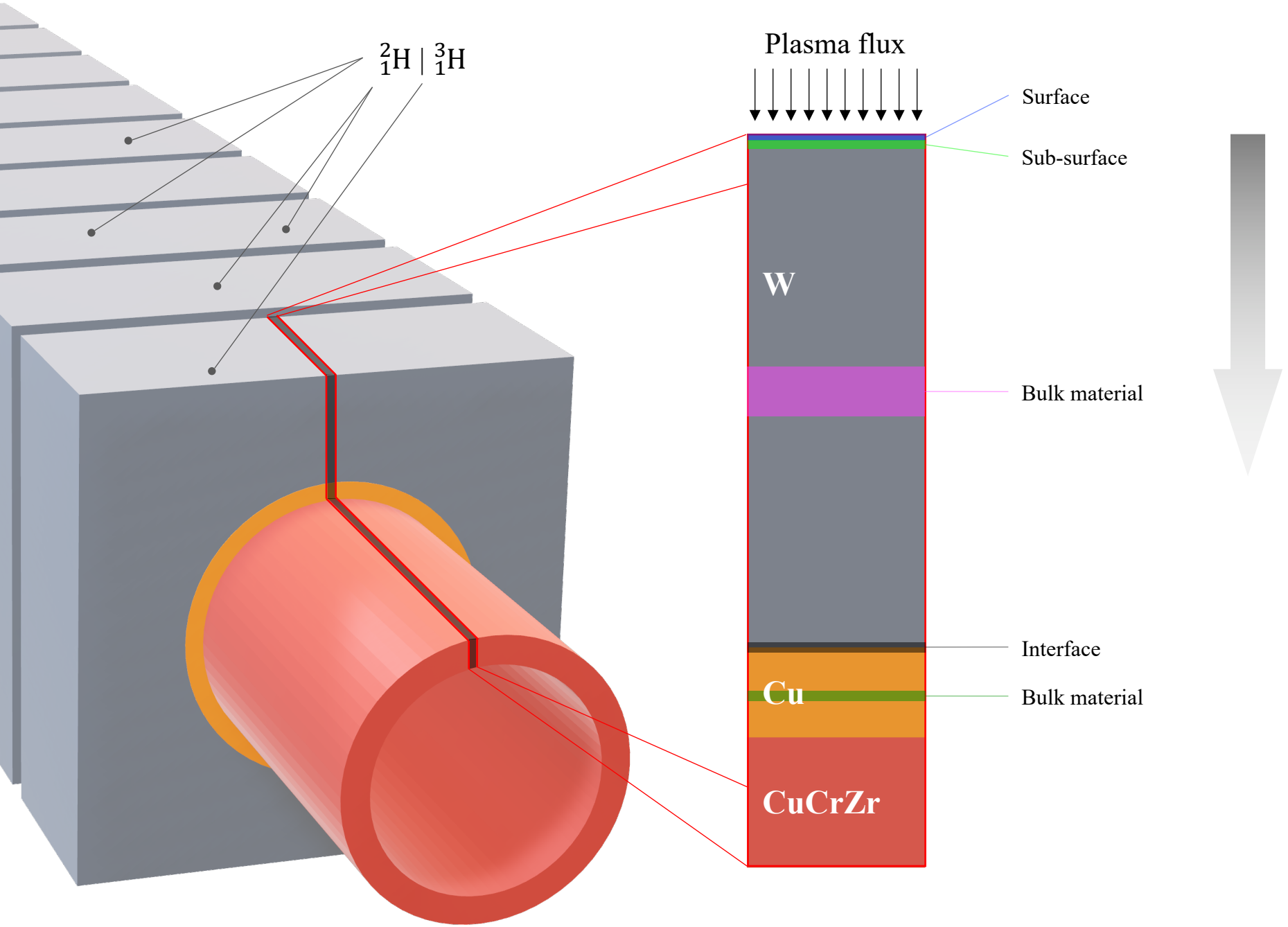
Strong interaction with the plasma

Plasma-facing units



Effect of H atoms

What are we interested in?



Hydrogen concentration

Multi-scale modeling

(Interactions of H with the materials)

- DFT (electronic and phonons)
- Statistical thermodynamics
- Kinetic models
- Molecular Dynamics

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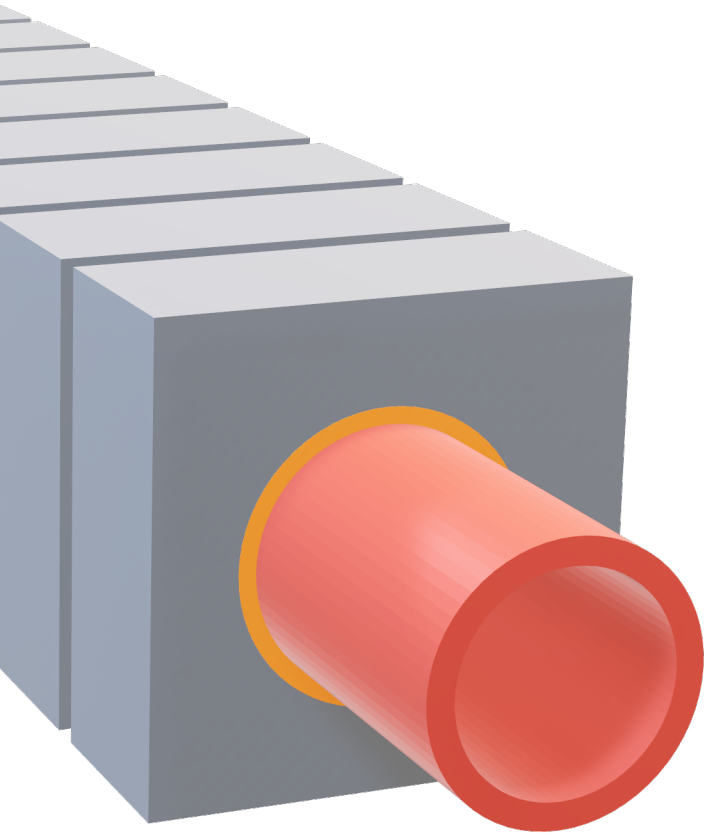
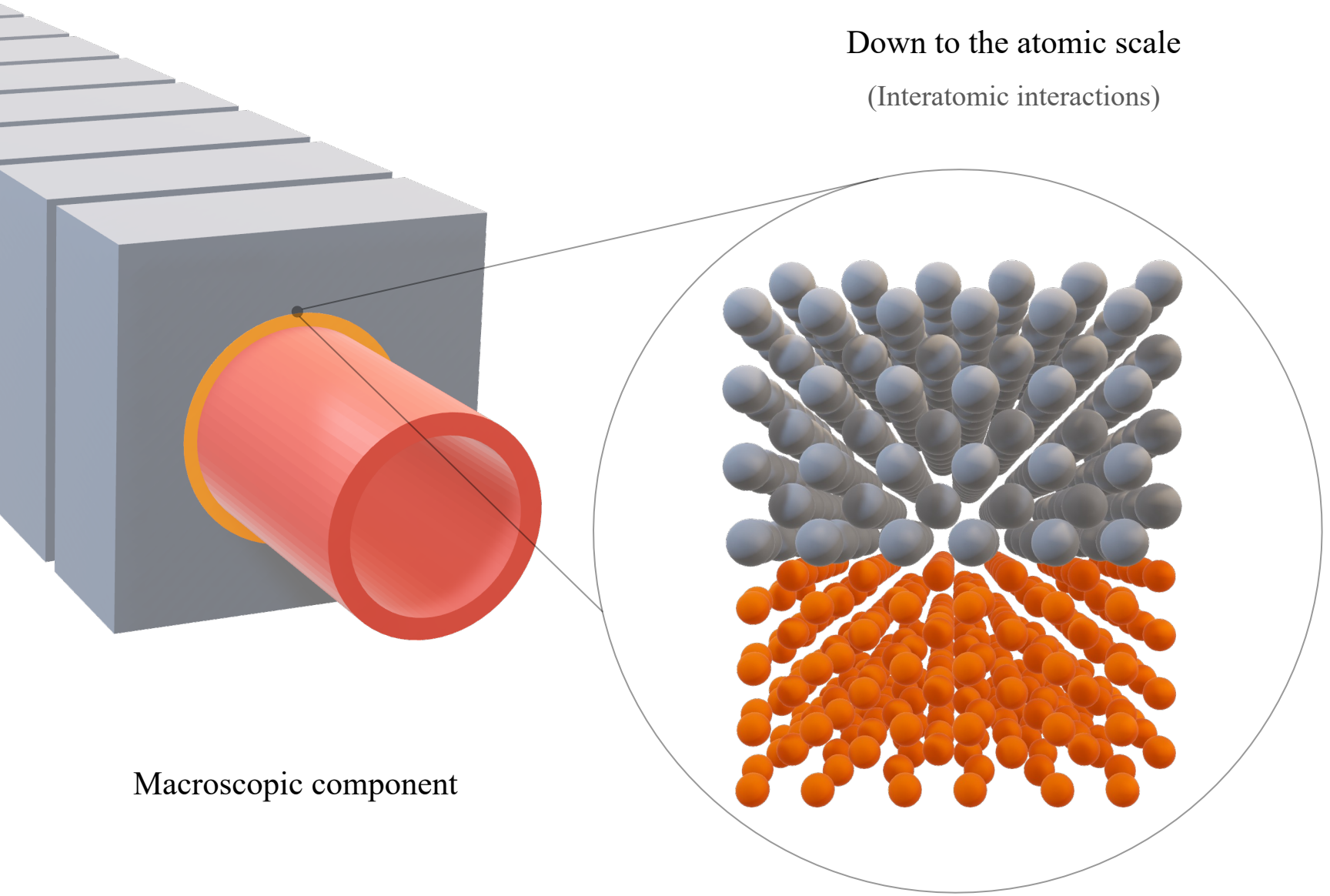
Outline

2.1. Methodology – Electronic structure by DFT



Macroscopic component

2.1. Methodology – Electronic structure by DFT

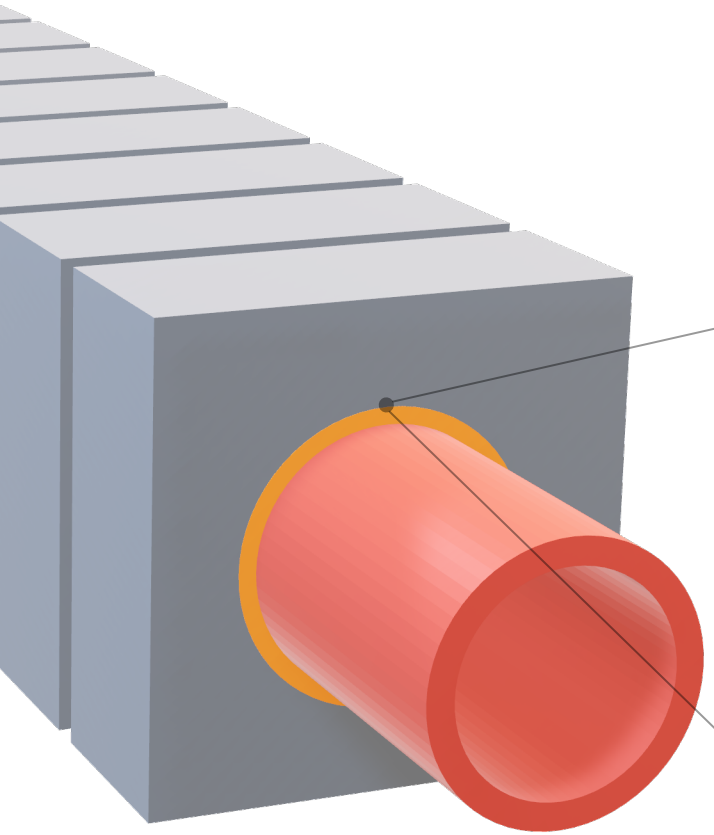


Down to the atomic scale

(Interatomic interactions)

Macroscopic component

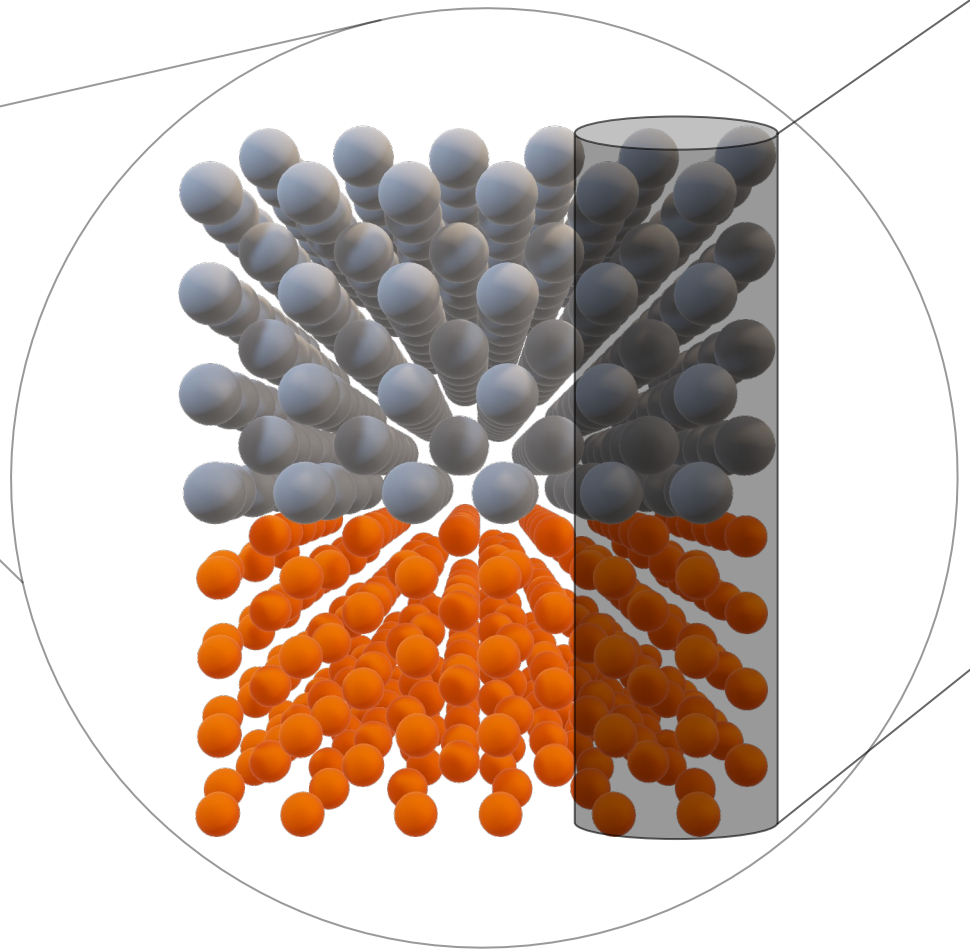
2.1. Methodology – Electronic structure by DFT



Macroscopic component

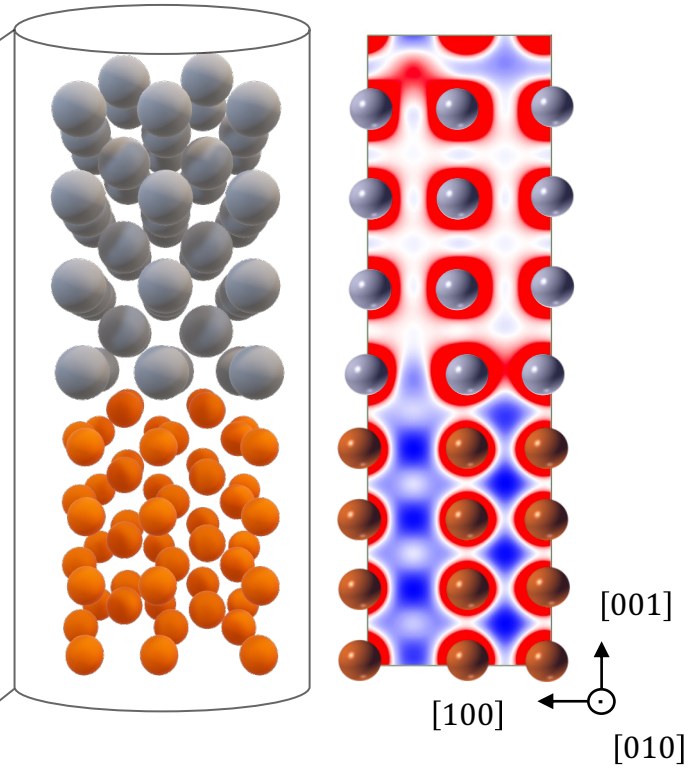
Down to the atomic scale

(Interatomic interactions)



Electronic properties

(Electronic structure calculations)



- Accurate, but not exact.
- Computationally expensive.
- Systems with few atoms.

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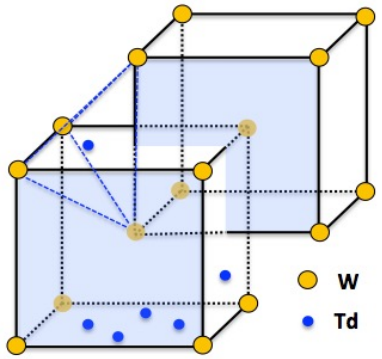
H in W bulk by DFT calculations

H — H



Molecule H_2 Interstitial H_i

Electronic energies by DFT

$e^{DFT}_{H_2}$ $e^{DFT}_{H_i}$

Vibrational frequencies by DFT

ν_{H_2} $\sum_{k=1}^{3} \nu_k$

H in W bulk by DFT calculations

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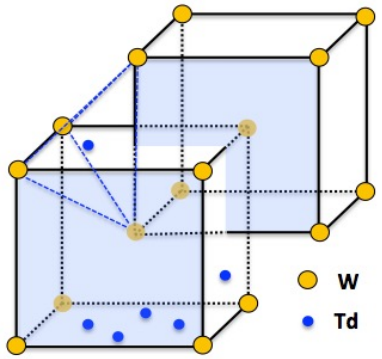

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Statistical thermodynamics

Gibbs free energy of the system based on DFT

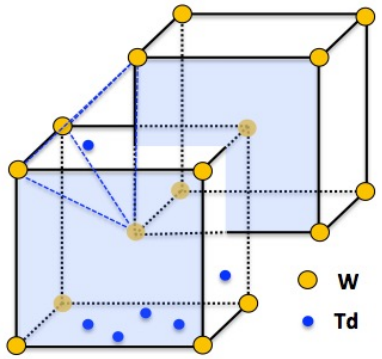
H_2 gas

$$g_{H_2} = g^{\circ}_{H_2} + k_B T \ln\left(\frac{P}{P^{\circ}}\right)$$

$$g^{\circ}_{H_2} = \left(e^{DFT}_{H_2} + e^{vib}_{H_2} + e^{rot}_{H_2} + e^{trans}_{H_2} + P\Delta V\right) - T\left(s^{vib}_{H_2} + s^{rot}_{H_2} + s^{\circ trans}_{H_2}\right)$$

H in W bulk by DFT calculations

H — H



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Macroscopic system

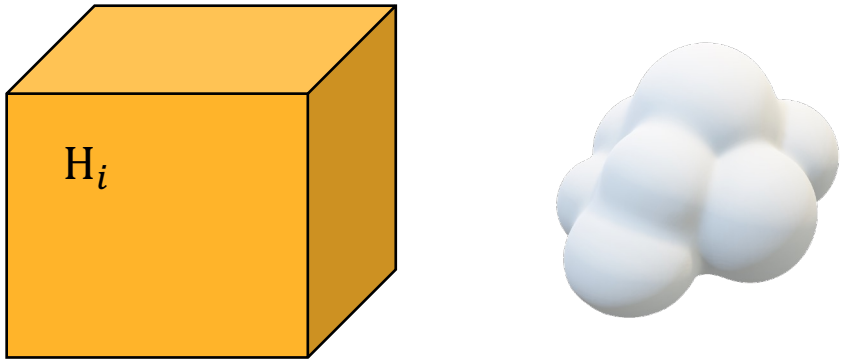
Any sub-system j

$$g_j = e_j - T s_j$$

Potential to be minimized

$$G = \frac{1}{2}\left(N_H - n_{int} - \sum_{j=0}^{12} j\, n_j\right)\mu_{H_2} + n_{int}\; g_{int} + \left(\sum_{j=0}^{12} j\, n_j\; g_j\right) - T\, S_{conf}$$

W Bulk $\rightleftharpoons$ H_2 gas



H fraction in W at. %

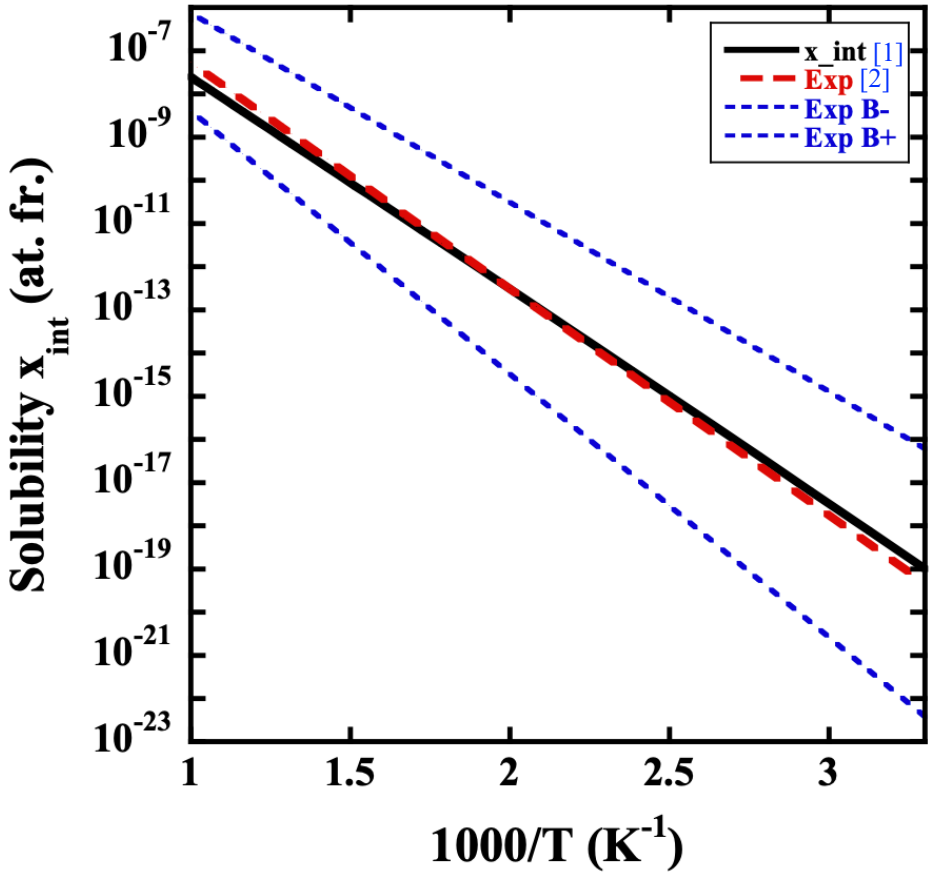
$$x_{H_i}(T) \approx \gamma \exp\left[-\frac{g_{H_i} - \mu}{k_B T}\right]$$

Chemical potential H_2 ideal gas

$$\mu = \frac{1}{2}\left(g^{\circ}_{H_2} + k_B T \ln \frac{P}{P^{\circ}}\right)$$

H reservoir was treated as real and ideal gas [1]

Solubility of H in W without defects



Comparison against experiments

[1] E. A. Hodille, *Physical Review Materials*, 2 (2018) 093802..
[2] R. Frauenfelder, J. Vac. Sci Technol 6 (1969).

