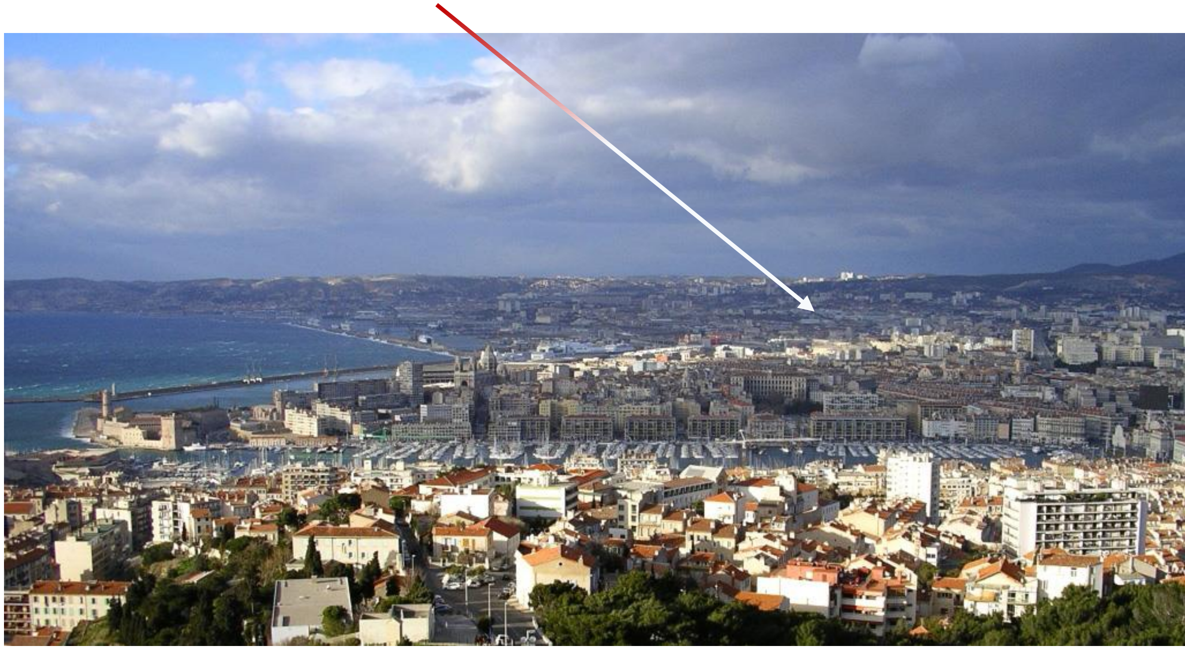
Simultating plasma-wall interaction in fusion reactors with beam-surface experiments

Plasma-Surface team / PIIM laboratory
Aix-Marseille University - CNRS
Marseille, France