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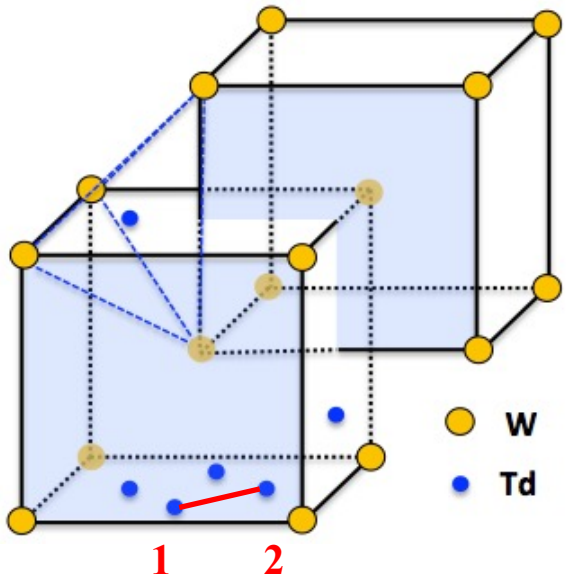
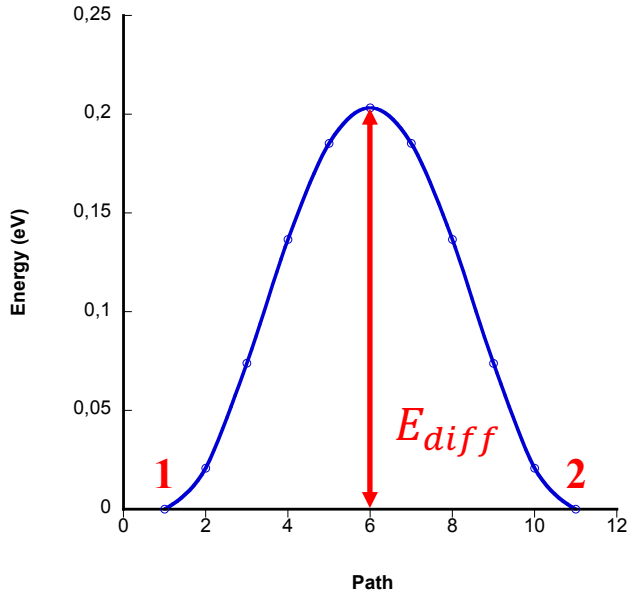
Diffusion of H atoms in perfect W bulk



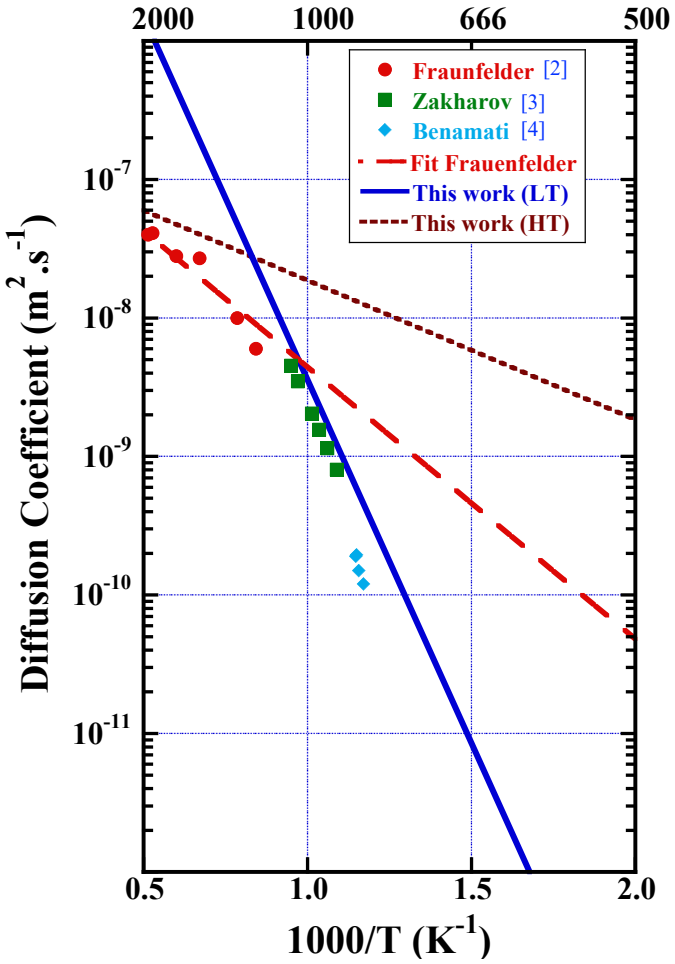
Interstitial H_i

Energy profile by DFT



Diffusion coefficient

$$D(T) \approx D_o \exp\left[-\frac{E_{diff}}{k_B T}\right]$$



N. Fernandez, et al., Acta Materialia 94 (2015), 307-318.

[2] R. Frauenfelder, J. Vac. Sci Technol 6 (1969).
[3] A. P. Zakharov et.al., SSR 9 (1975), 149–153.
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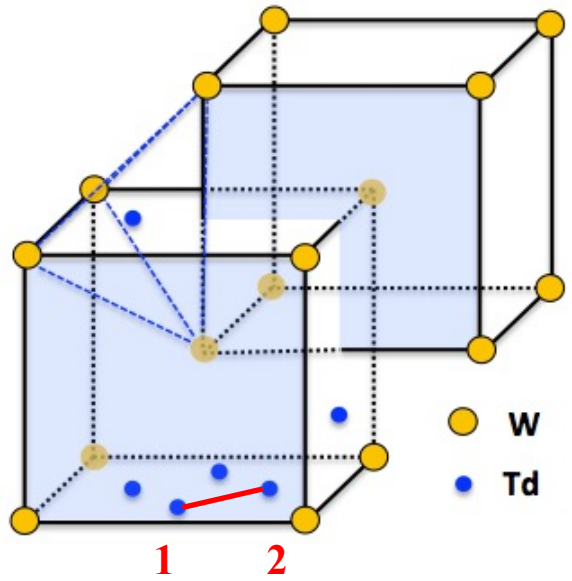

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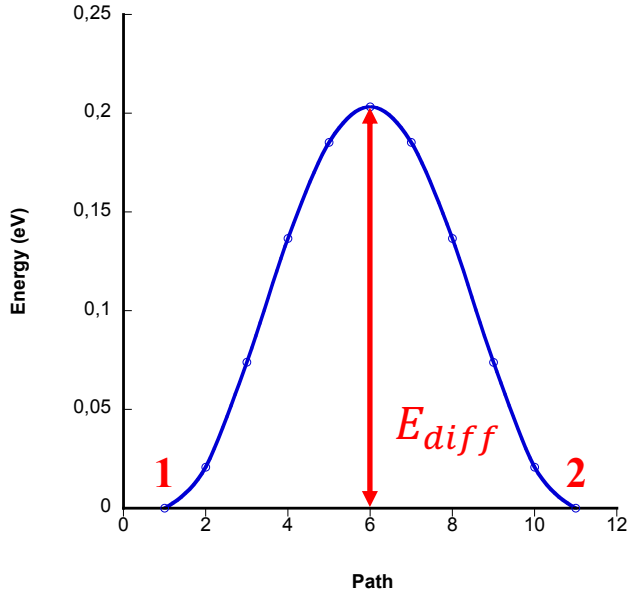

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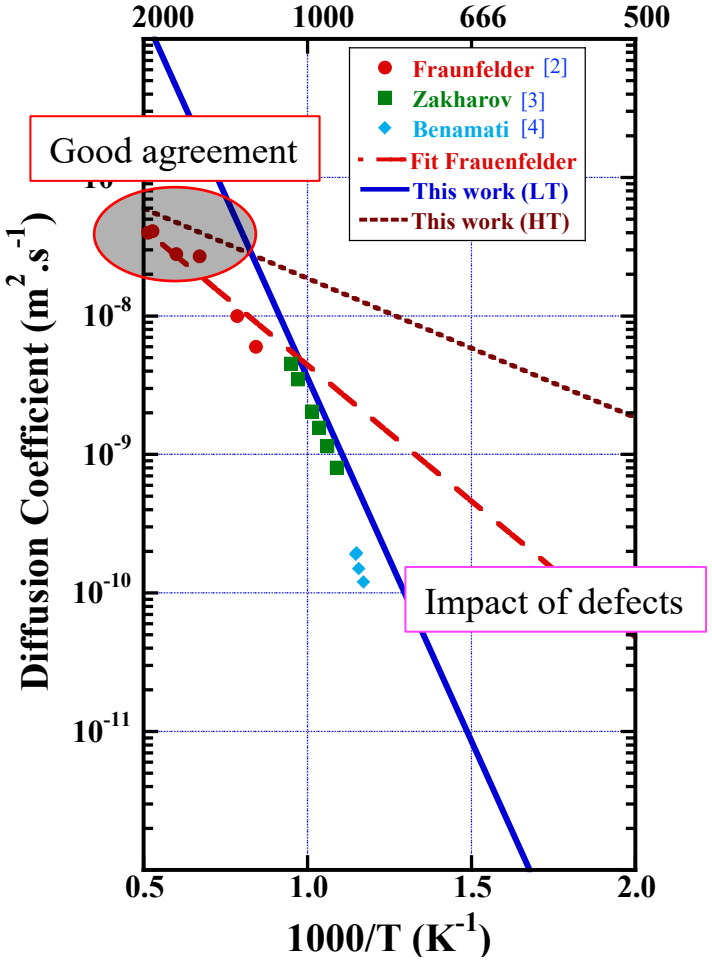

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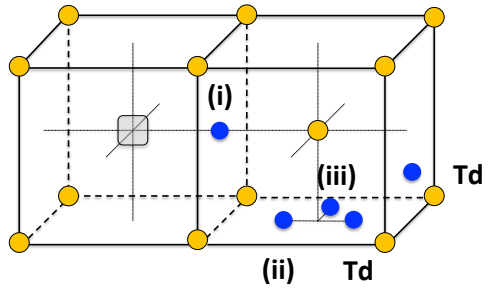
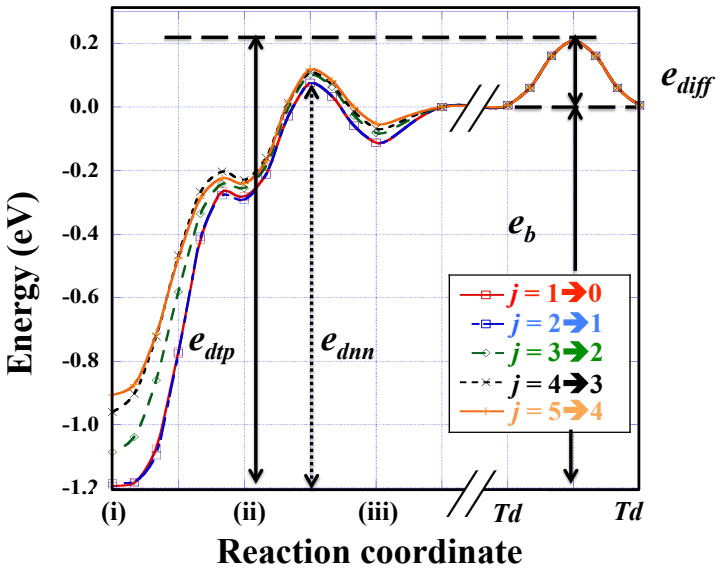
Diffusion and trapping in complex environments

Vacancy in W





N. Fernandez, et al., Acta Materialia 94 (2015), 307-318.

Reaction diffusion models

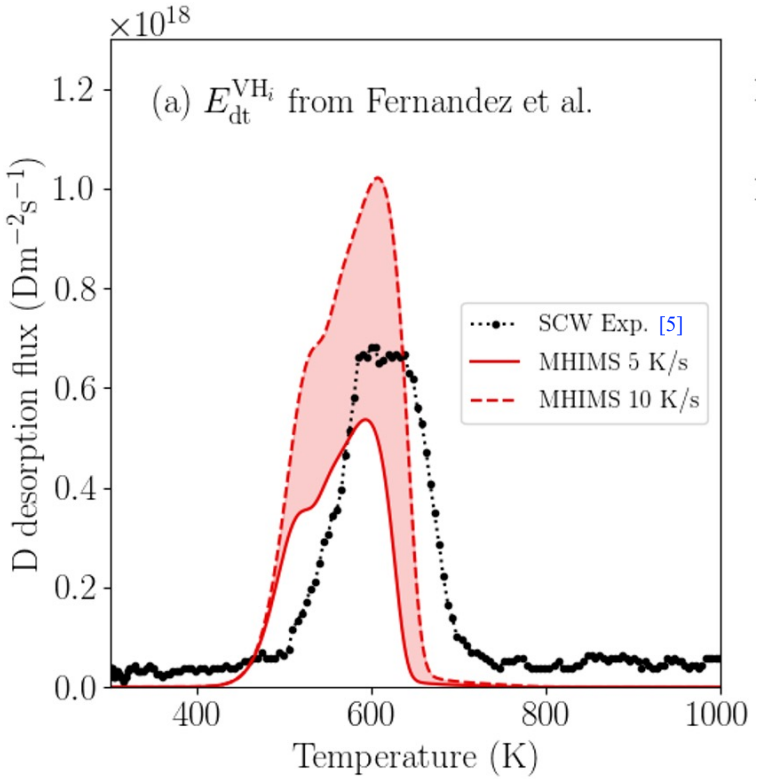
$$\nu_i = \nu_o \exp\left[-\frac{E_{diff}}{k_B T}\right]$$

MHIMS code

$$\frac{\partial c_{\mathrm{m}}}{\partial t} = \nabla \cdot (D(T)\nabla c_{\mathrm{m}}) - \sum \frac{\partial c_{\mathrm{t},i}}{\partial t} + S_{\mathrm{ion}}(x)$$

$$\frac{\partial c_{t,i}}{\partial t} = \nu_{t,i}(T) c_m \frac{(n_i - c_{t,i})}{n_{IS}} - \nu_{dt,i}(T) c_{t,i}$$

Experimental comparison with TDS



[5] M. Poon *et al JNM* 374 (2008) 390

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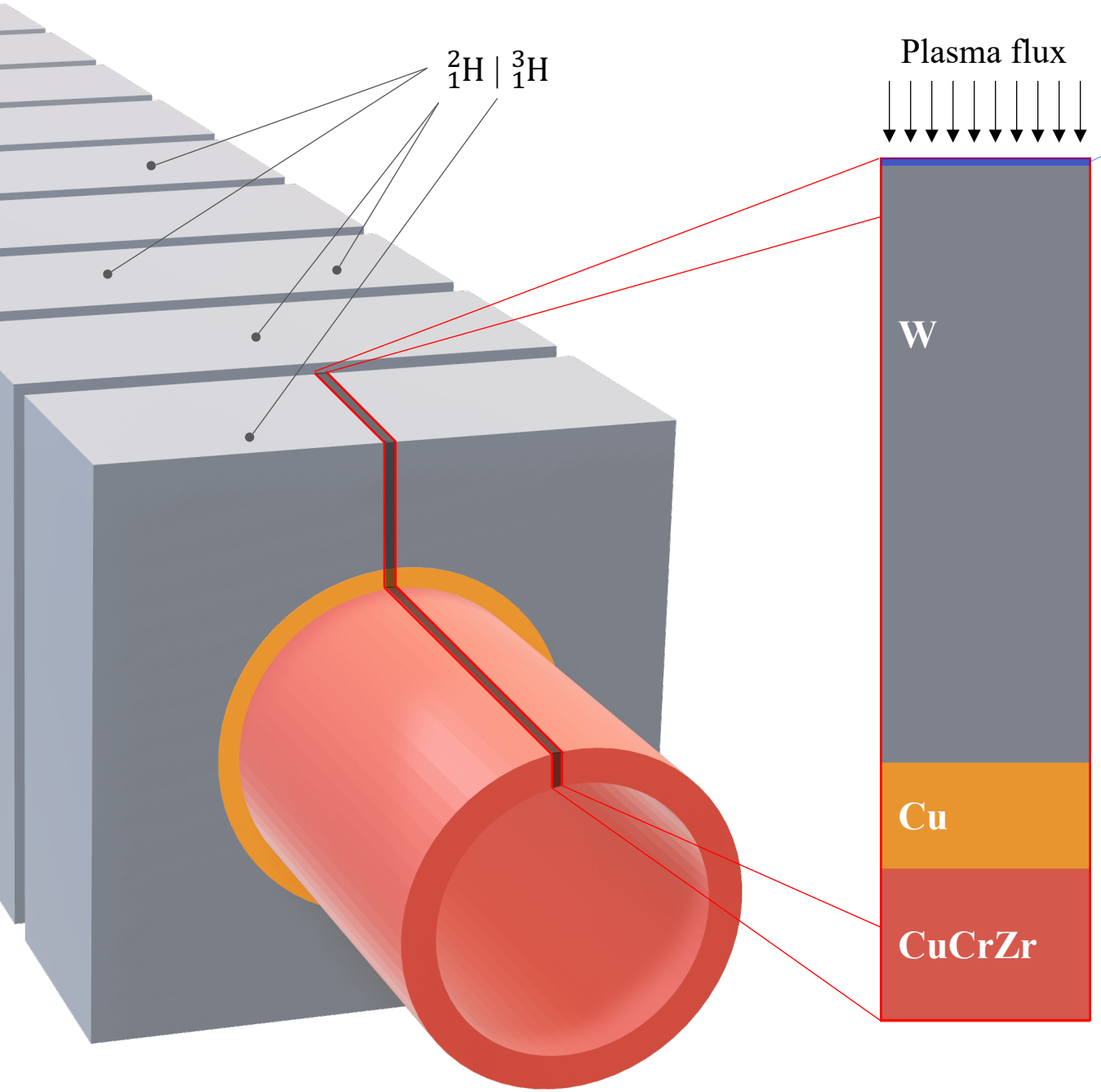
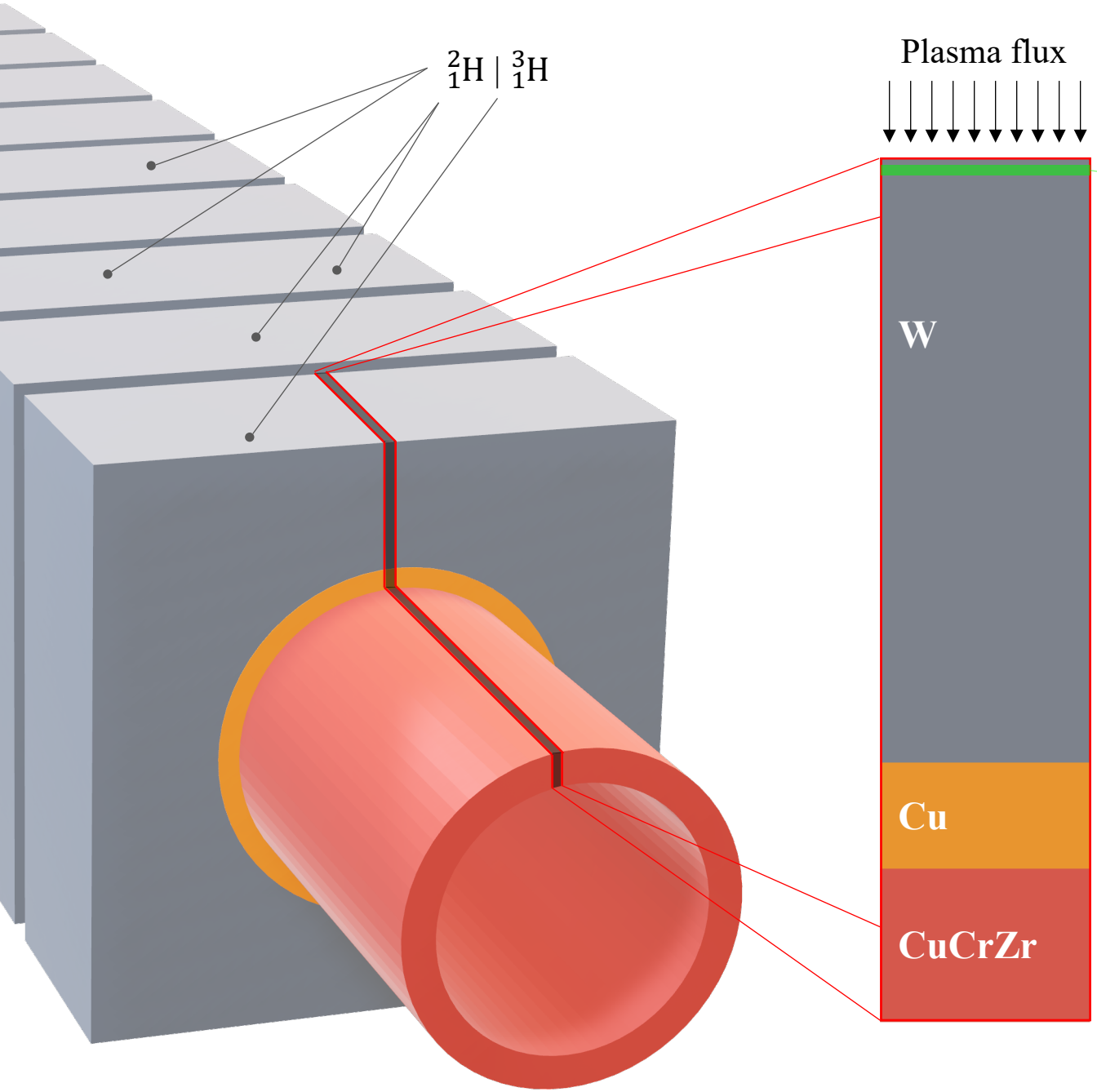


Hydrogen concentration

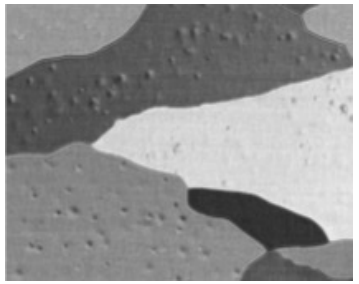
Surface models

- H recycling depends on the surface.
- E_{des} depending on the coverages.
- Impact of H and O was modelled.

3. Surface, sub-surface and bulk phenomenon



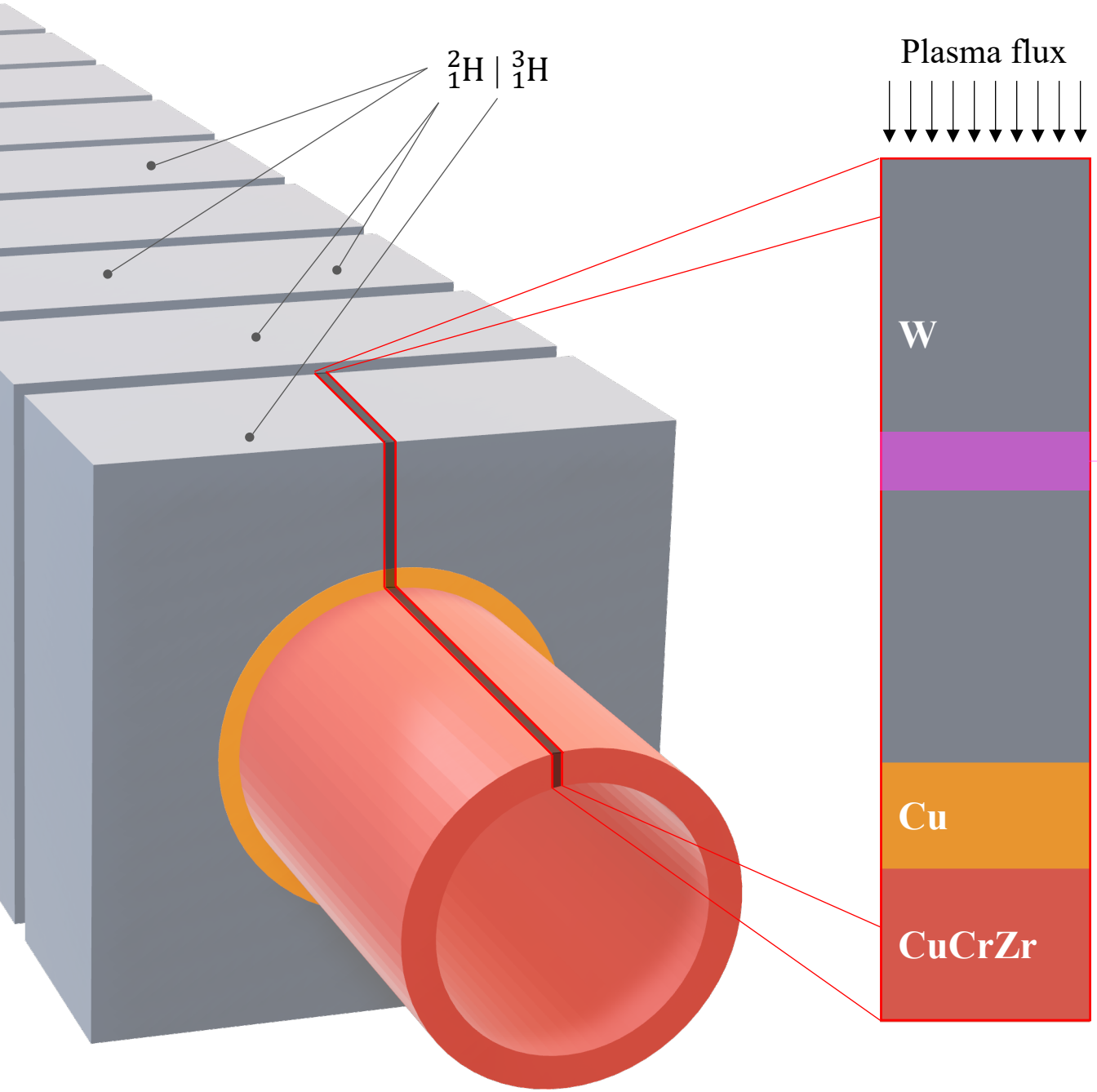
Hydrogen concentration



Super-saturated layers (SSL)

- H flux to the surface, high H concentration.
- Induces VH_j formation.
- Lead to the formation of SSL.

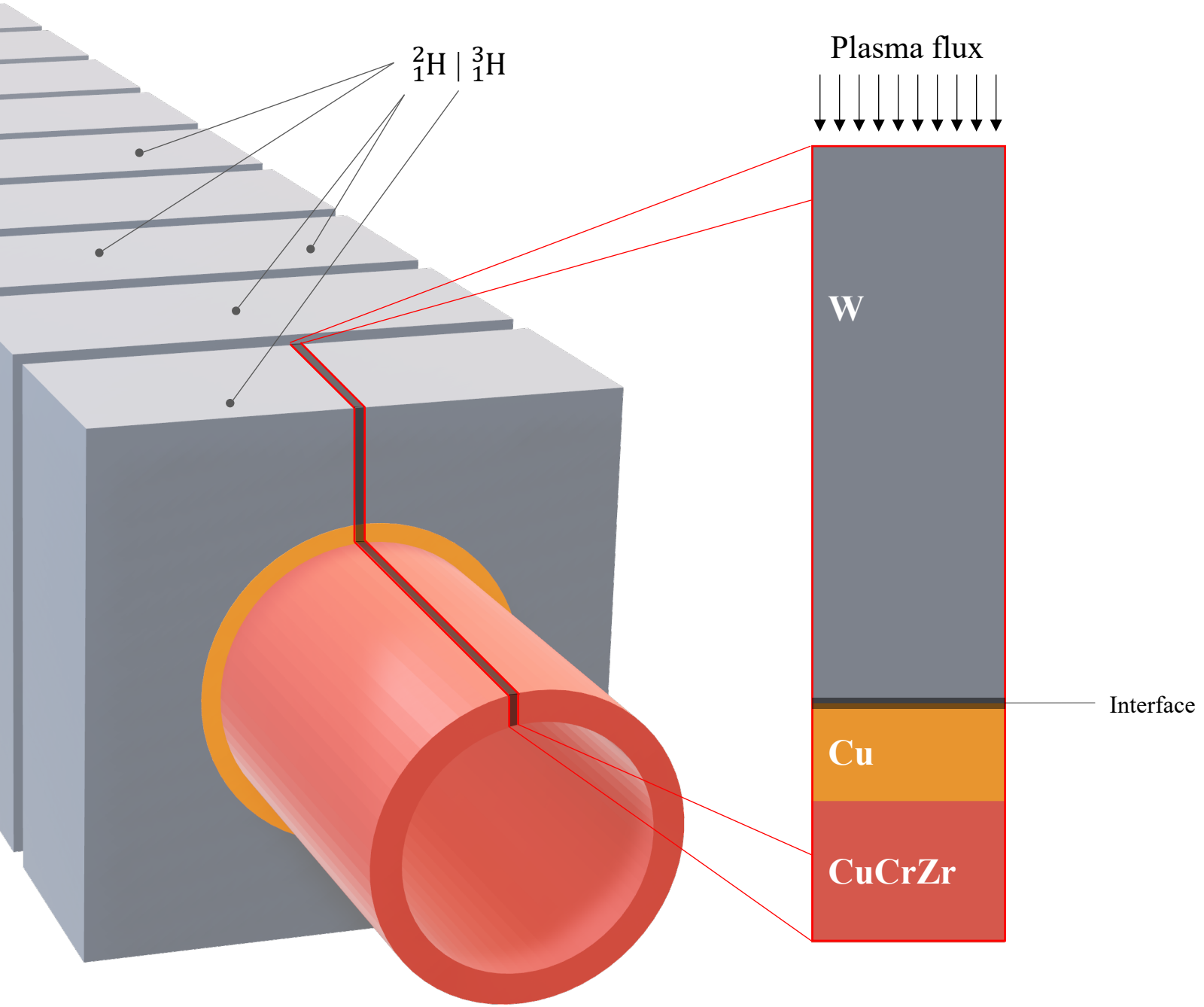
3. Surface, sub-surface and bulk phenomenon



Vacancies and vacancy clusters

- Kinetic and thermo models.
- H trapping and VH_j formation.
- Vacancies form in large number under high H concentration.

Interface: W/Cu in the PFUs



Hydrogen concentration

How much H is retained?

Model H diffusion at the interface.

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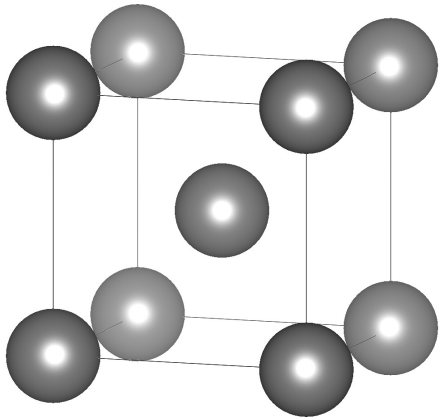
   - 4.1. Atomic scale model of the W/Cu interface.
   - 4.2. H solubility at the W/Cu interface.
   - 4.3. H diffusivity at the W/Cu interface.
   - 4.4. Propagation of defects towards the W/Cu interface.

5. Conclusions.

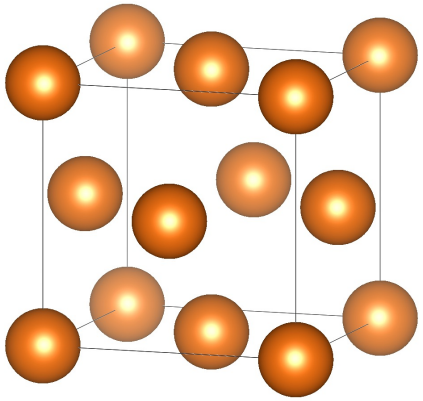
How to match the W and Cu bulks?

1. Different cell parameters and Bravais lattice.
2. Different crystallographic orientations can be considered.



W body centered cubic (bcc)

$a = 3.187$ Å



Cu face centered cubic (fcc)

$a = 3.620$ Å

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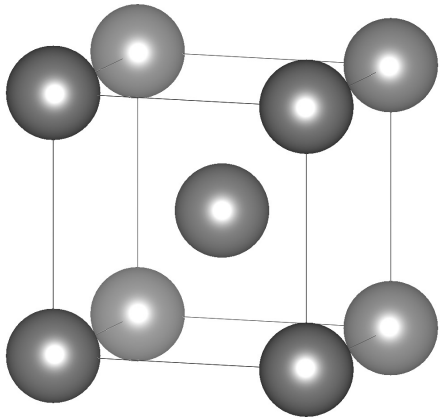

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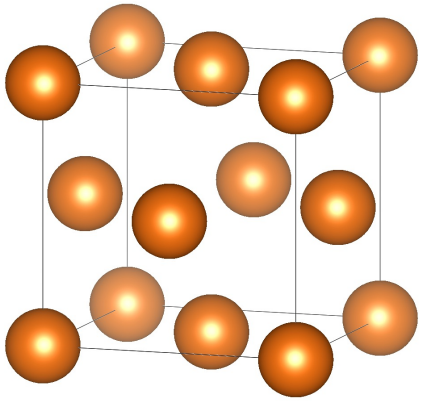

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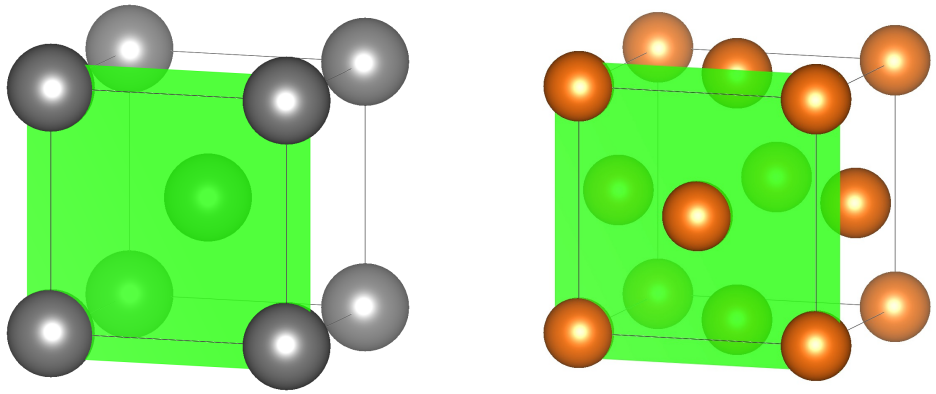
W(001)/Cu(001)R45°

High energy of separation.

W(001) is known to reconstruct.

W(001)/Cu(001)R45°



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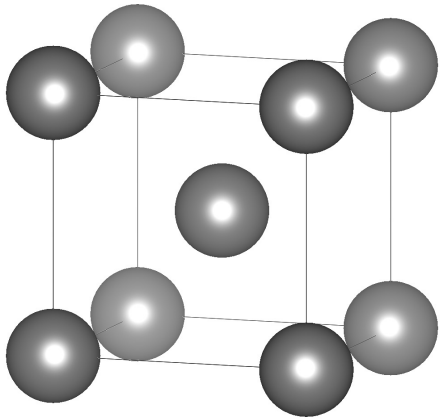
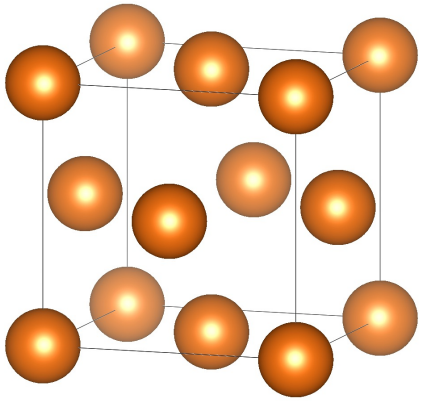


W body centered cubic (bcc)

$a = 3.187$ Å



Cu face centered cubic (fcc)

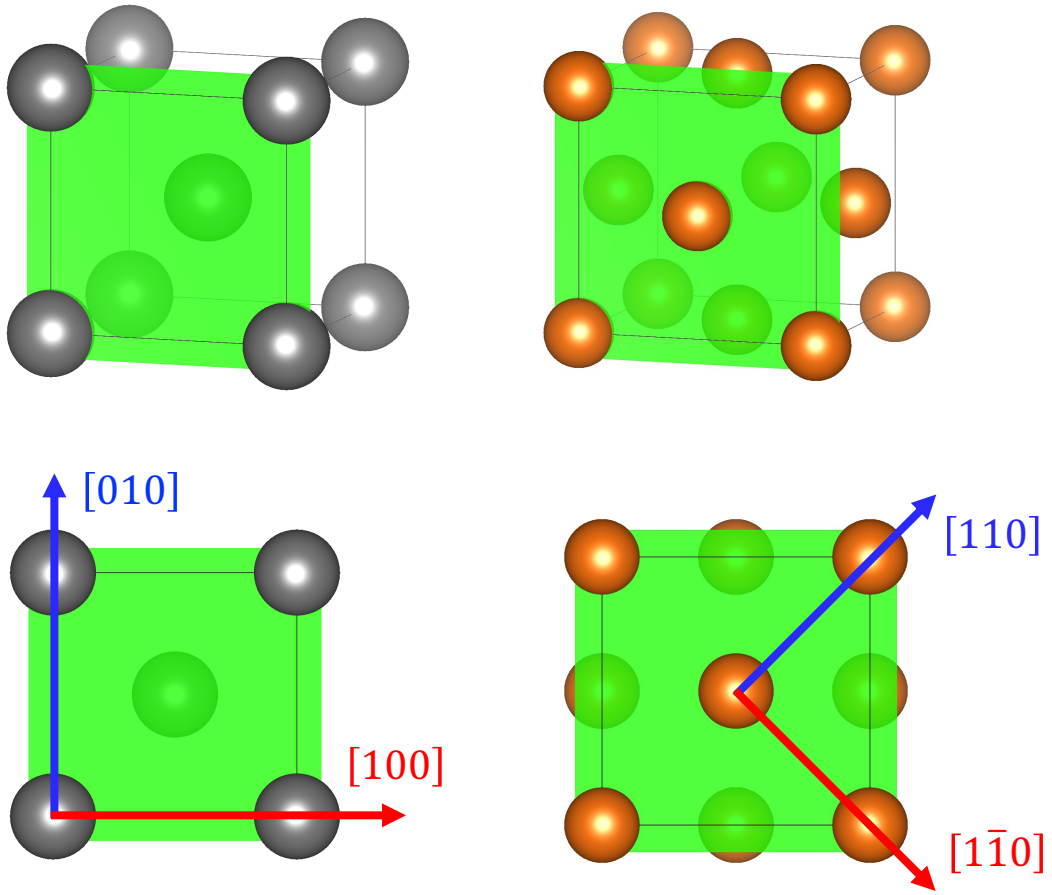
$a = 3.620$ Å

W(001)/Cu(001)R45°

High energy of separation.

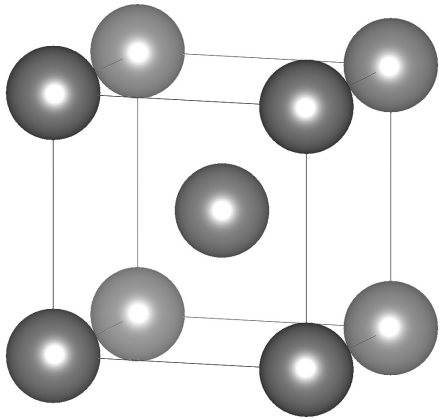
W(001) is known to reconstruct.

W(001)/Cu(001)R45°



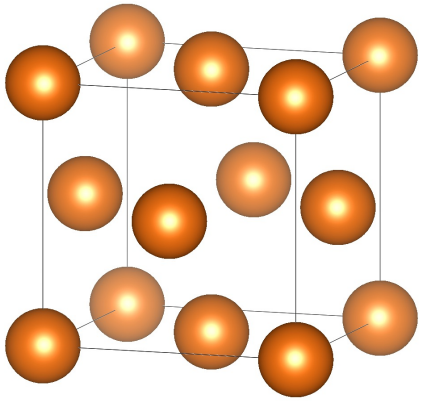
How to match the W and Cu bulks?

1. Different cell parameters and Bravais lattice.
2. Different crystallographic orientations can be considered.



W body centered cubic (bcc)

$a = 3.187$ Å



Cu face centered cubic (fcc)

$a = 3.620$ Å

W(001)/Cu(001)R45°

High energy of separation.

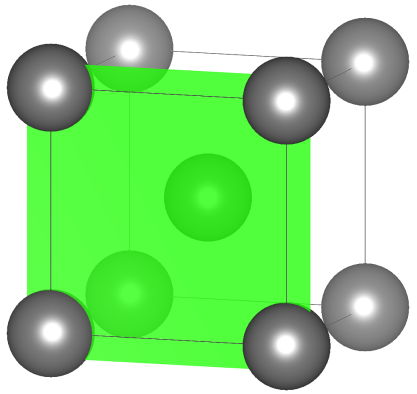
W(001) is known to reconstruct.

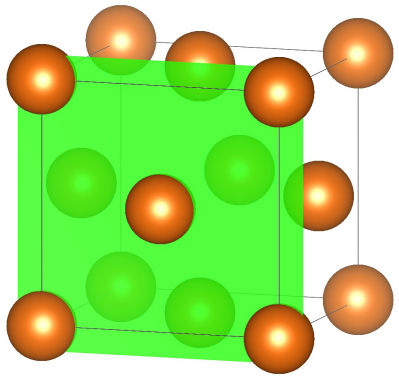
W(110)/Cu(111)

Most compact layers.

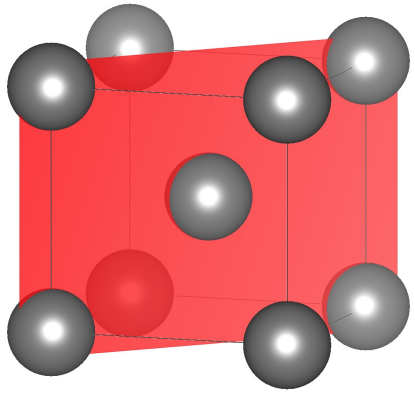
Lower energy of the interface.

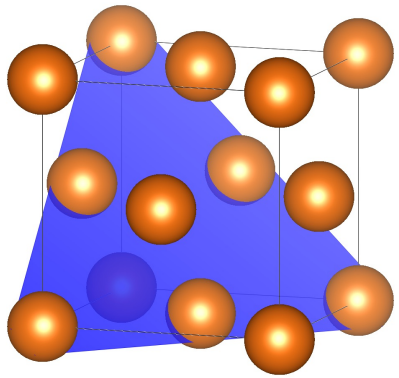
W(001)/Cu(001)R45°





W(110)/Cu(111)

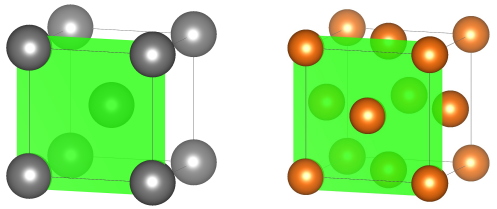


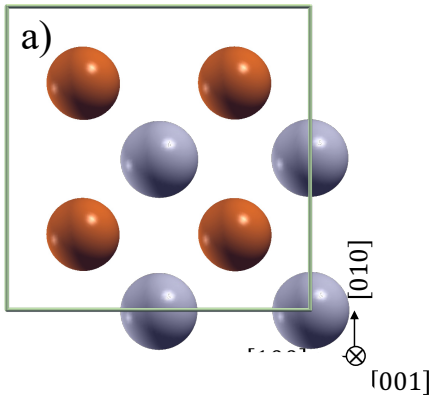


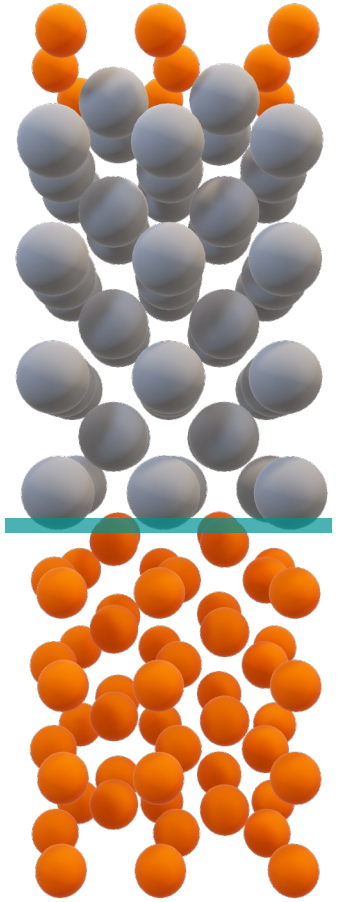
4.1. Atomic scale model of the W/Cu interface

W(001)/Cu(001)R45°

- Cu atoms
- W atoms







[6] Y. Silva-Solís et. al., Nuclear Materials & Energy 37 (2023) 101516.
[7] H. Wormeester et. al., Surf. Sci. 377 (1997) 988–991.
[8] T.R.J. Bollmann et. al., Phys. Rev. B 85 (2012) 125417.

4.1. Atomic scale model of the W/Cu interface

W(001)/Cu(001)R45°

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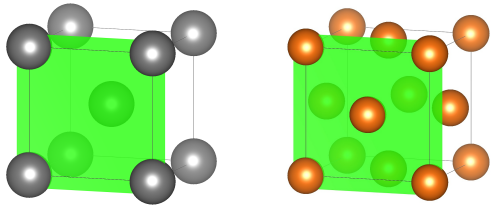
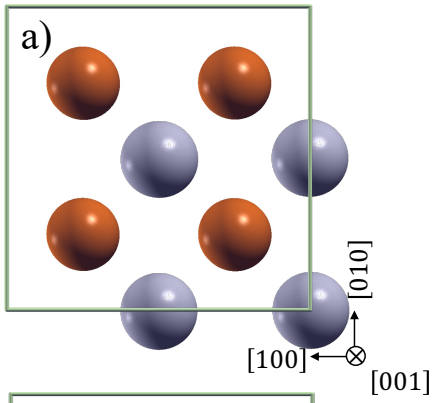
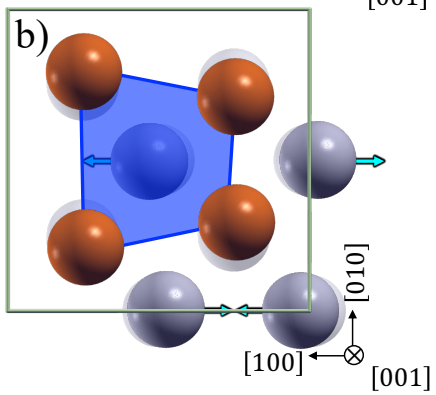
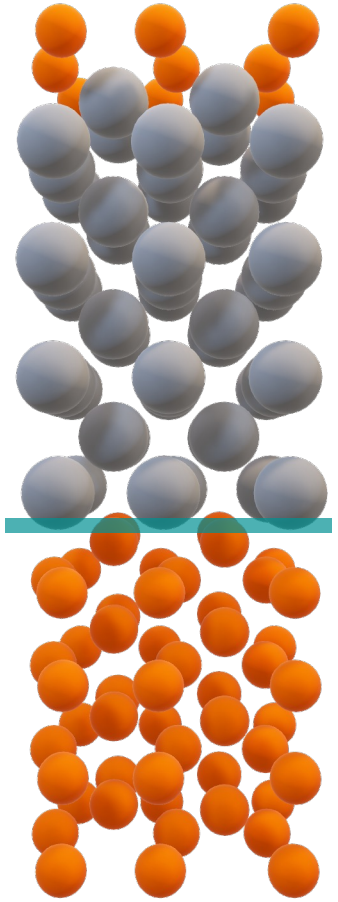
- W atoms







Relaxed structure



[6] Y. Silva-Solís et. al., Nuclear Materials & Energy 37 (2023) 101516.
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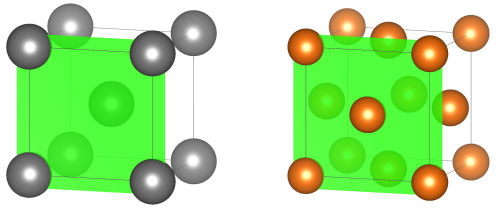
[8] T.R.J. Bollmann et. al., Phys. Rev. B 85 (2012) 125417.

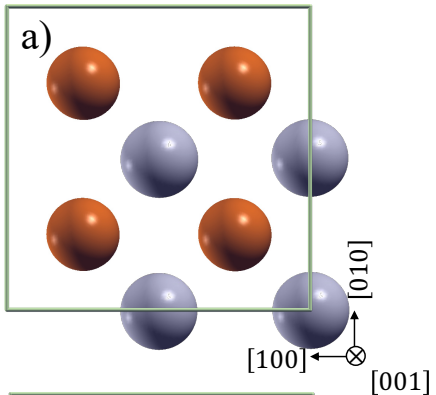
4.1. Atomic scale model of the W/Cu interface

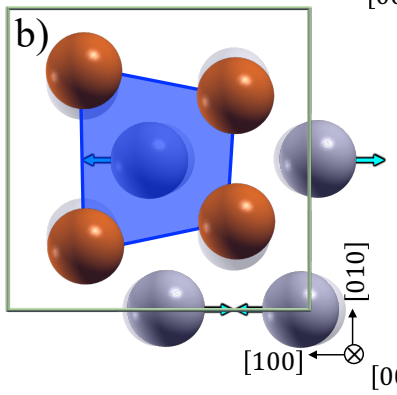
W(001)/Cu(001)R45°

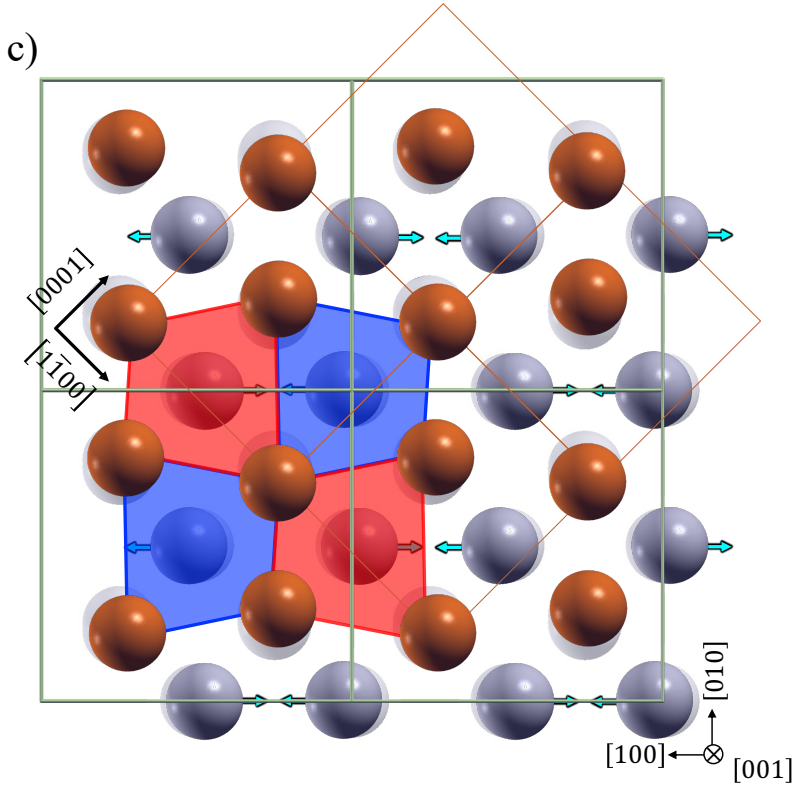
- Cu atoms
- W atoms



Our model [6]

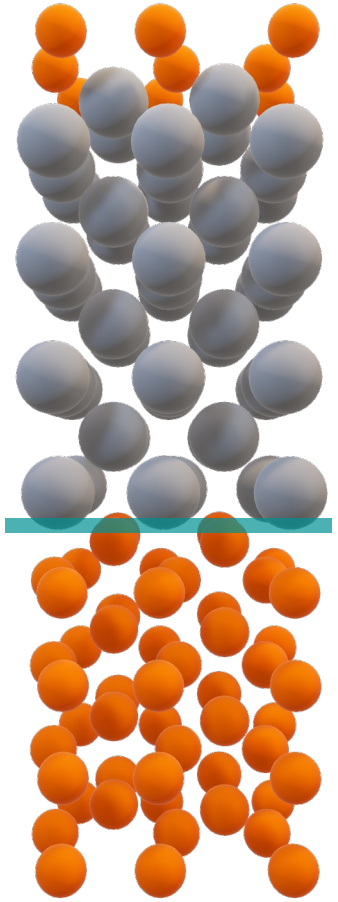






Relaxed structure

Significant reconstruction



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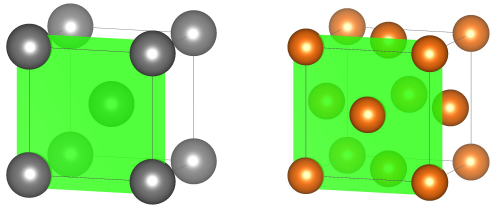
4.1. Atomic scale model of the W/Cu interface