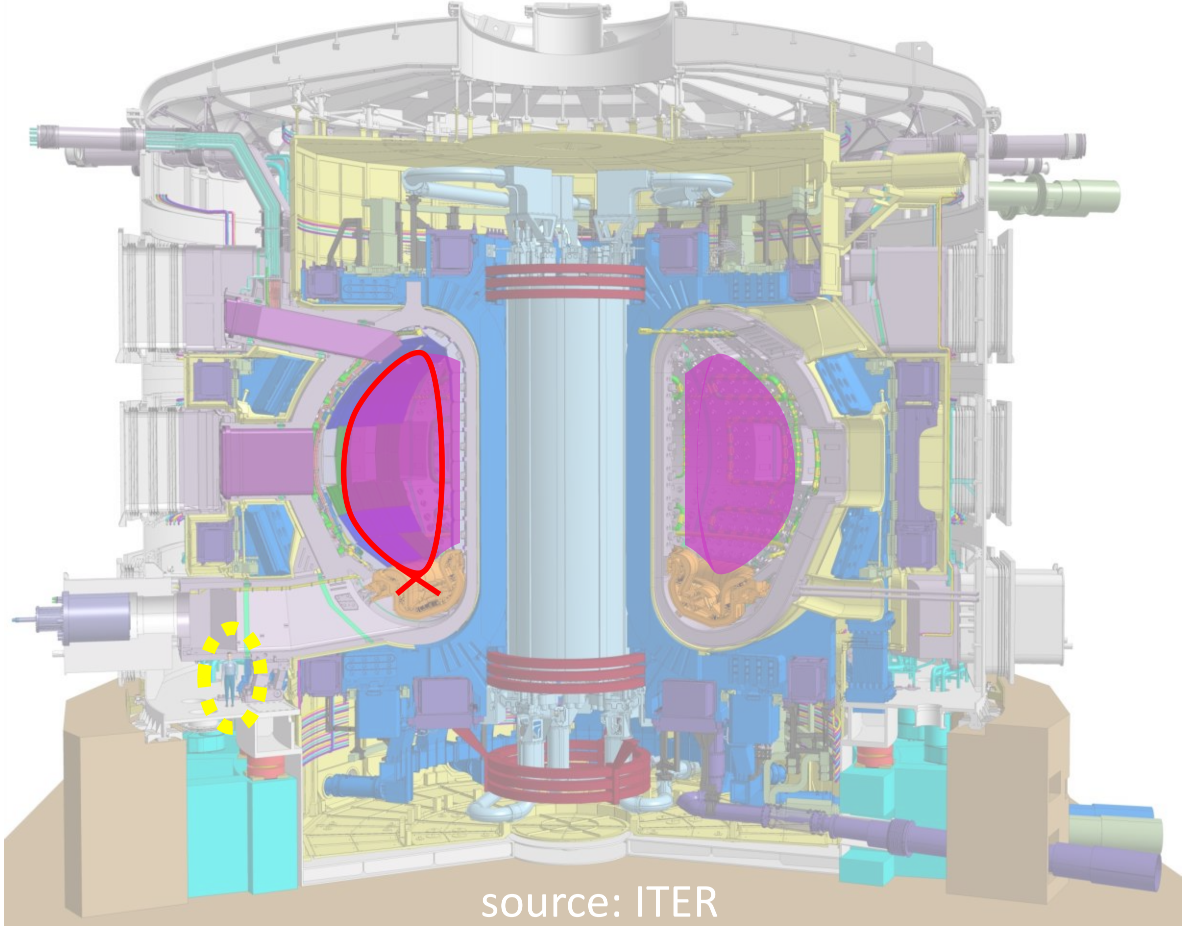
30th Summer School and International Symposium on the Physics of Ionized Gases
August 24-28, 2020

Context - the international fusion experiment ITER

$$^{2}H^{+} + {}^{3}H^{+} \xrightarrow[\text{100 000 000 K}]{} {}^{4}He^{2+} + n^{0}$$

- ➢ Magnetic confinement of the fusion plasma to protect reactor inner walls
- ➢ Power and particle exhaust at the divertor

~ 10^{24} part.$m^{-2}.s^{-1}$ (<50 eV)
(10 MW.m^{-2})
~ ^{3}H up to ~ 1 g.$m^{-2}.s^{-1}$
1 kg of $^{3}H^{+}$ allowed to be retained in inner walls
→ strong recycling needed