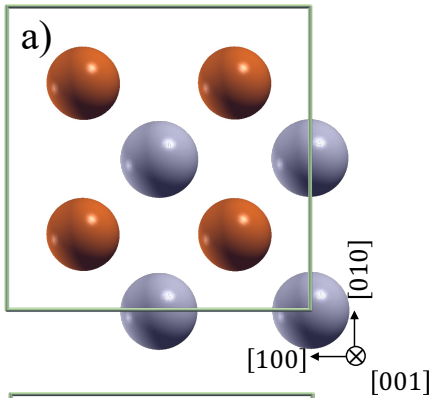
W(001)/Cu(001)R45°

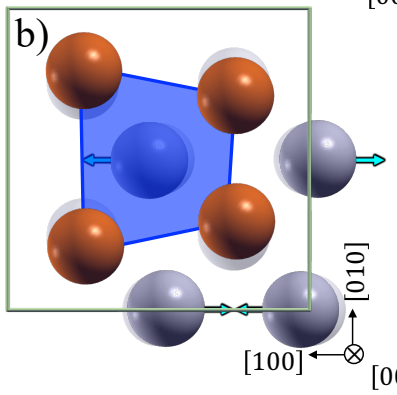
- Cu atoms
- W atoms



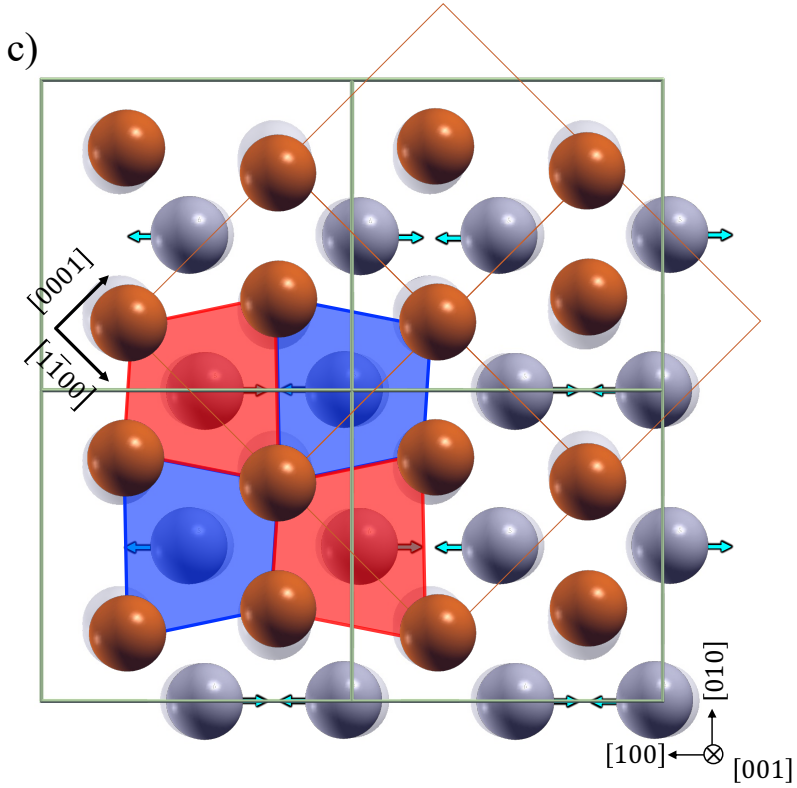
Our model [6]

Experiments [7, 8]

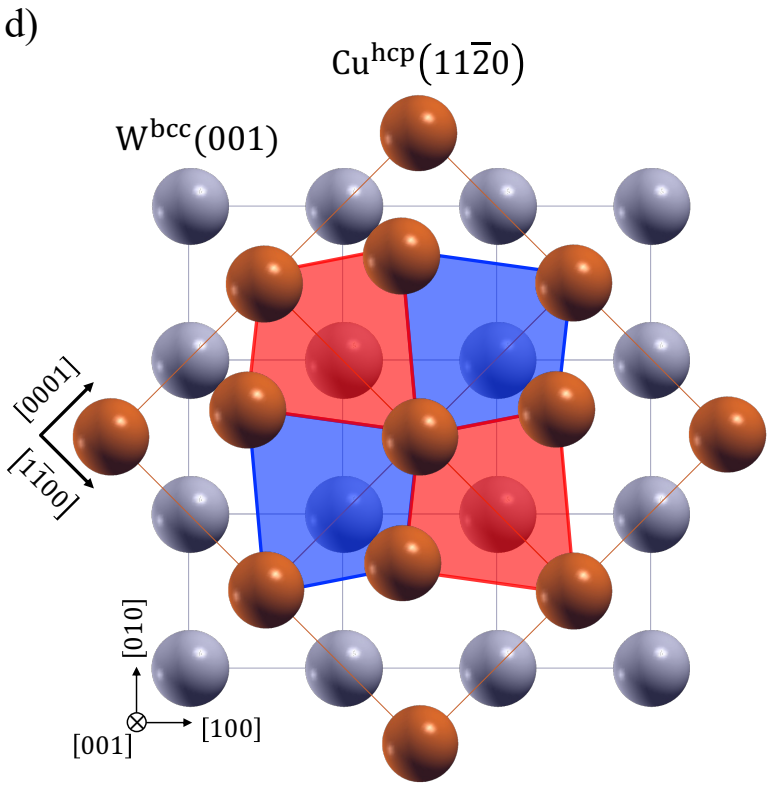


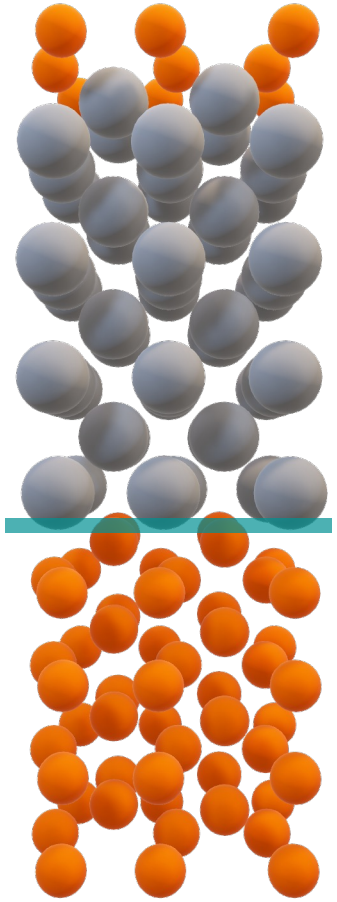


Relaxed structure



Significant reconstruction





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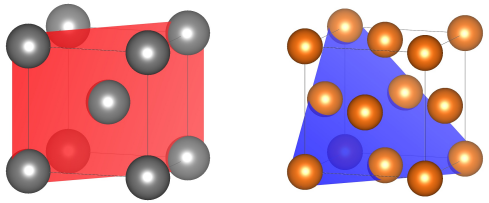
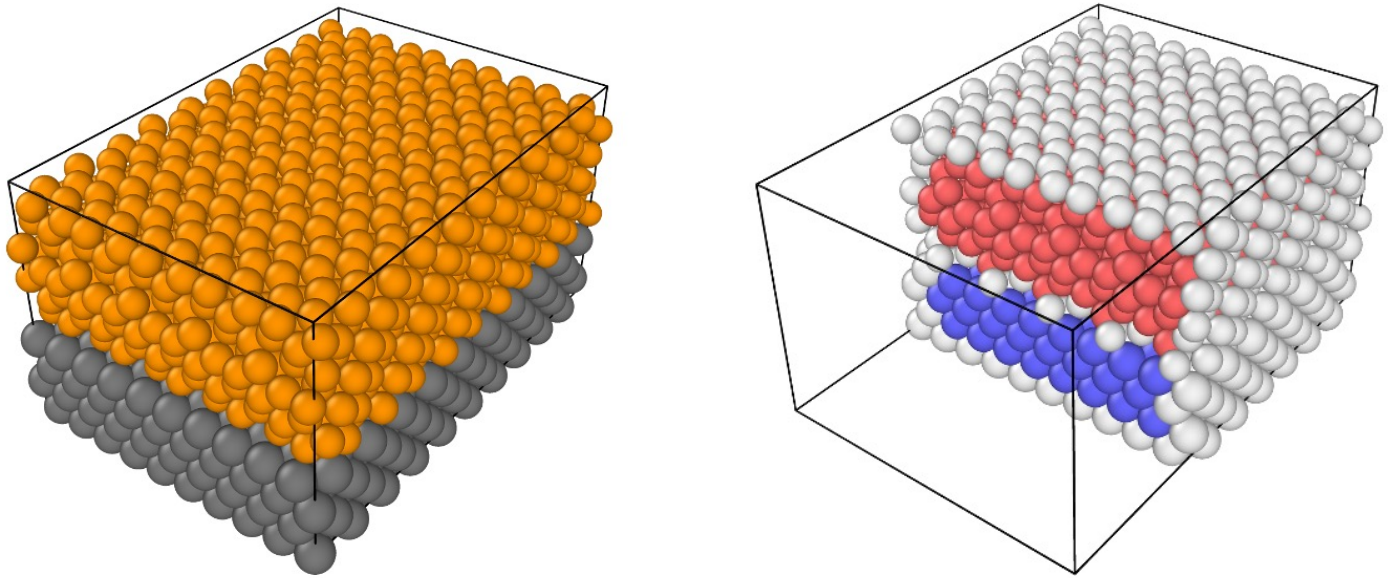
4.1. Atomic scale model of the W/Cu interface

W(110)/Cu(111)

- Cu atoms
- W atoms





Other	1200	49.5%
FCC	0	0.0%
HCP	869	35.8%
BCC	356	14.7%
ICO	0	0.0%

4.1. Atomic scale model of the W/Cu interface

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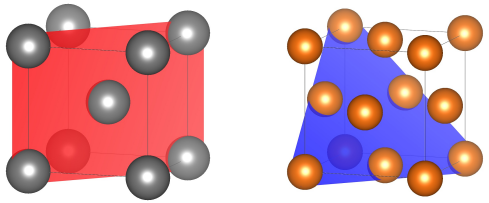

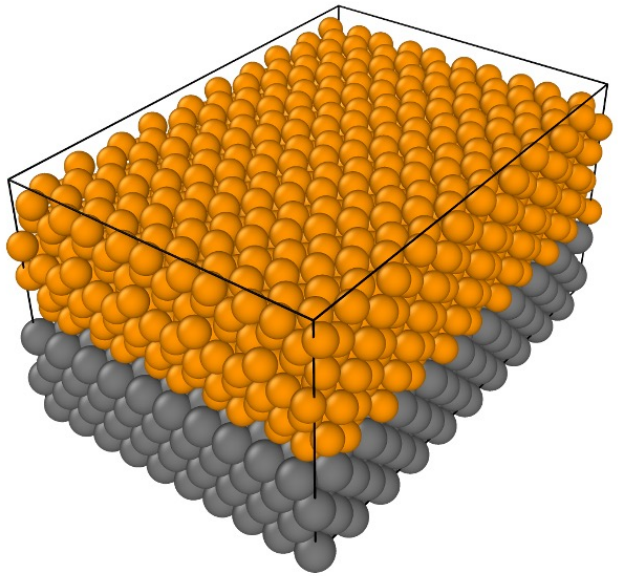

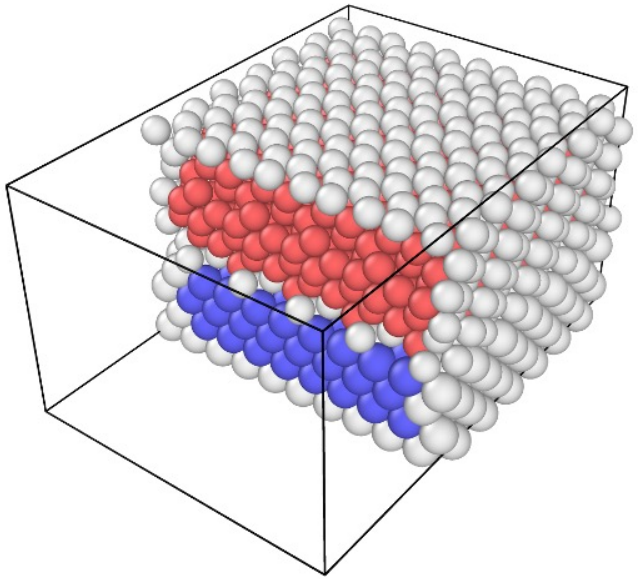

Other	1200	49.5%
FCC	0	0.0%
HCP	869	35.8%
BCC	356	14.7%
ICO	0	0.0%

At both the W(001)/Cu(001) and W(110)/Cu(111) interfaces

Copper reconstructs in a hexagonal compact structure

Common feature to both interface despite they are different models

Outline

1. Introduction.

2. Methodology.

3. Surface, sub-surface and bulk phenomenon.

4. Interface: W/Cu in the PFUs.

   - 4.1. Atomic scale model of the W/Cu interface.
   - 4.2. H solubility at the W/Cu interface.
   - 4.3. H diffusivity at the W/Cu interface.
   - 4.4. Propagation of defects towards the W/Cu interface.

5. Conclusions.

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   - 4.1. Atomic scale model of the W/Cu interface.
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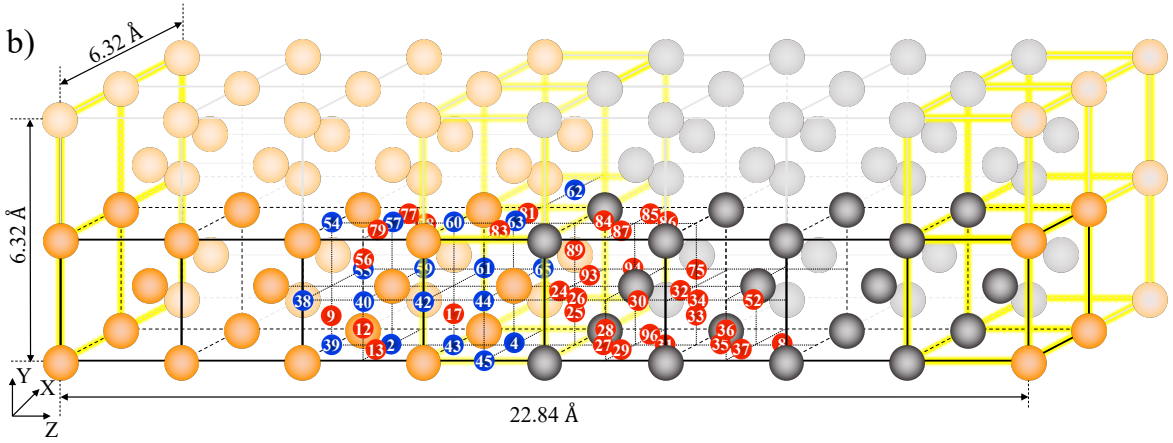
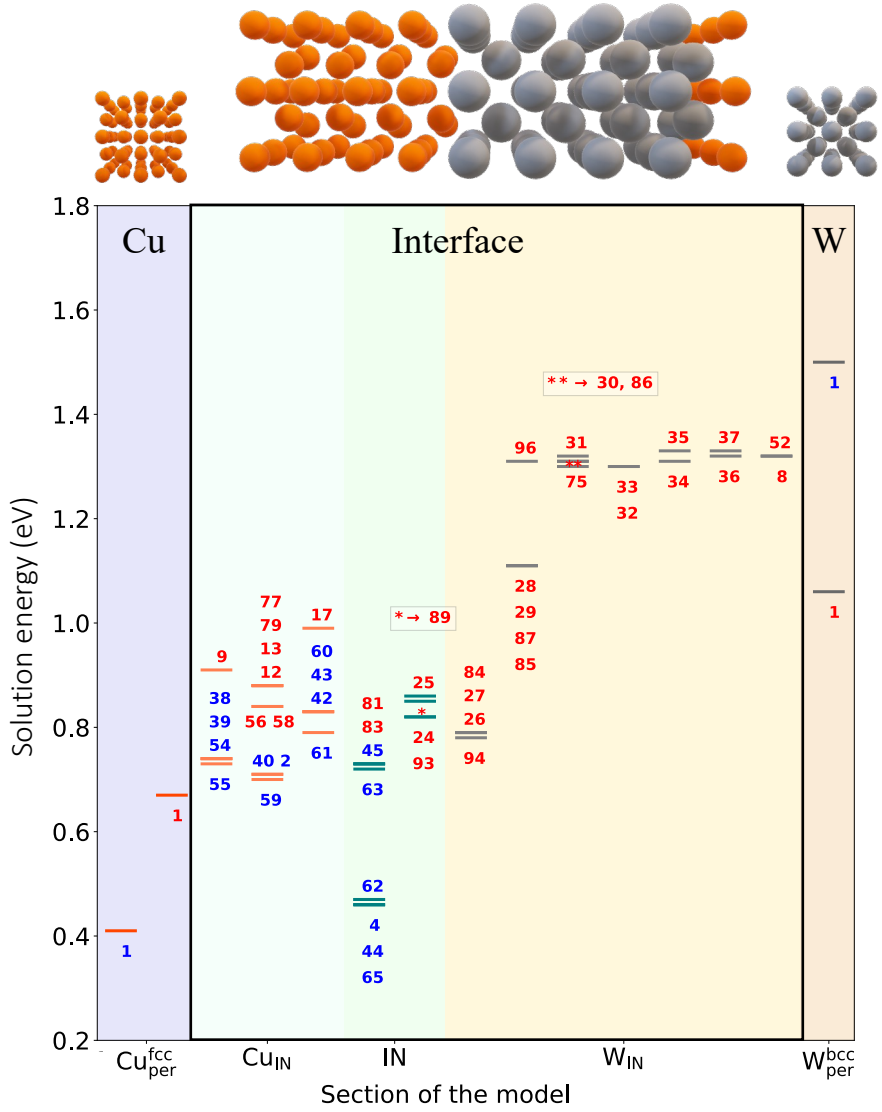
5. Conclusions.

4.2. H solubility at the W/Cu interface

DFT calulations at the W(001)/Cu(001)R45° + H

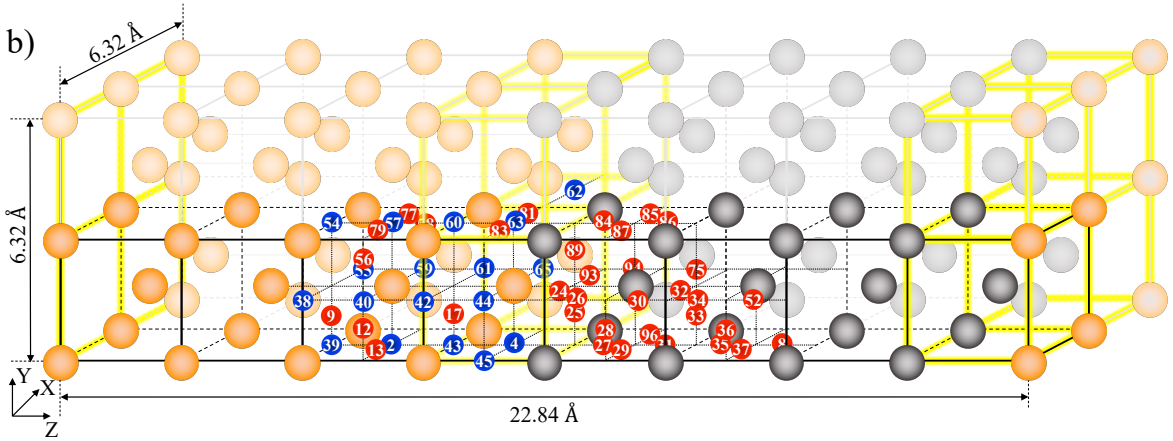


H as interstitial Tetrahedral sites Octahedral sites



4.2. H solubility at the W/Cu interface

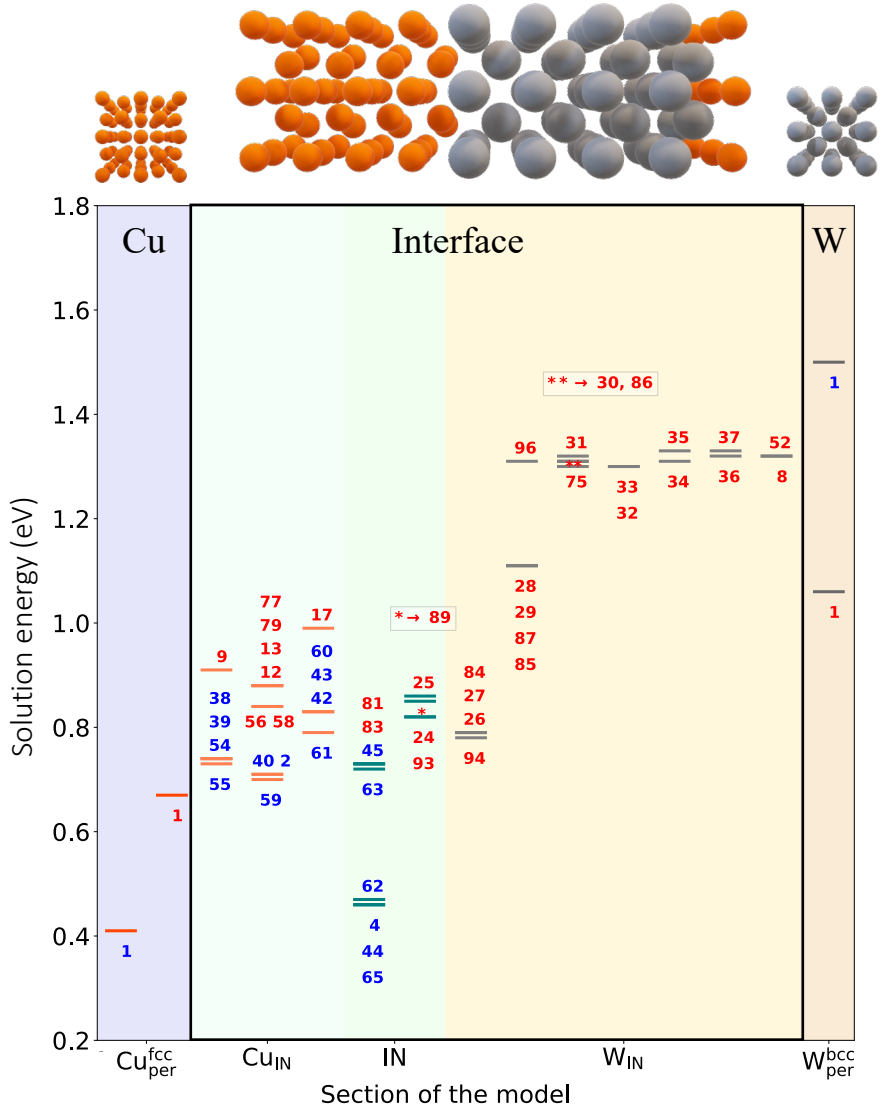
DFT calulations at the W(001)/Cu(001)R45° + H



H as interstitial Tetrahedral sites Octahedral sites

Solubility is higher in the **Cu** than in **W**

Solution energy is lowest at the **interface**



4.2. H solubility at the W/Cu interface

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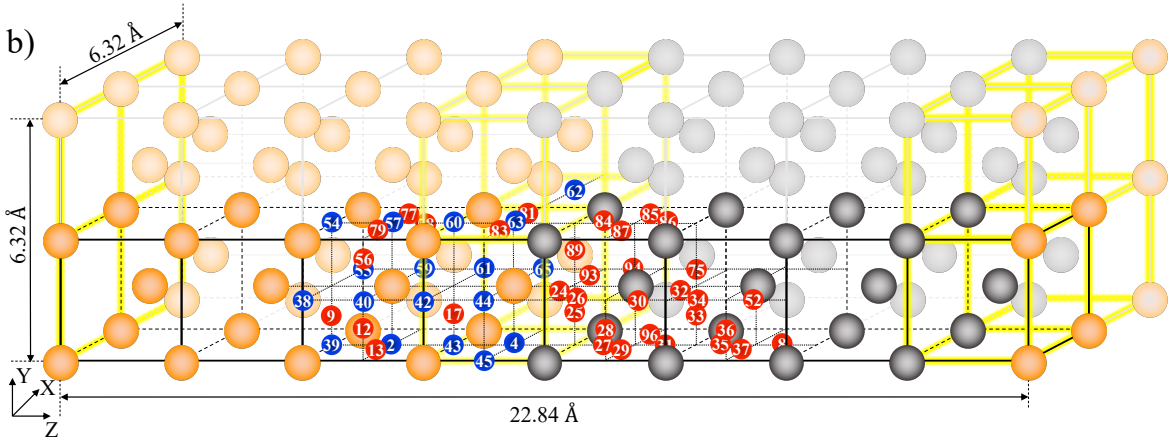
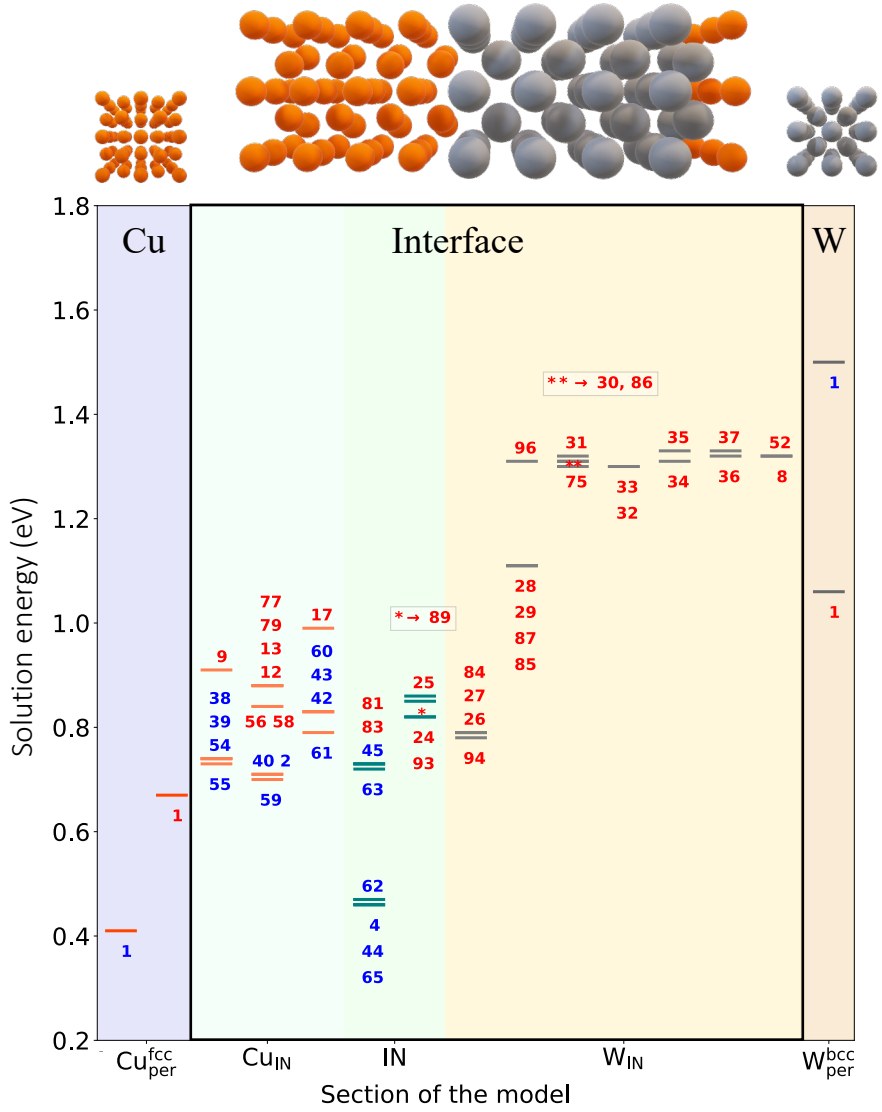


H as interstitial Tetrahedral sites Octahedral sites

Solubility is higher in the **Cu** than in **W**

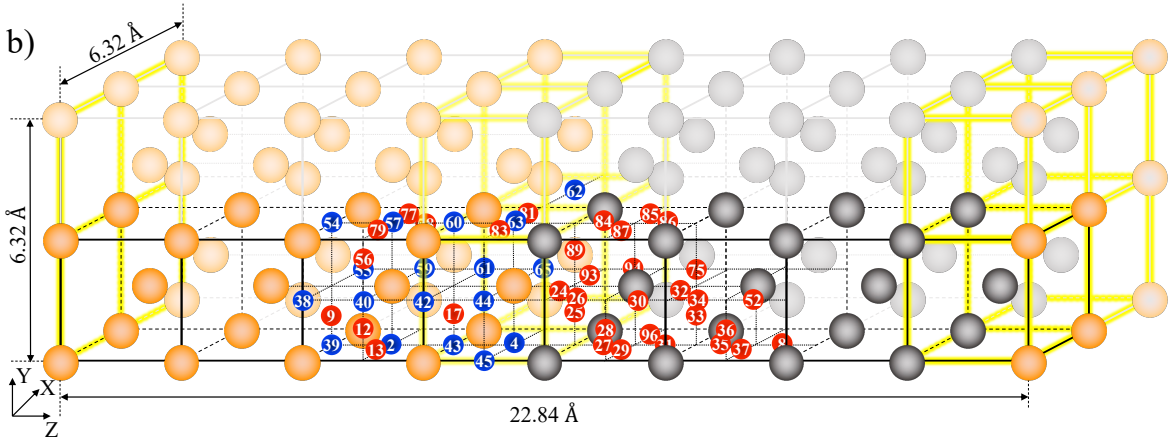
Solution energy is lowest at the **interface**

Hydrogen solubility is high at the interface



4.2. H solubility at the W/Cu interface

DFT calulations at the W(001)/Cu(001)R45° + H



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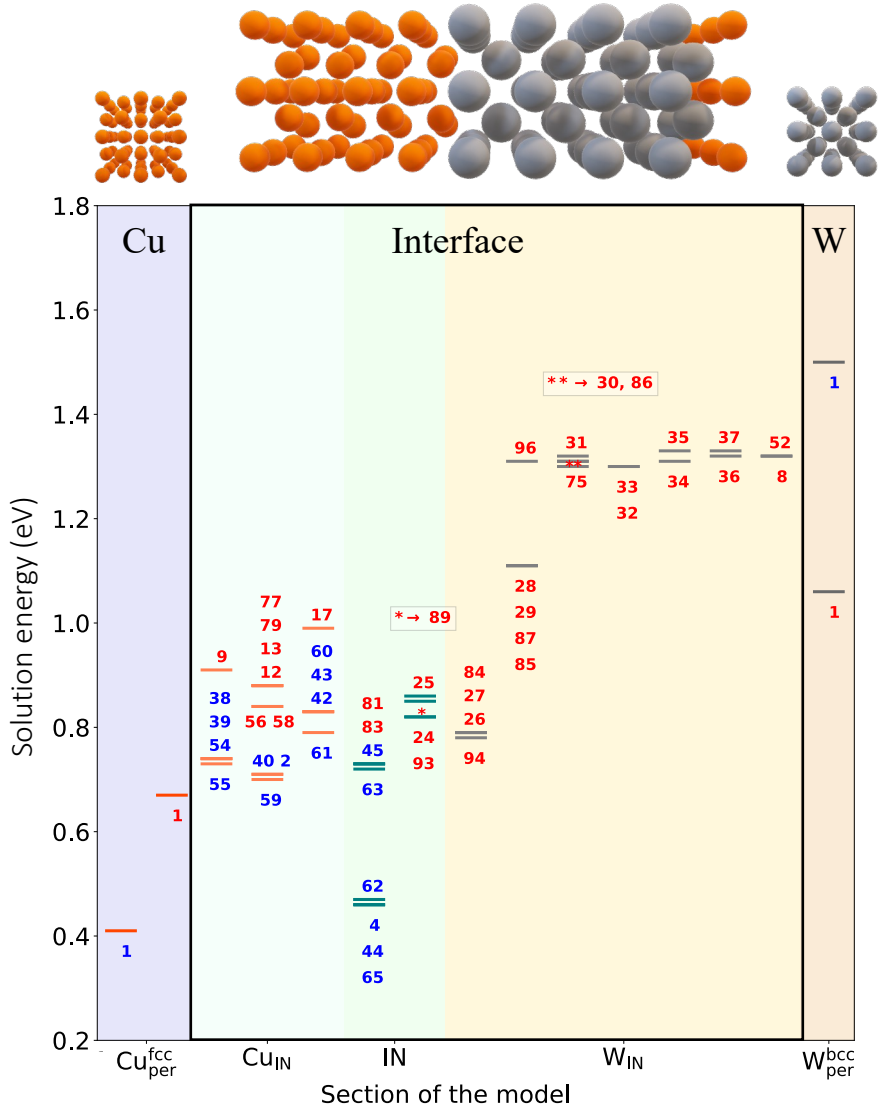
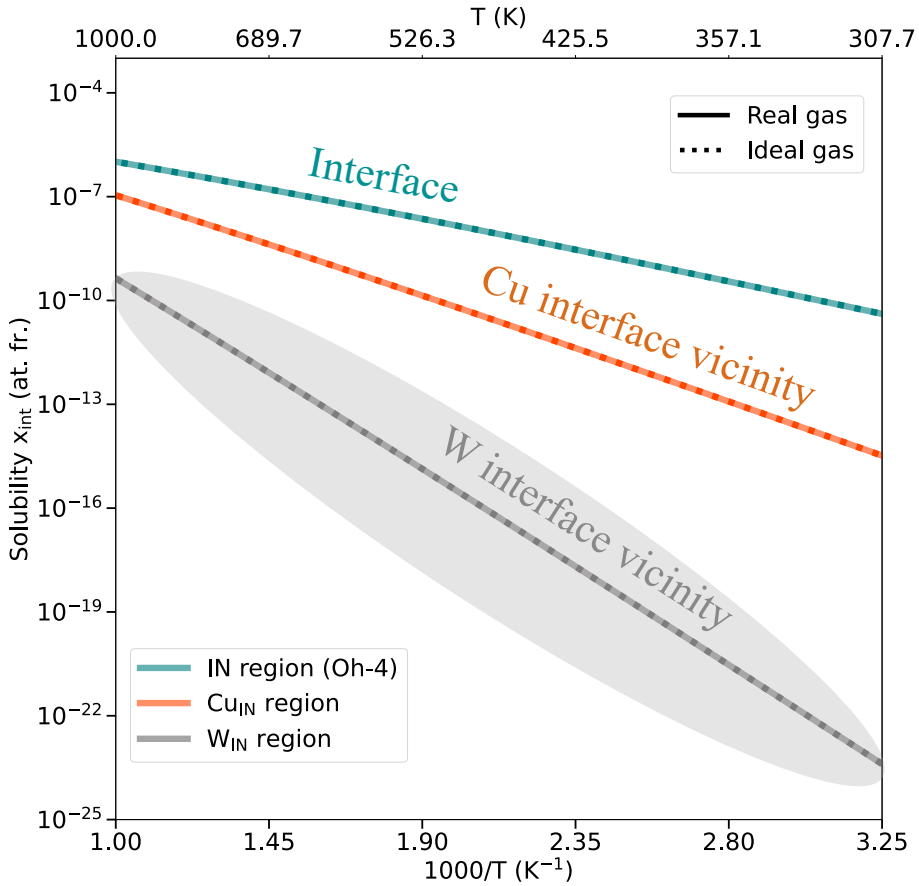
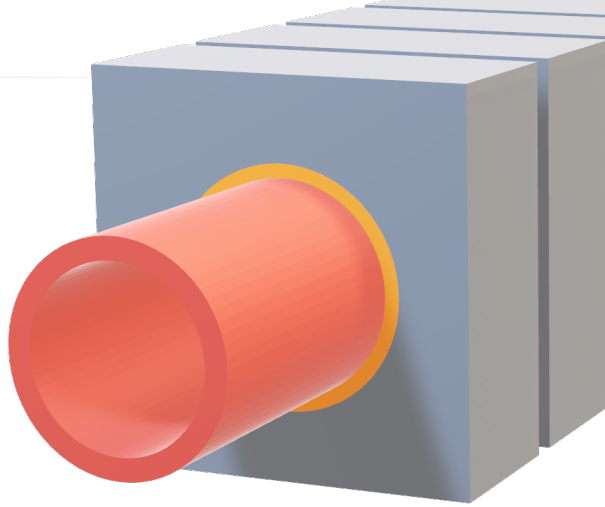


How to consider the effect of temperature?

4.2. H solubility at the W/Cu interface

Solubility of H at the W/Cu interface and in the W and Cu bulks





Tungsten

The hydrogen solubility is lower in the vicinity of the interface.

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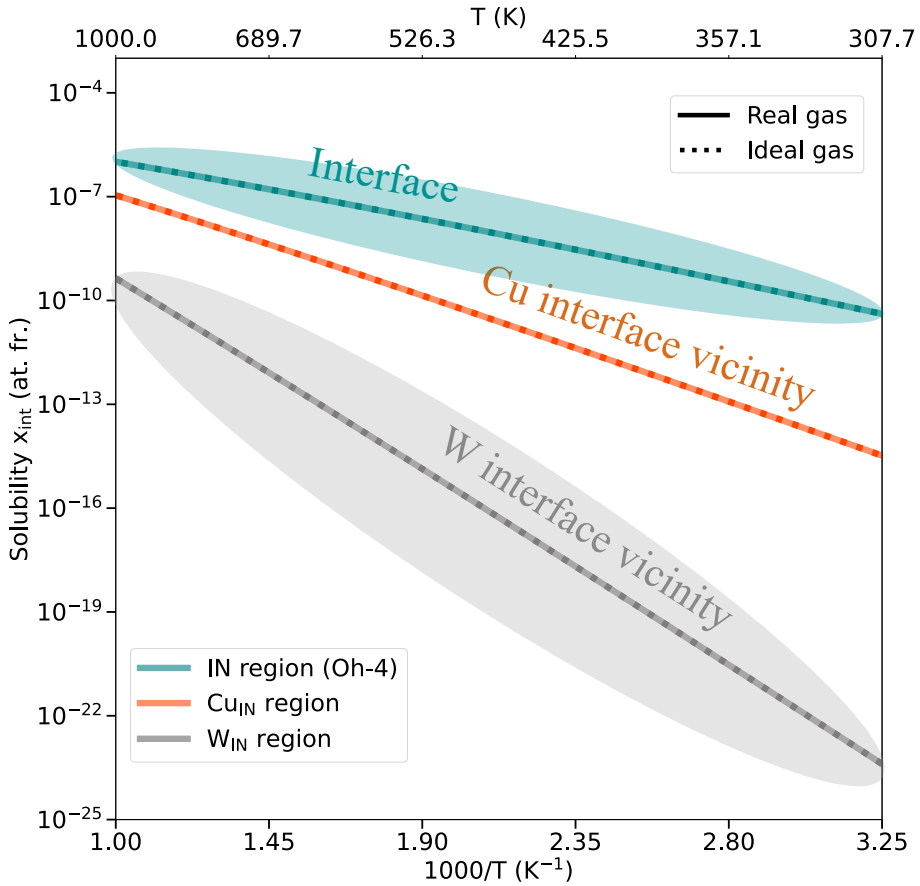
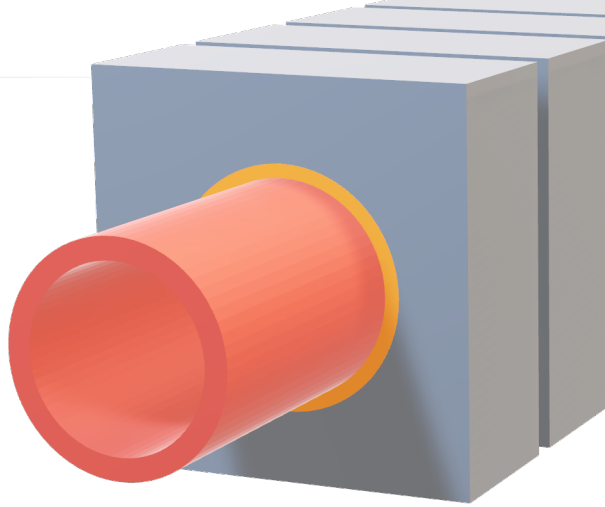
Solubility of H at the W/Cu interface and in the W and Cu bulks





Tungsten

The hydrogen solubility is lower in the vicinity of the interface.

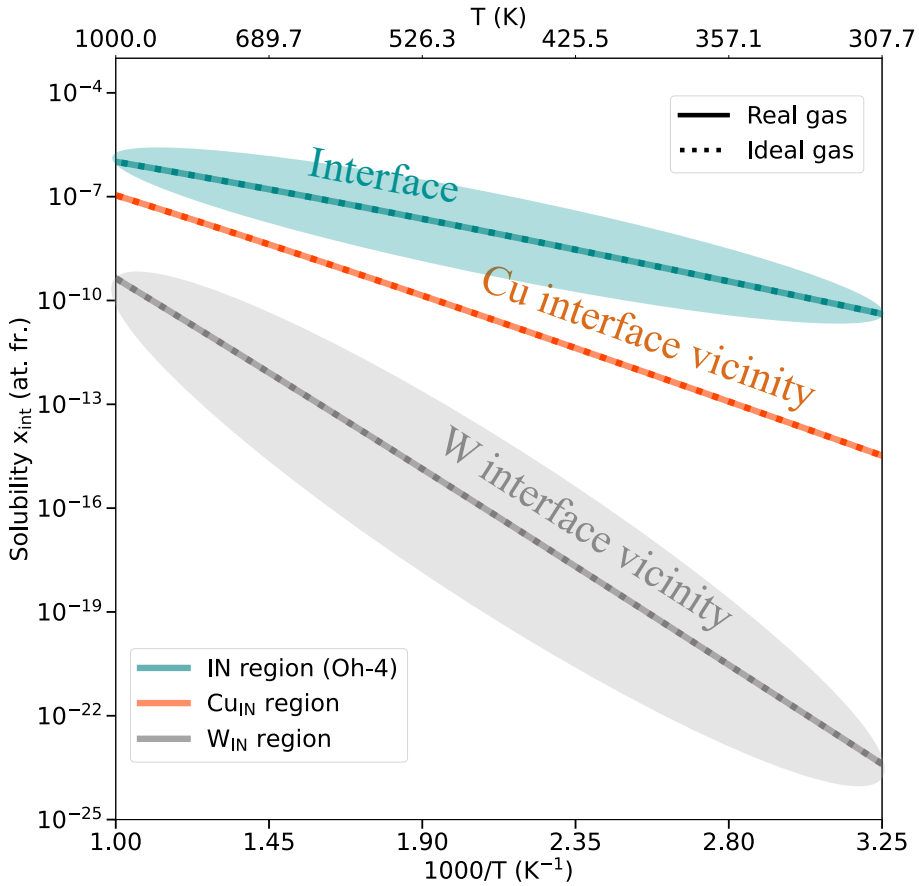
Interface

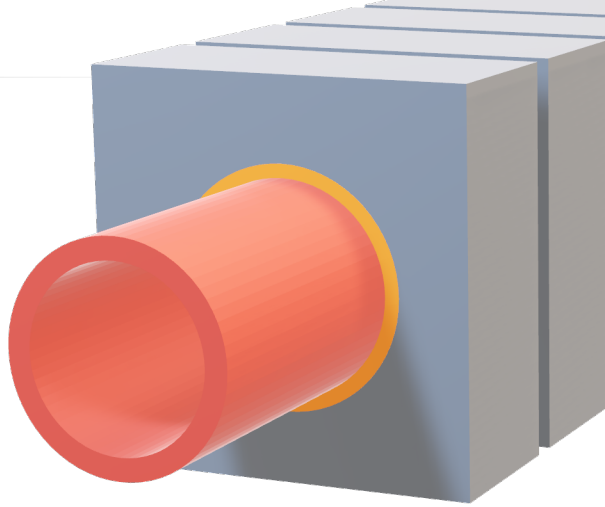
The hydrogen solubility is similar to that in perfect **Cu**.

The hydrogen solubility is higher at the plane of the interface.

4.2. H solubility at the W/Cu interface

Solubility of H at the W/Cu interface and in the W and Cu bulks





Tungsten

The hydrogen solubility is lower in the vicinity of the interface.

Interface

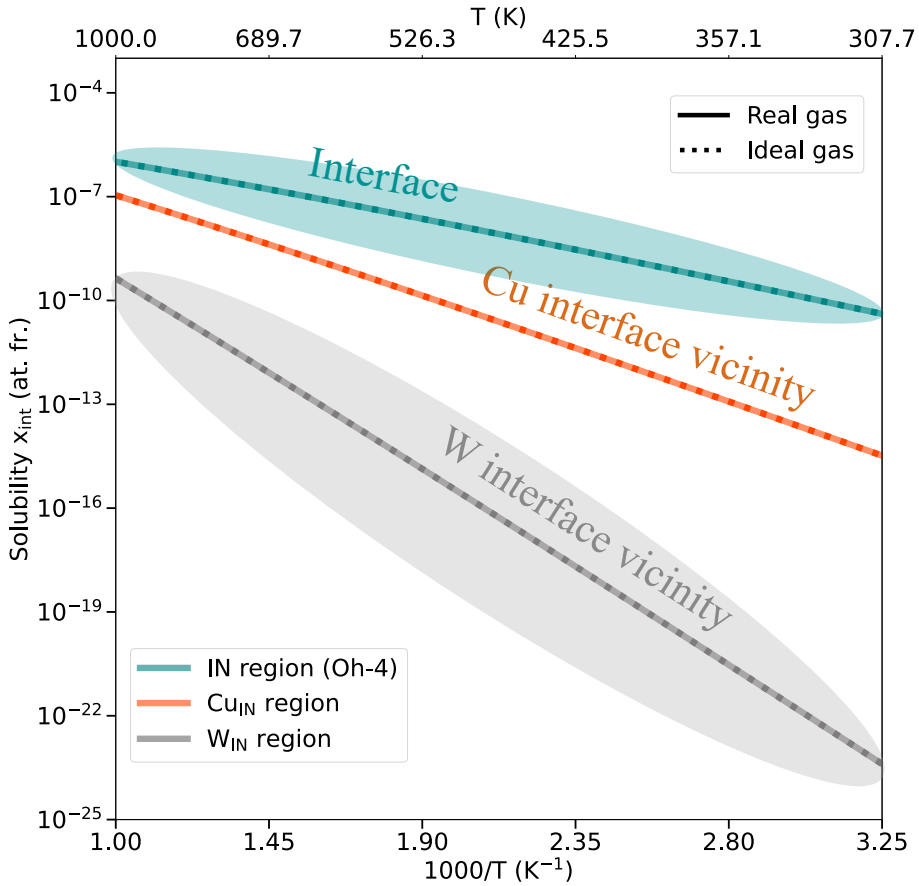
The hydrogen solubility is similar to that in perfect **Cu**.

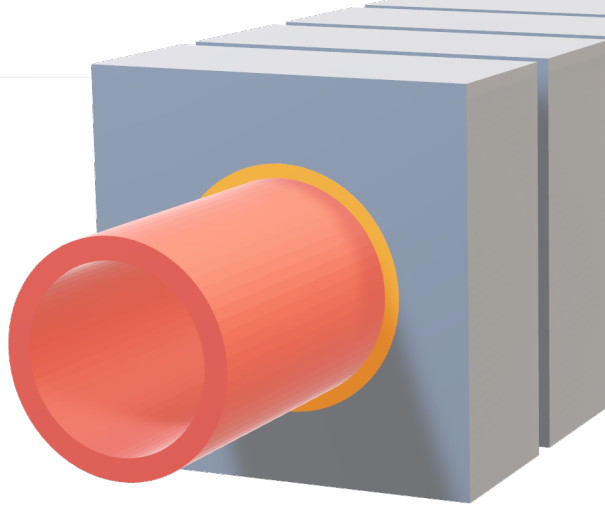
The hydrogen solubility is higher at the plane of the interface.

Hydrogen might segregate at the interface

4.2. H solubility at the W/Cu interface

Solubility of H at the W/Cu interface and in the W and Cu bulks





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What about diffusion?

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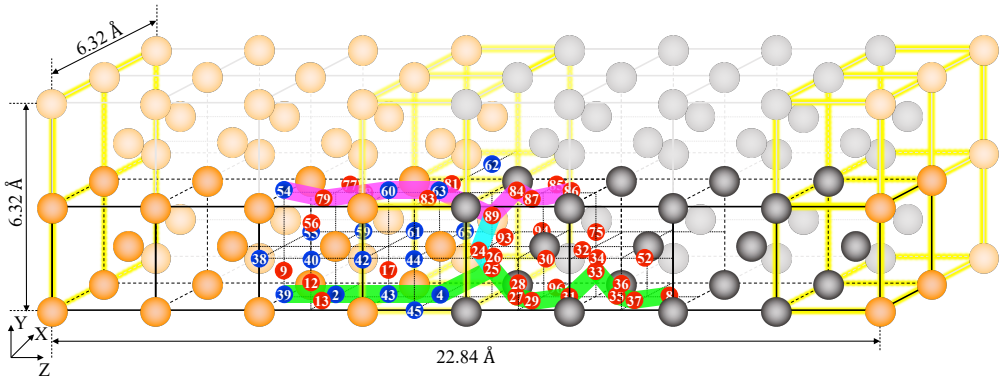
4.3. H diffusivity within the W/Cu interface

Minimum energy path for H across the W/Cu interface



- 2 paths across the **interface**
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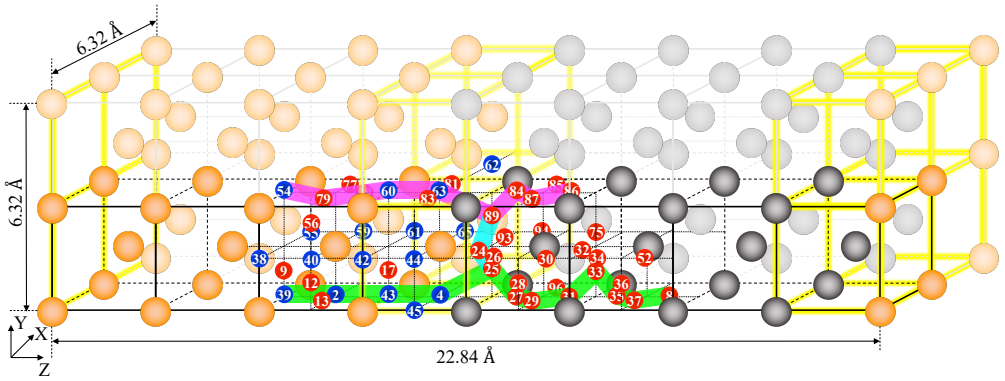

- 2 paths across the **interface**
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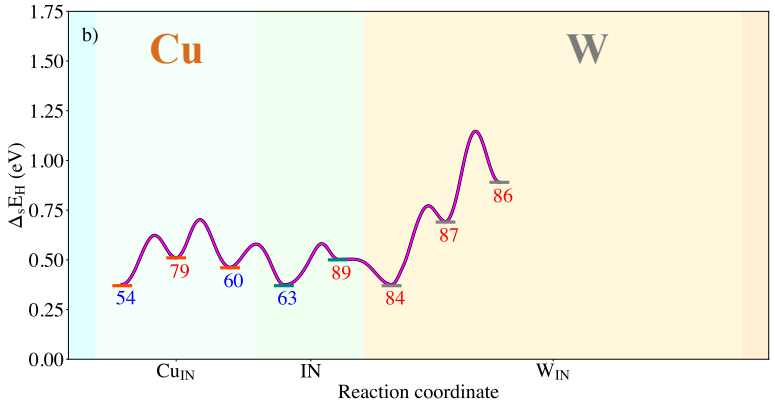
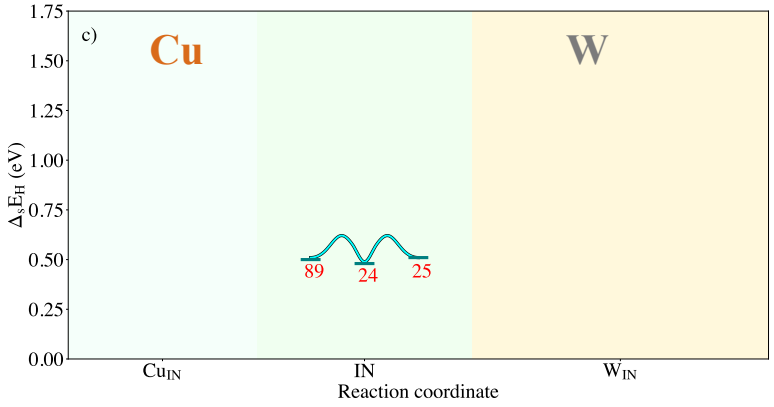
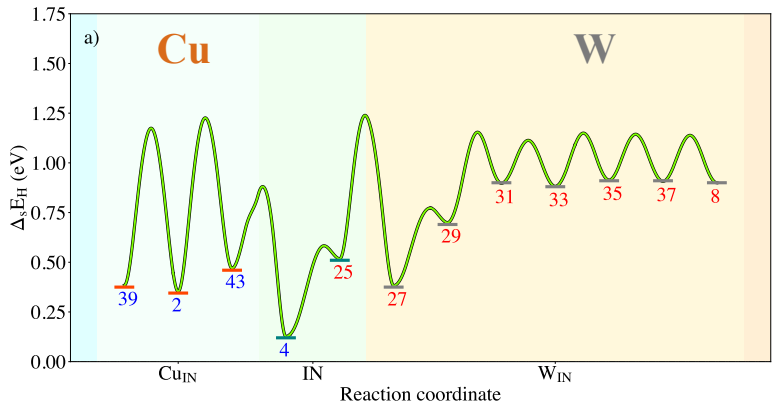
Energy barriers along all the paths at the interface







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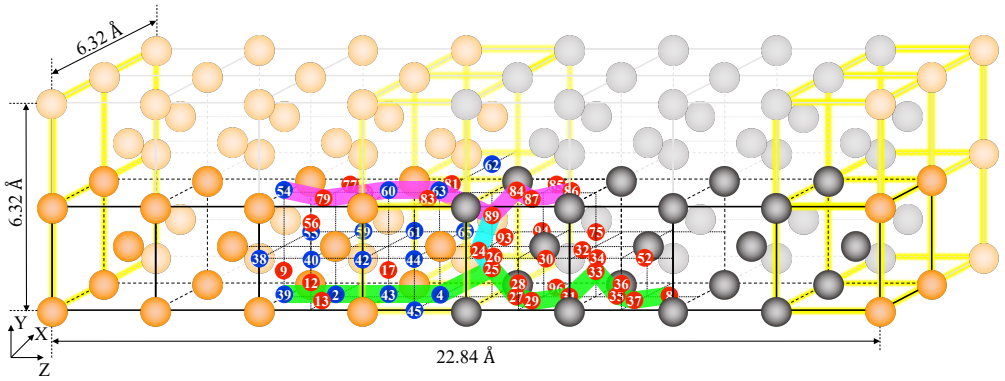

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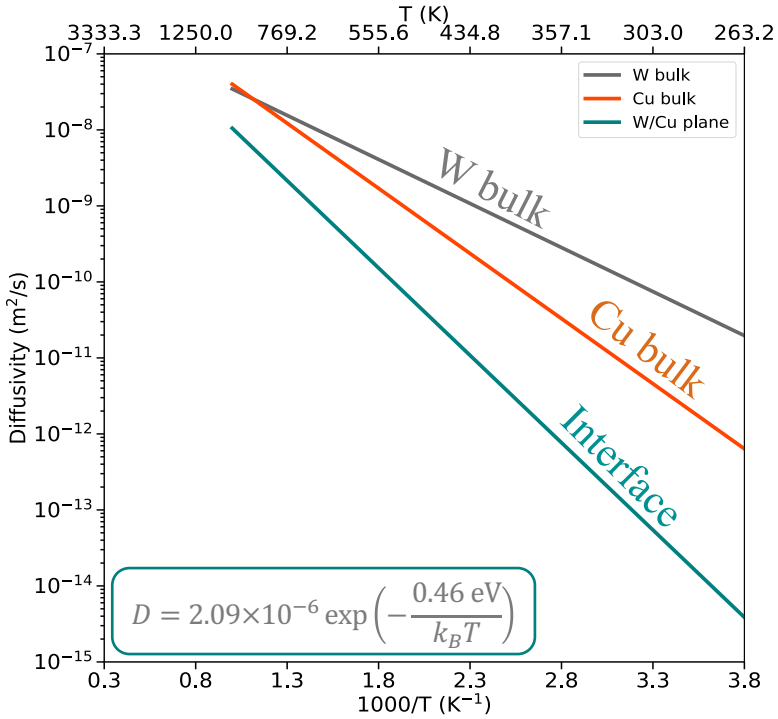
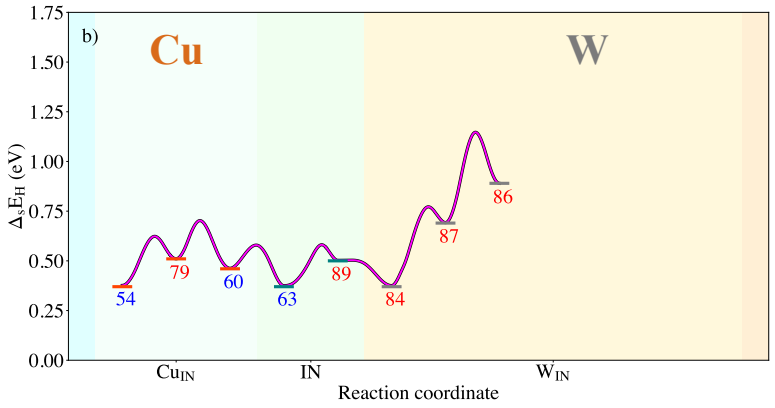
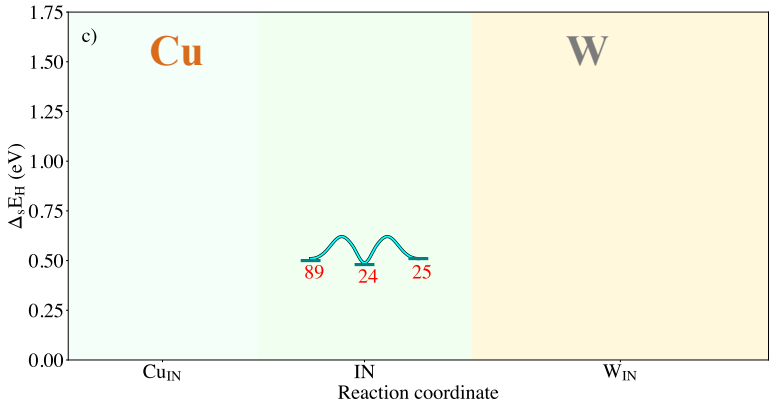
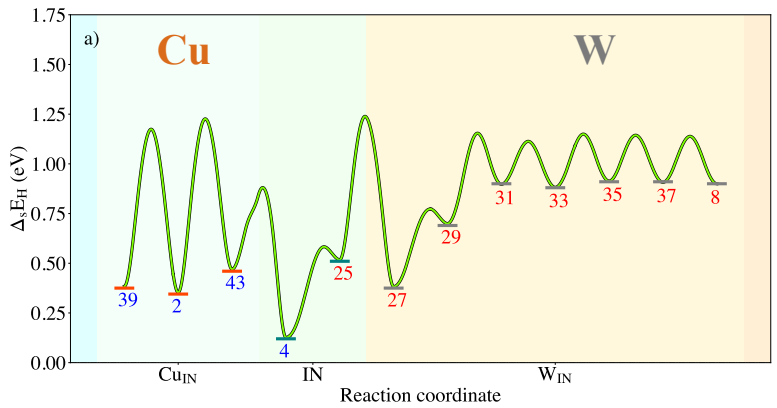
Diffusivity of H parallel to the **interface**



Energy barriers along all the paths at the interface







4.3. H diffusivity within the W/Cu interface

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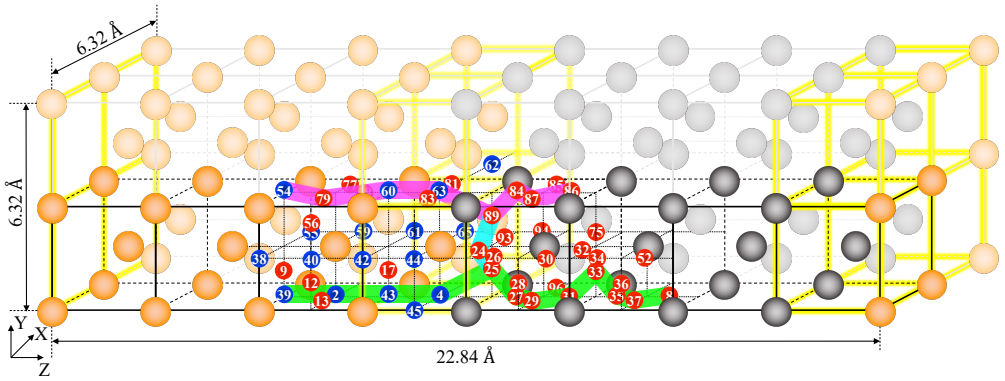

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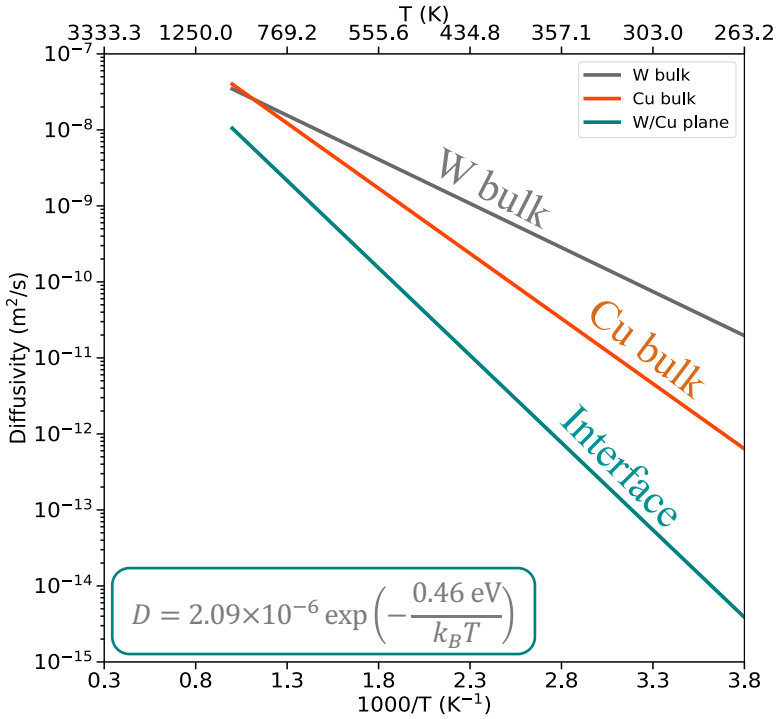


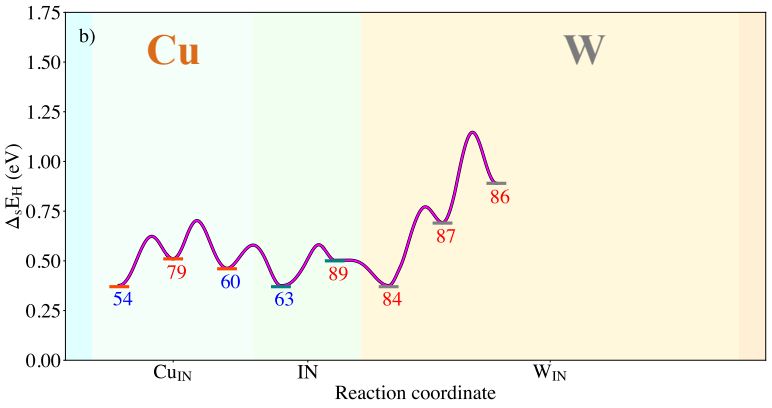
Diffusivity of H

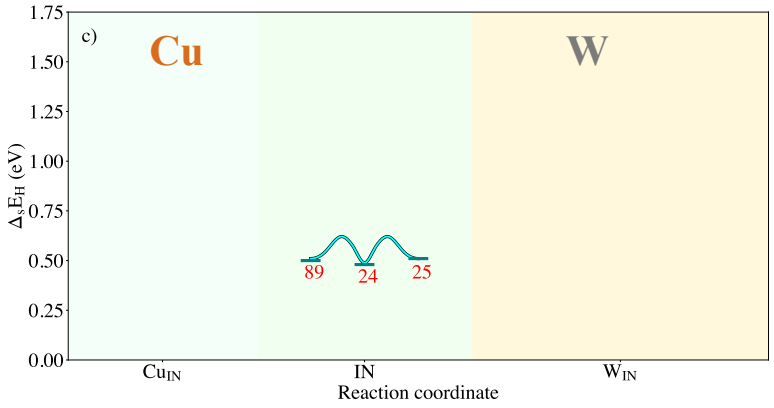
Plane W/Cu < Cu < W

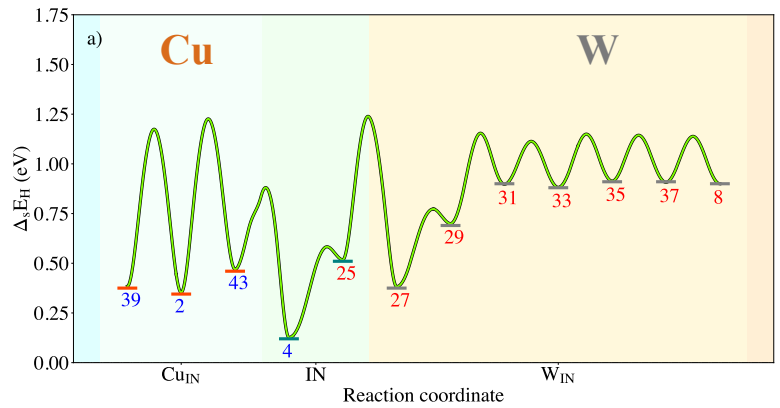
Solubility of H (thermo model)

Plane W/Cu > Cu > W

Energy barriers along all the paths at the interface







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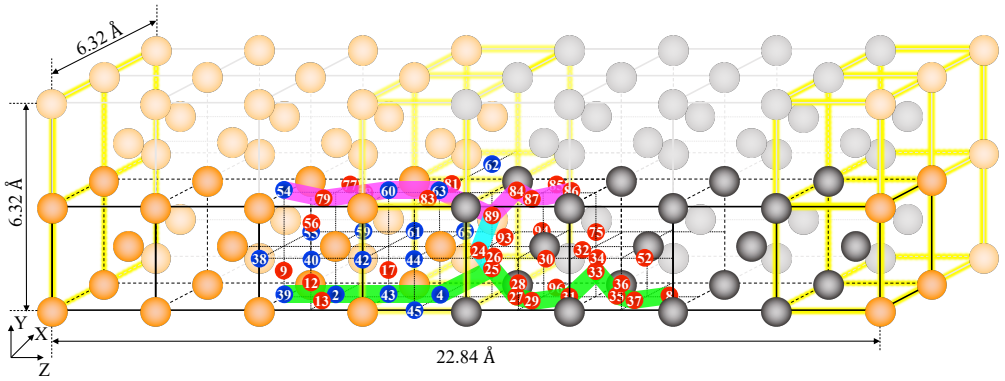

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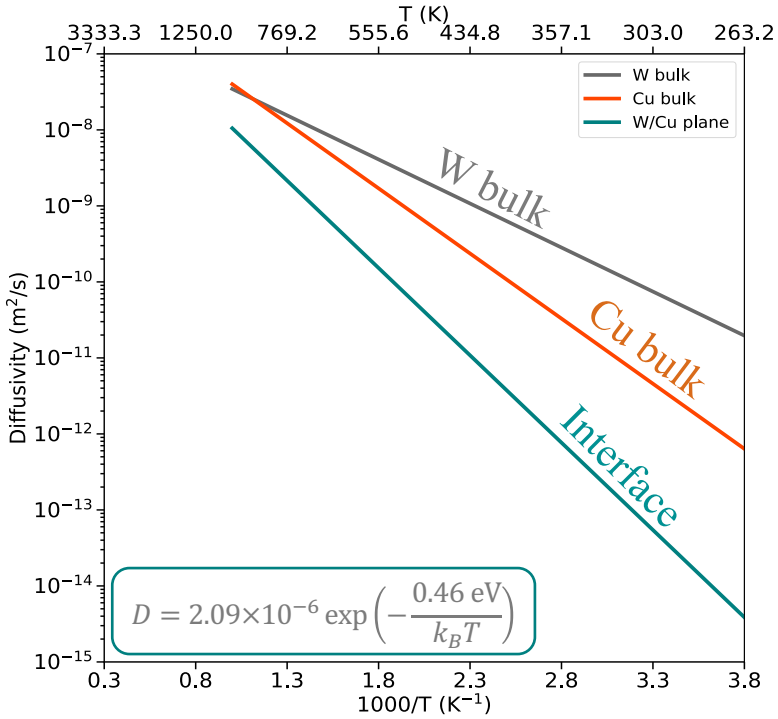

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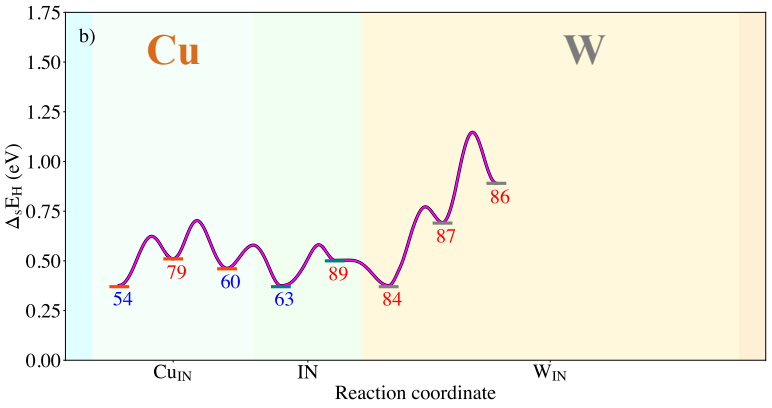
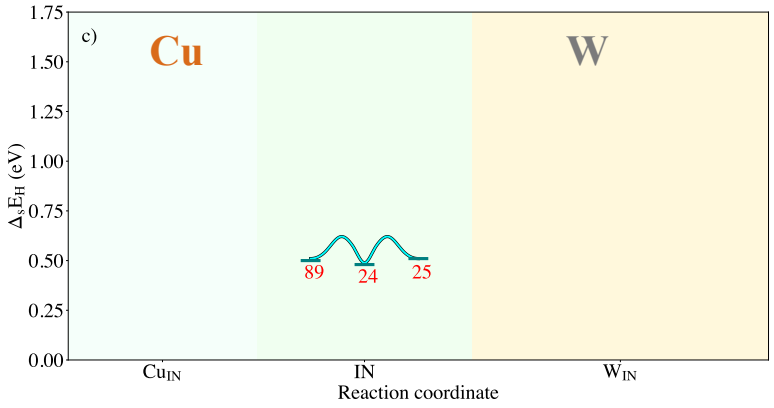
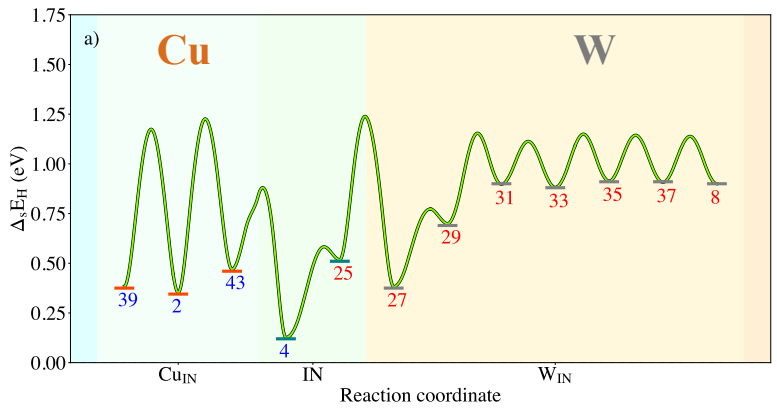
The interface behaves as a sink

Energy barriers along all the paths at the interface







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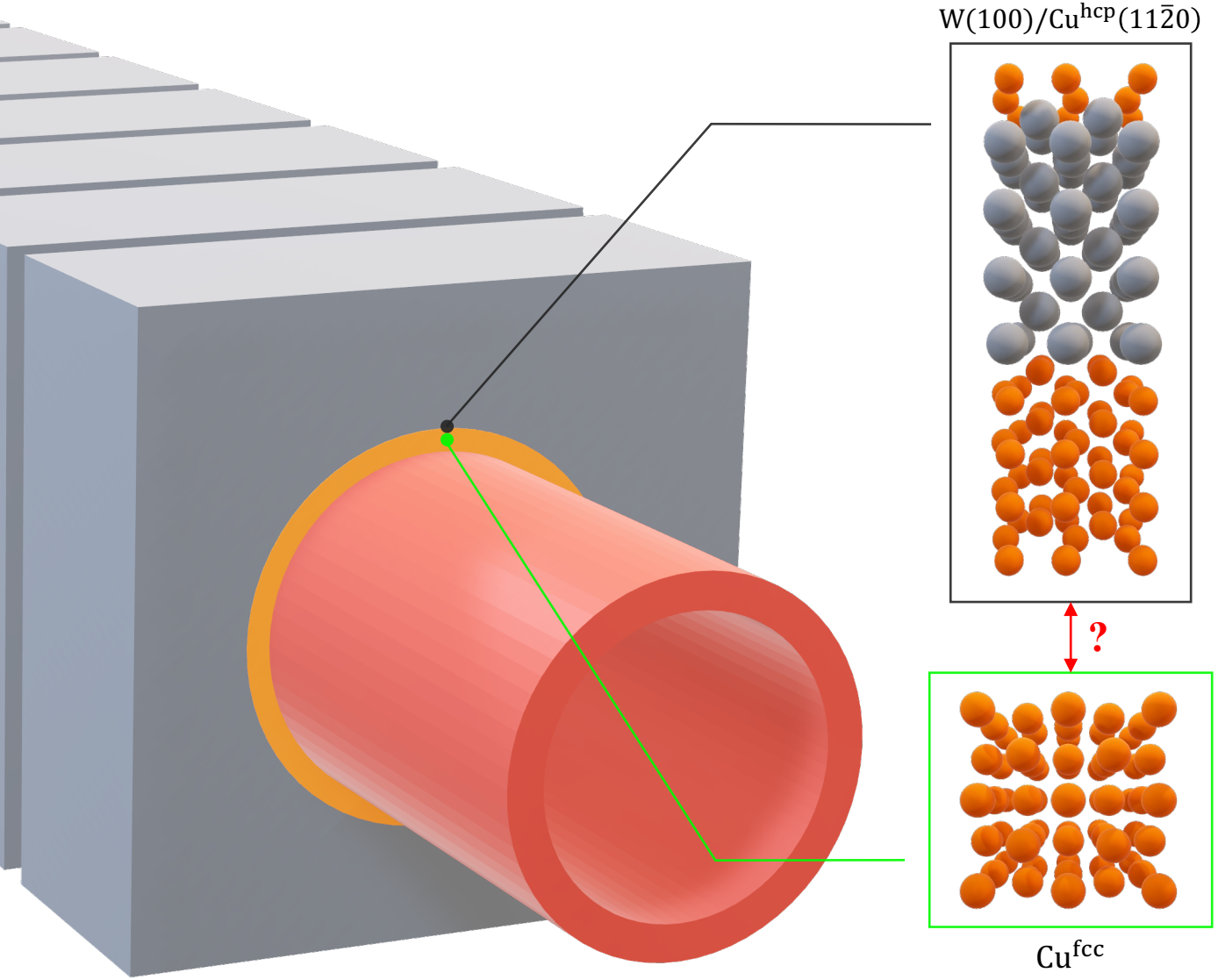
4.4. Porpagation of defects towards the W/Cu interface

Does the **hcp** reconstruction propagate into the **Cu** bulk?



MD simulations only in Cu bulk

vc-relax → NPT → NVE

100 ps 100 ns

T = [300, 430, 550, 700] K

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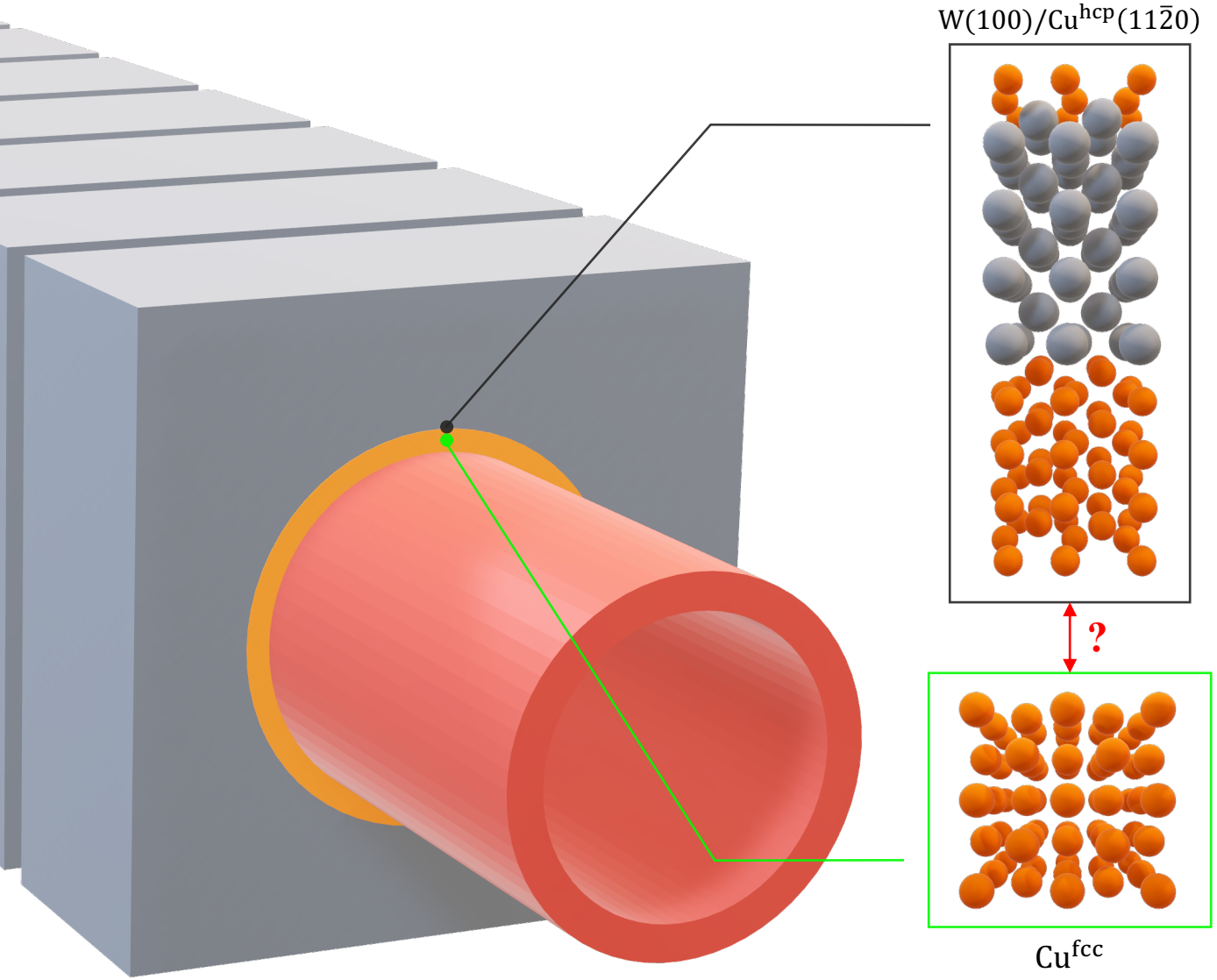

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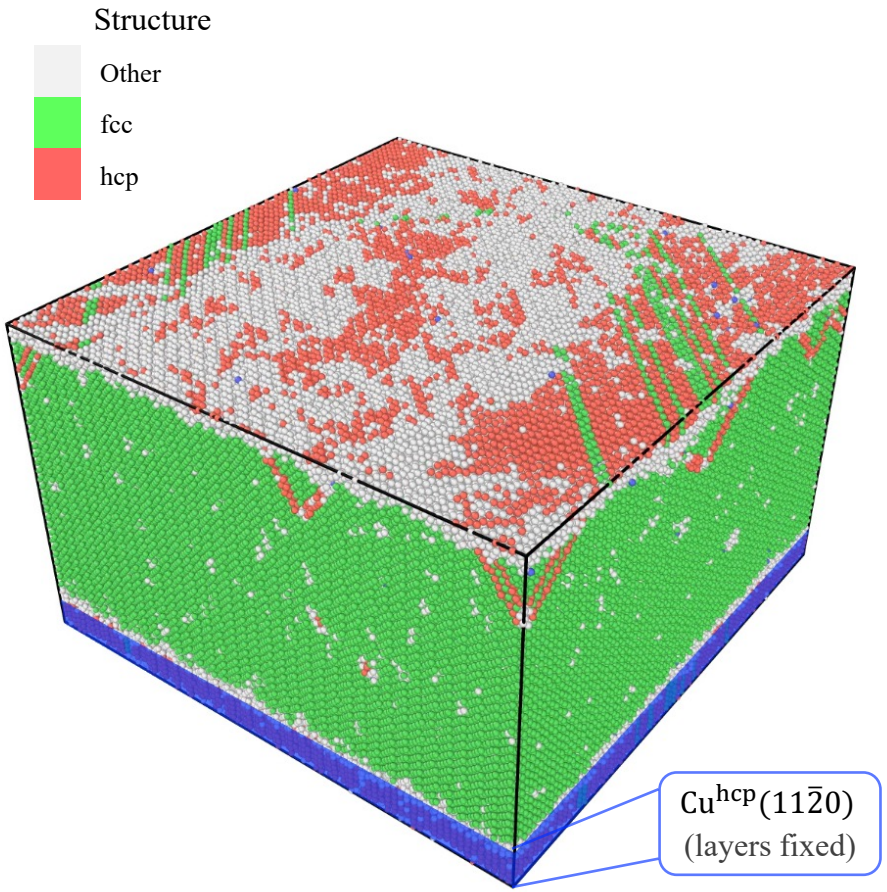

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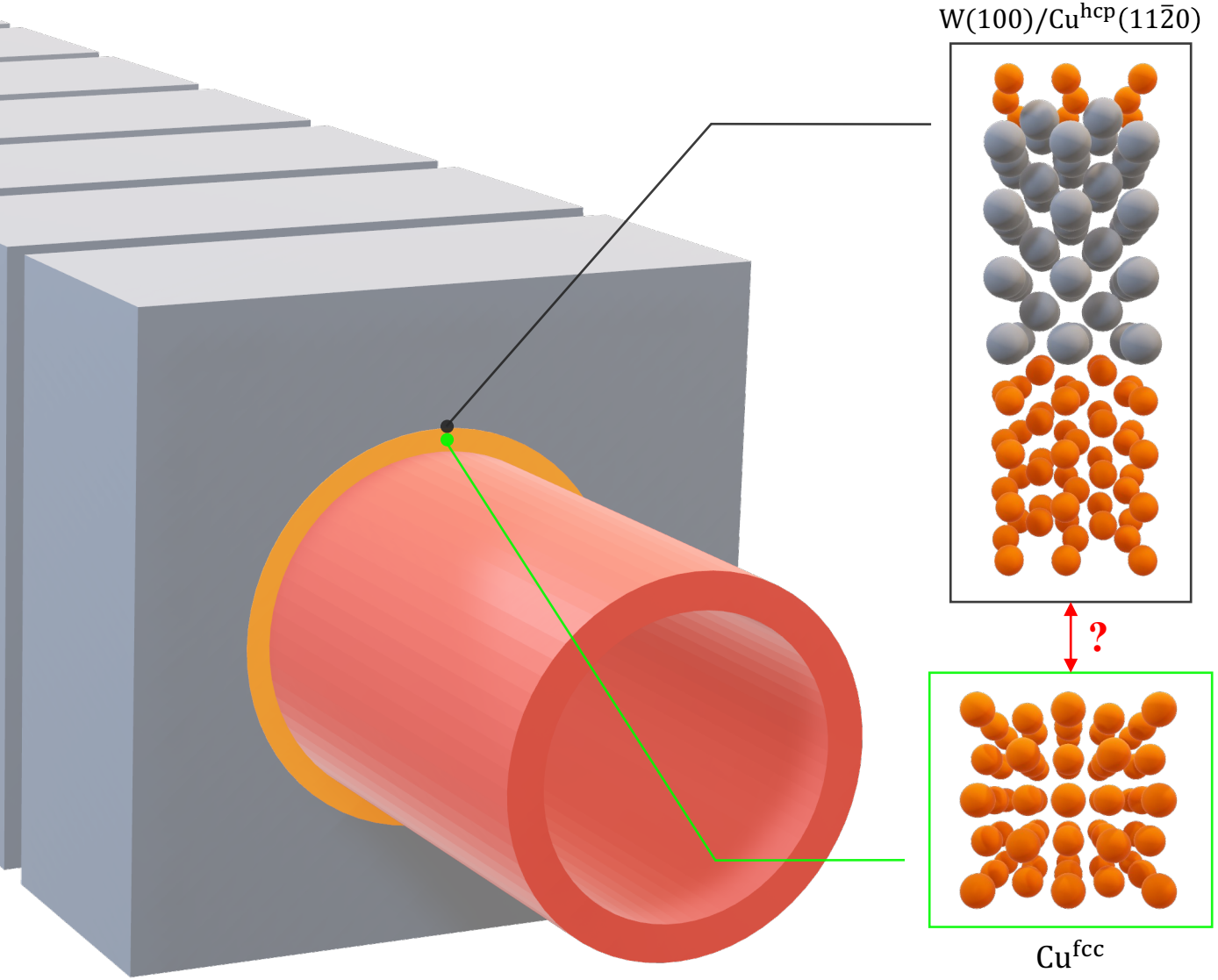
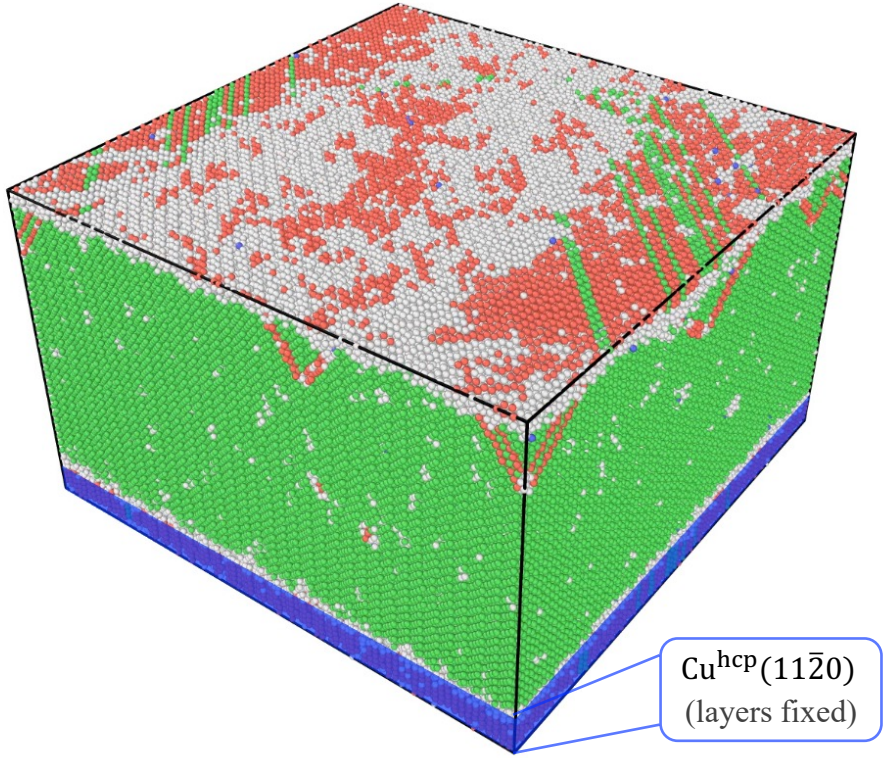
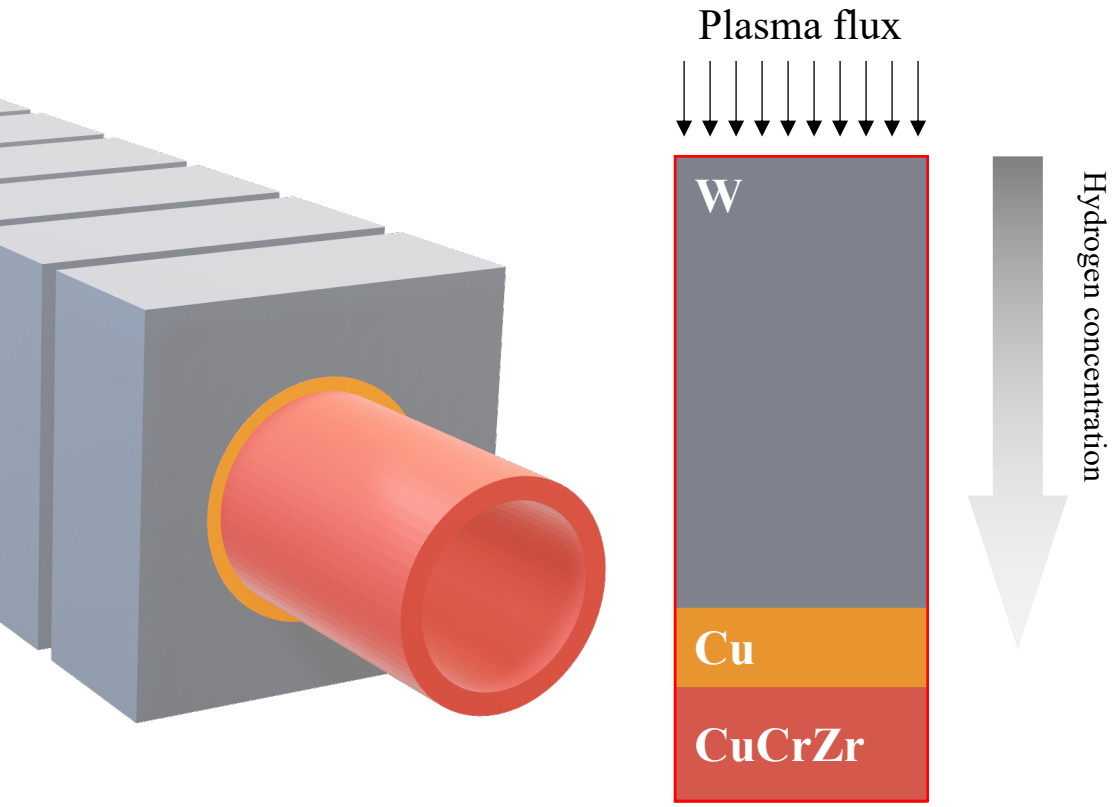


MD simulations only in Cu bulk

- Cu^{fcc} strucuture propagates into the Cu^{hcp} due to the recrystallization of the bulk.
- Point and extended defects propagate towards the W/Cu interface.





Summary of the W/Cu interface

- **Hydrogen solubility** is **high** at the plane of the **interface**.
- **Diffusivity of hydrogen** is **lower** at the plane of the **interface**.
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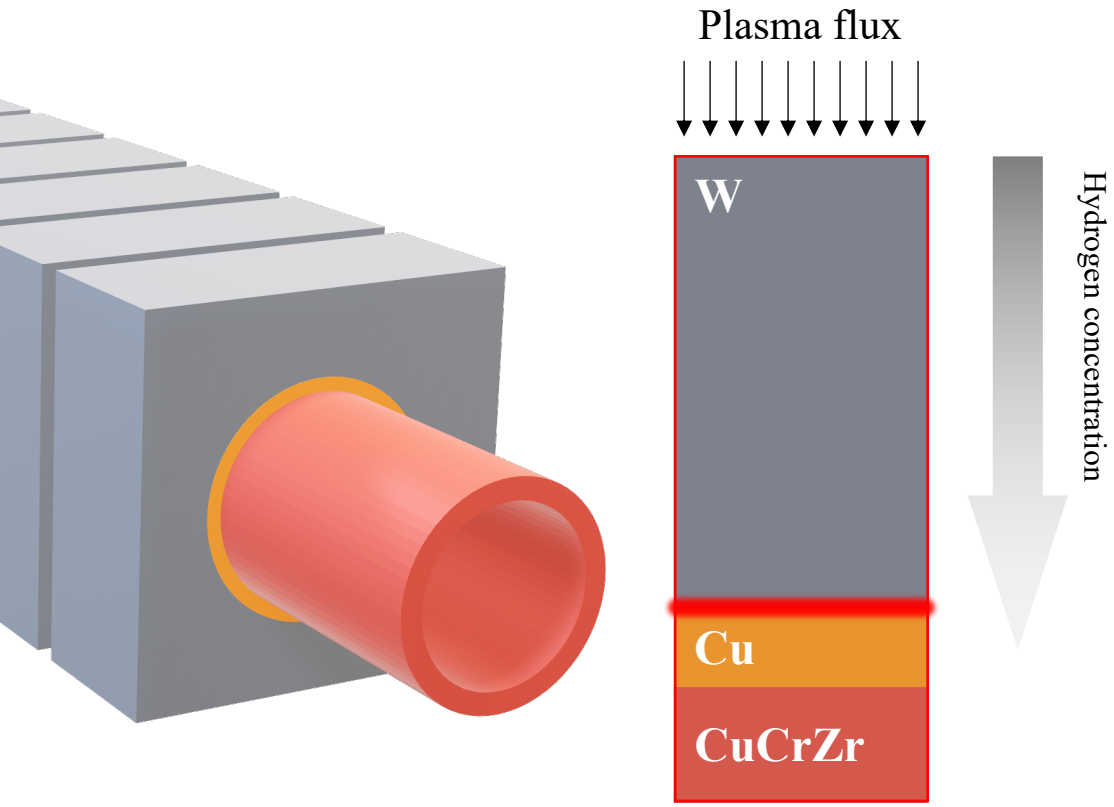

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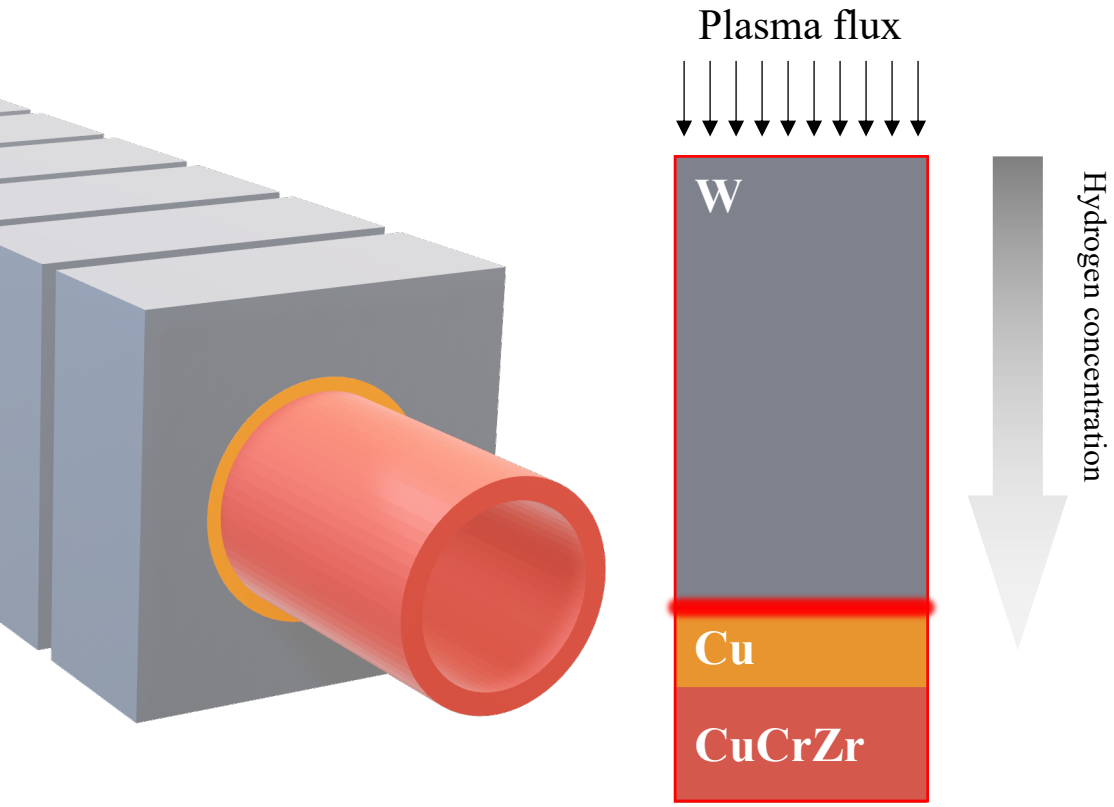
Segregation of H within the W/Cu interface



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Segregation of H within the W/Cu interface

The W/Cu interface behaves as a sink for H atoms

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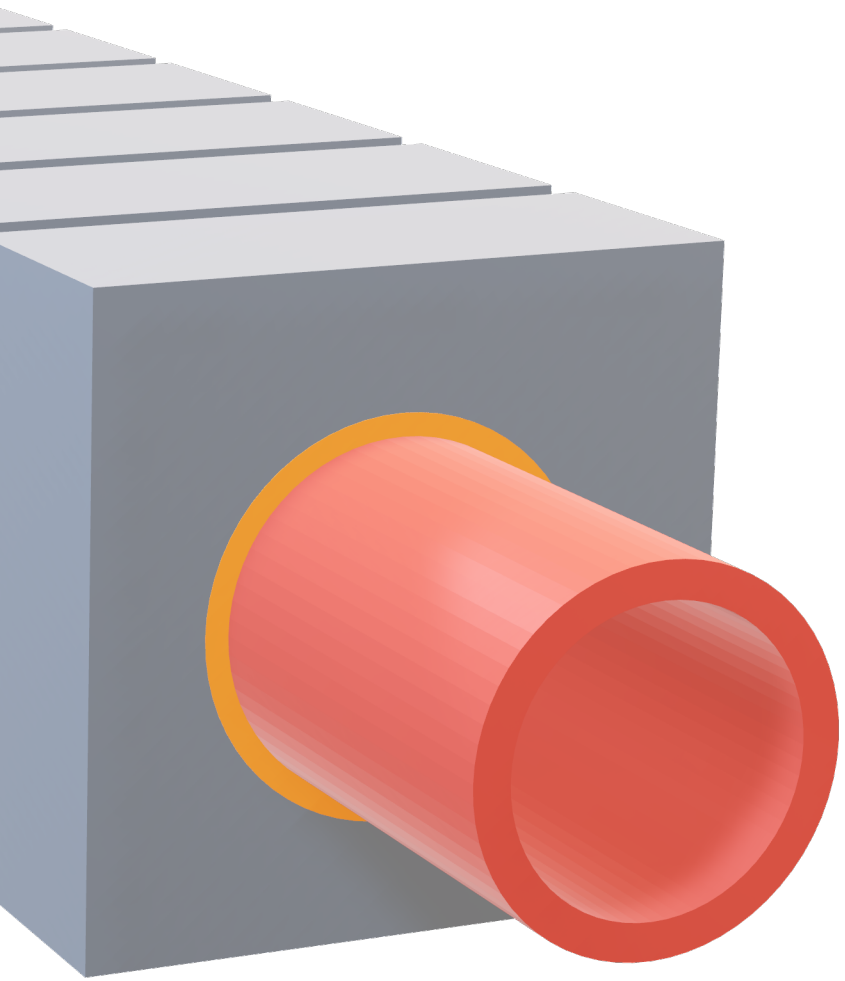


Material modeling starting from the atomic scale - Multiscale approach

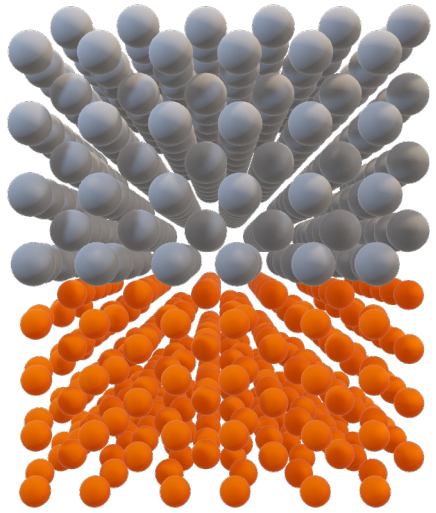
Equilibrium properties (Thermo model)

Dynamic properties (Kinetic model)

From the W surface to the W/Cu interface and beyond.

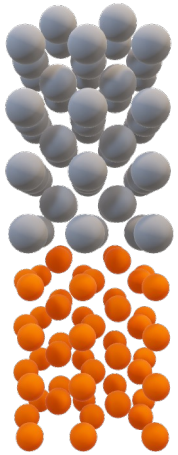
H segregation at the **W/Cu interface**

Future perspectives

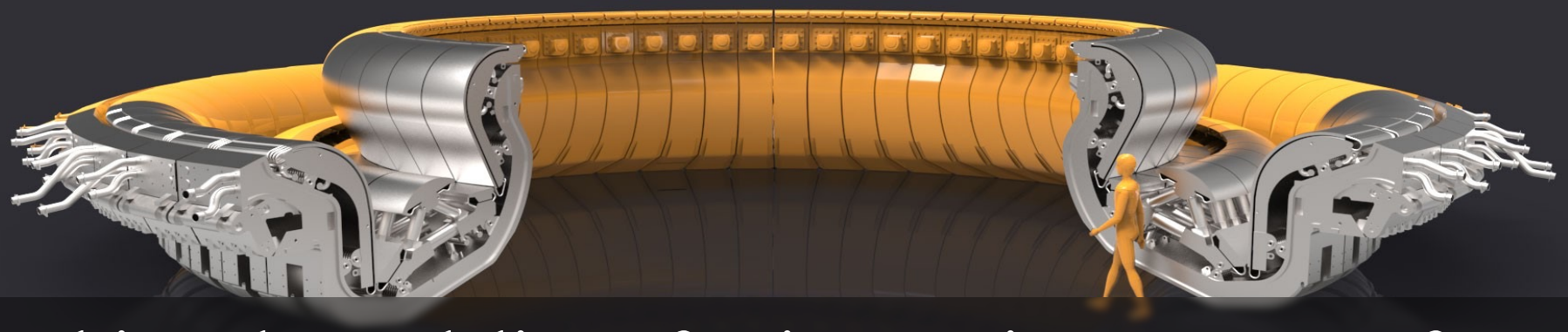


Building the interatomic potential W-Cu and W-Cu-H

Machine Learning Potential



Our team



Multi-scale modeling of H interactions on W surfaces and W/Cu interlayers

Y. Silva-Solís[1], J. D. Cremé[1], J. Denis[1], E. A. Hodille[2] and Y. Ferro[1]

[1]Aix-Marseille University, CNRS, PIIM, F-13013 Marseille, France

[2]CEA, IRFM, F-13108 Saint-Paul-lez-Durance, France

Backup slides

Y. Silva-Solís[1], J. D. Cremé[1], J. Denis[1], E. A. Hodille[2] and Y. Ferro[1]

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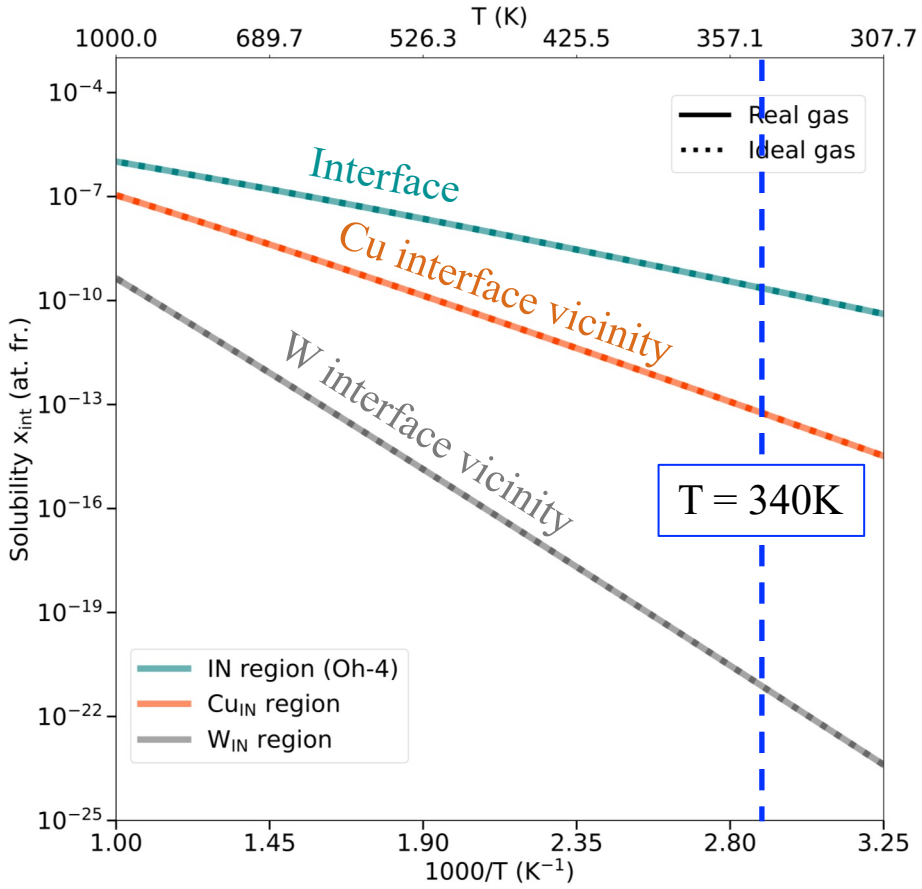
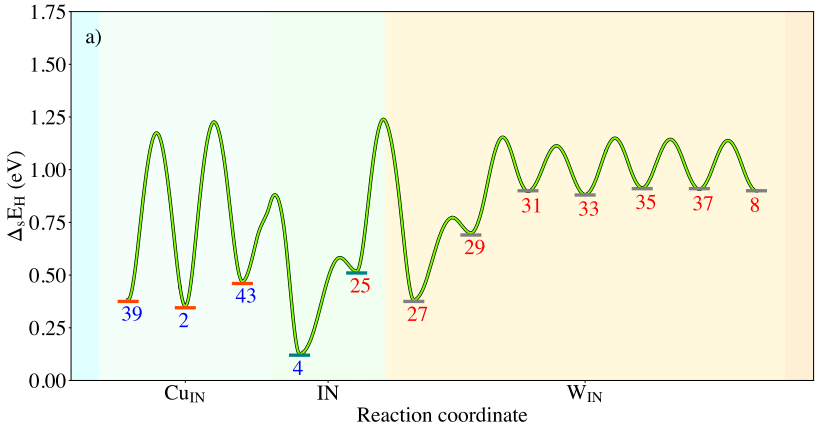
4.3. H diffusivity within the W/Cu interface

Thermodynamics vs Kinetic at steady-state

Thermo model
(H concentration at thermal equilibrium)



Kinetic model
(H concentration out of thermal equilibrium)



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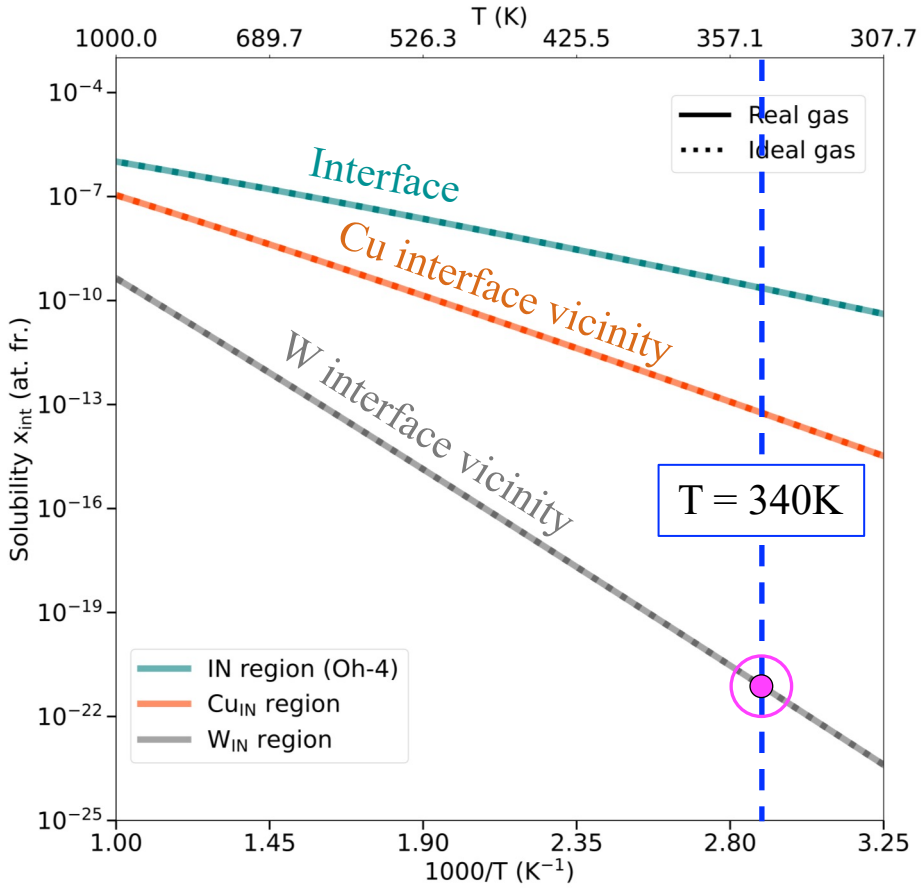

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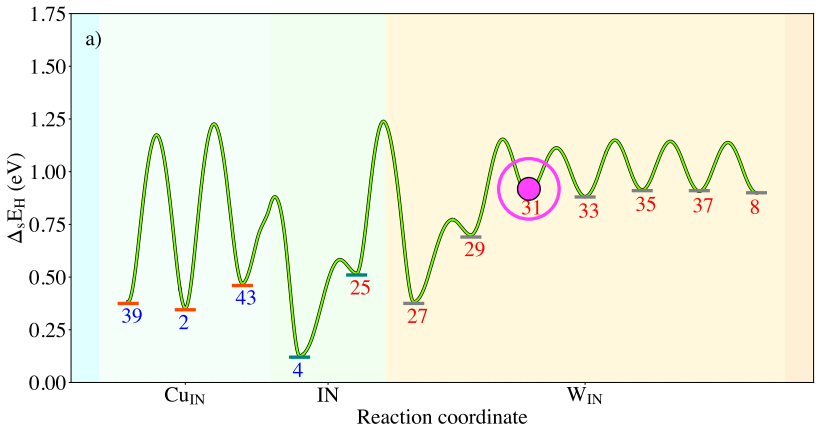

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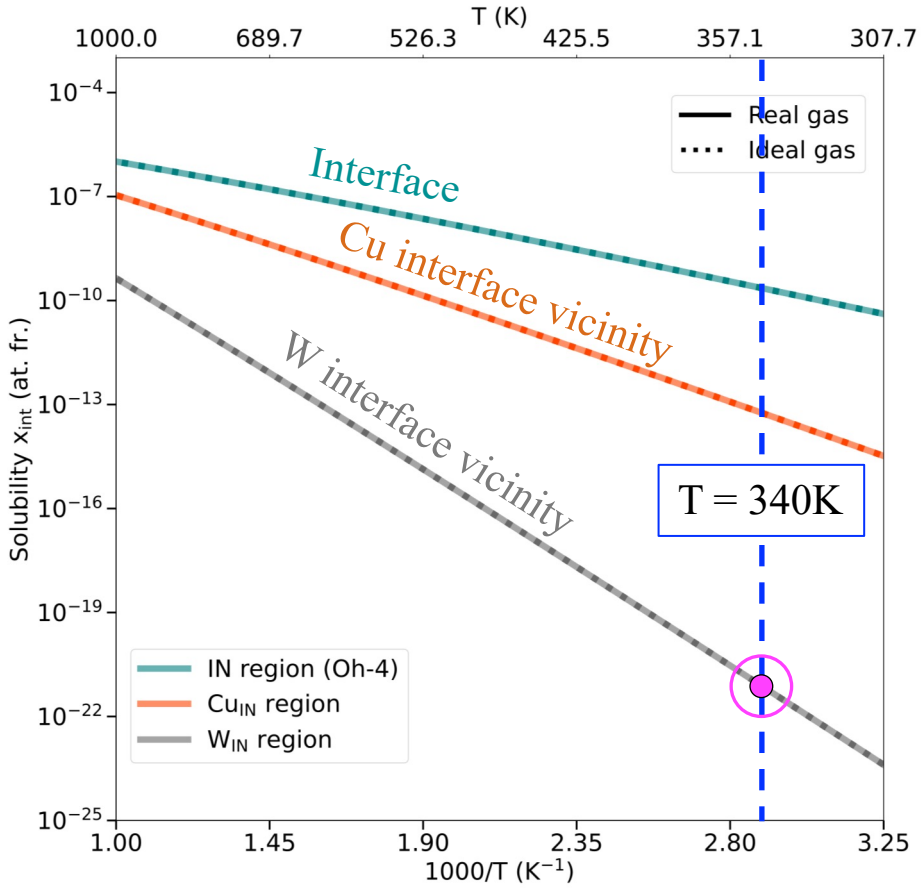

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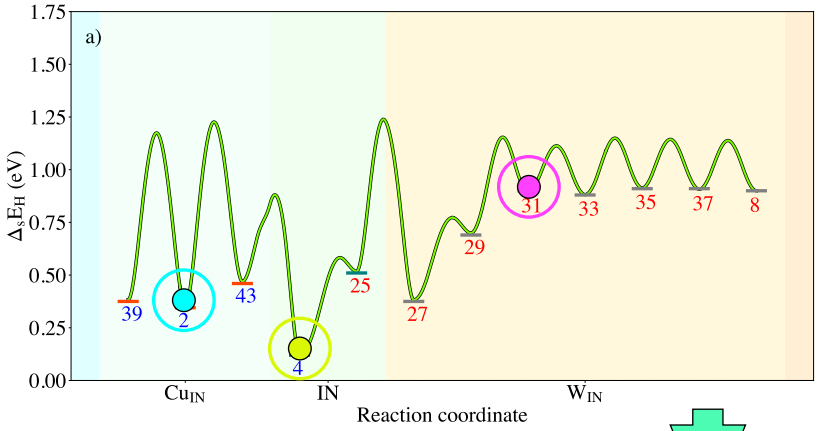
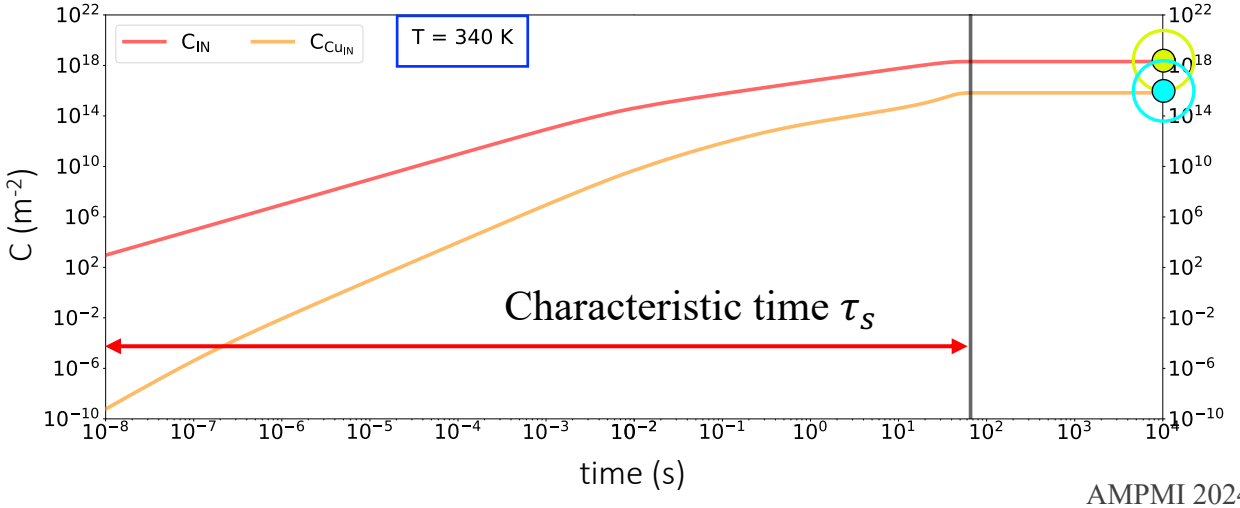


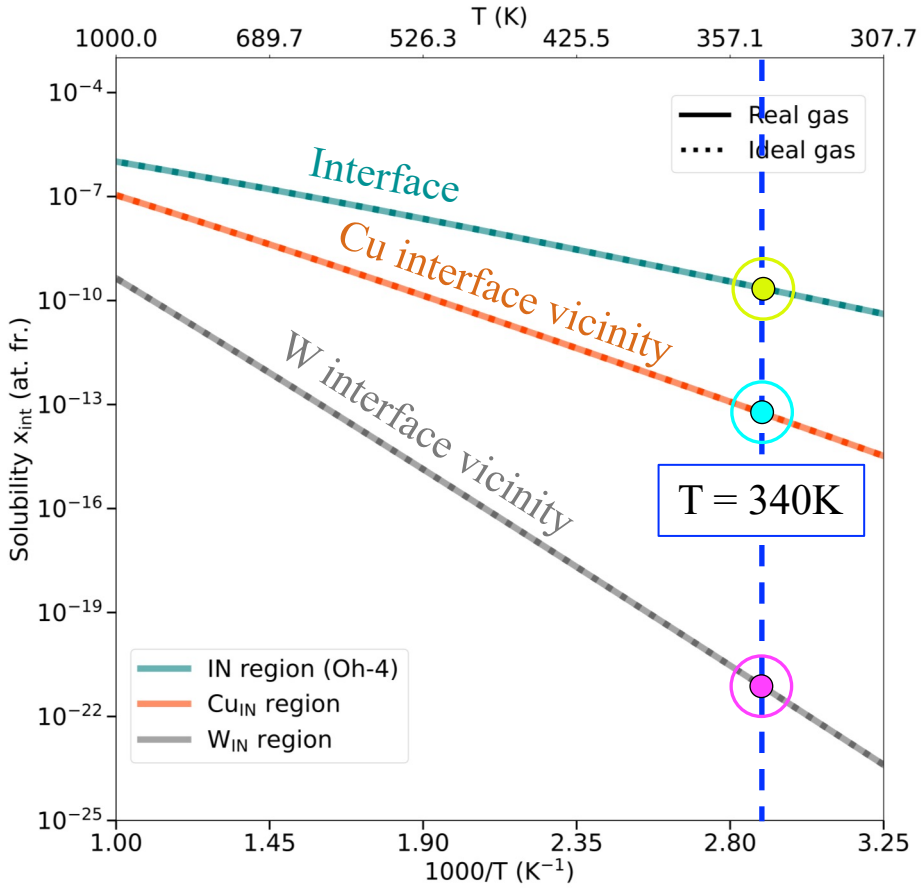


τ_s is the characteristic time to reach the steady-state

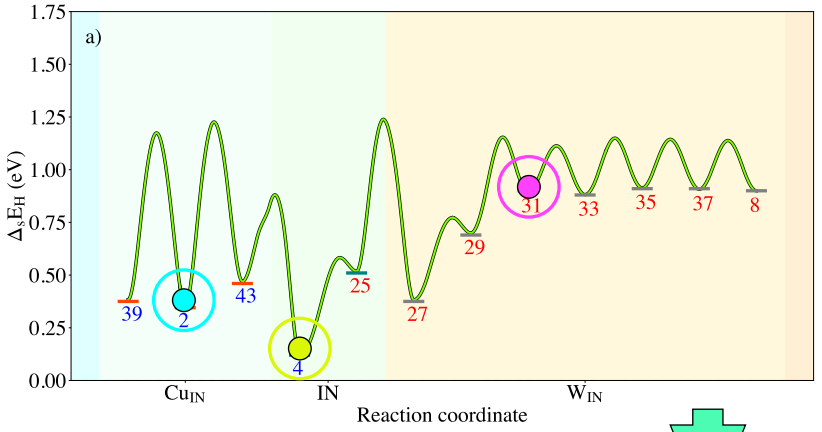
4.3. H diffusivity within the W/Cu interface

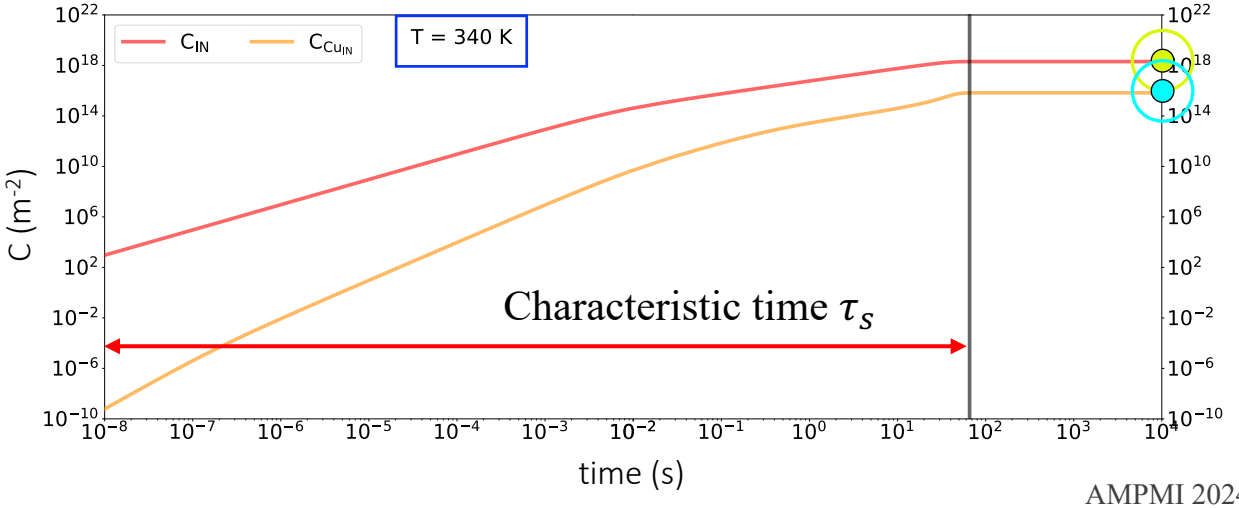
Thermodynamics vs Kinetic at steady-state

Thermo model
(H concentration at thermal equilibrium)



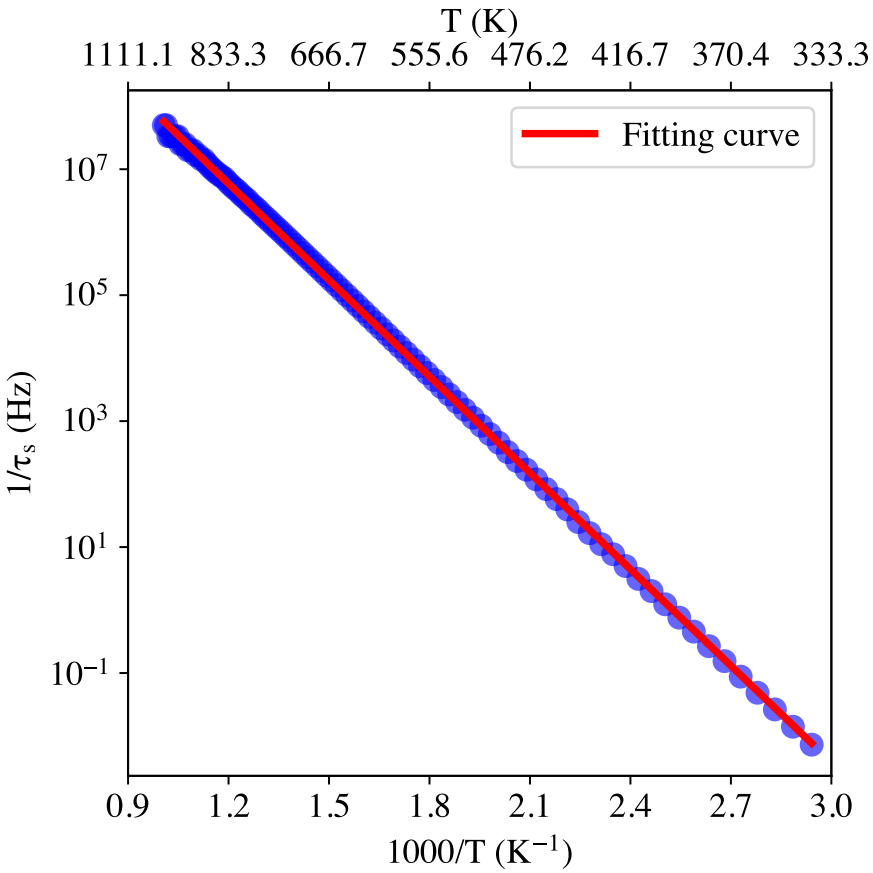
Kinetic model
(H concentration out of thermal equilibrium)





τ_s is the characteristic time to reach the steady-state

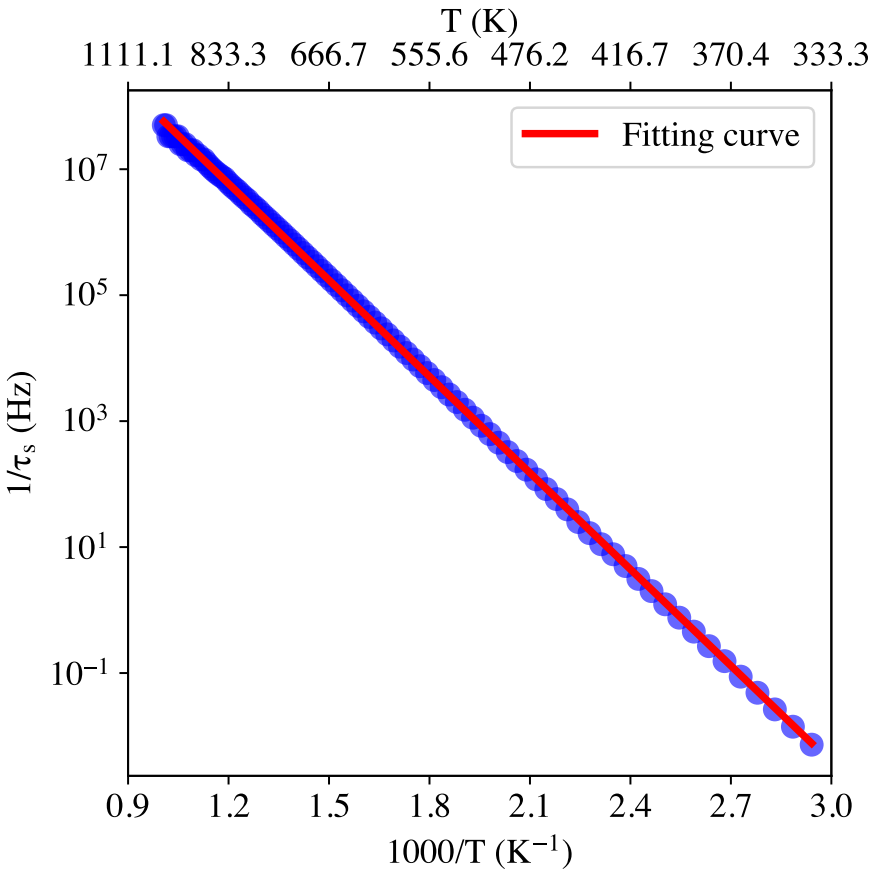
Simplifying the kinetic model



τ_s is determined from T = 340K to 1000K

$$\nu_s = 7.84 \times 10^{12} \exp\left(-\frac{1.01}{k_B T}\right)$$

Simplifying the kinetic model



τ_s is determined from T = 340K to 1000K

An Arrhenius fit is obtained.

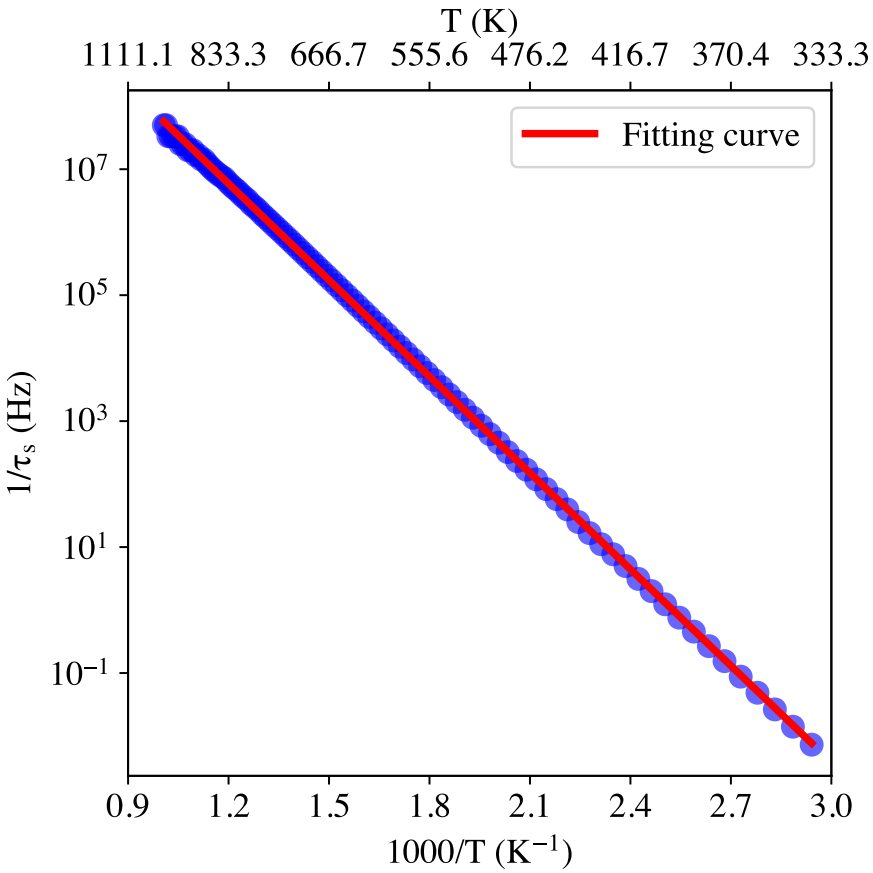
The complex energy profile behaves like a single step diffusion mechanism.

Kinetic model simplifies to a fictitious model with:

- Single diffusion step.
- $E_a = 1.01$ eV
- $\nu_0 = 7.84 \times 10^{12}$ Hz

$$\nu_s = 7.84 \times 10^{12} \exp\left(-\frac{1.01}{k_B T}\right)$$

Simplifying the kinetic model



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Diffusivity of H

Plane W/Cu < Cu < W

The interface behaves as a sink