source: ITER

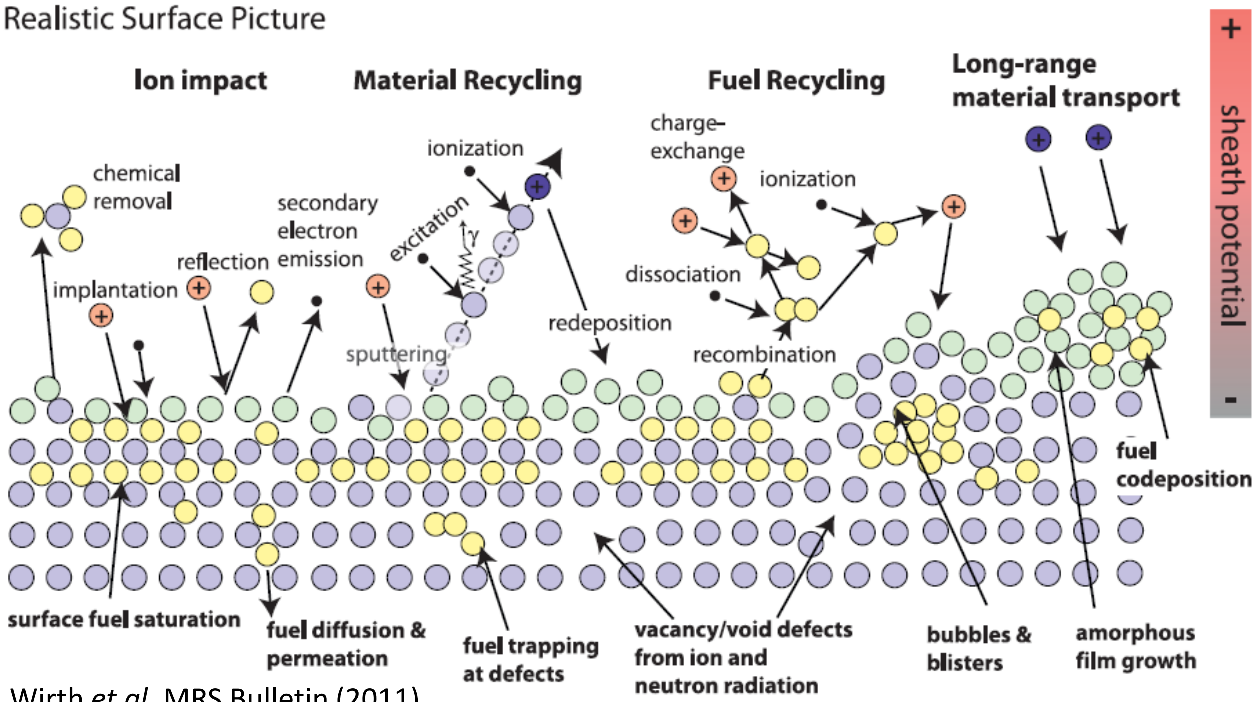
- ➢ Understand interaction of ^{3}H (i.e. ^{2}H) with tungsten to control its retention

Context - the international fusion experiment ITER

Study interaction of D with W to understand retention mechanisms

source: FZ-Jülich

realistic approach



Wirth *et al.* MRS Bulletin (2011)

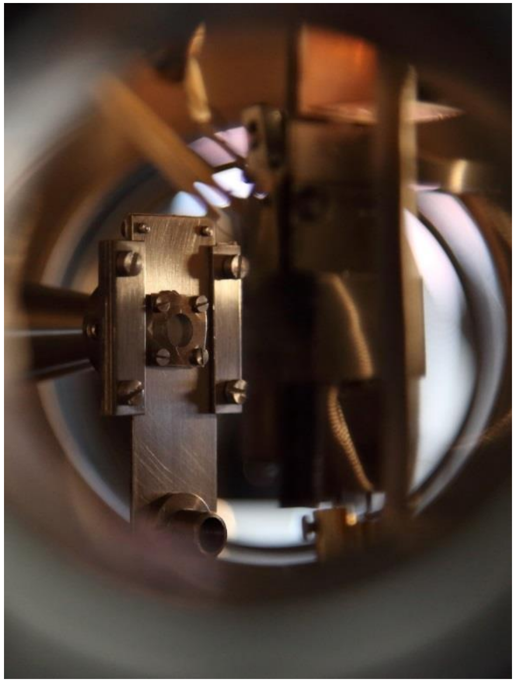
Linear plasma experiments

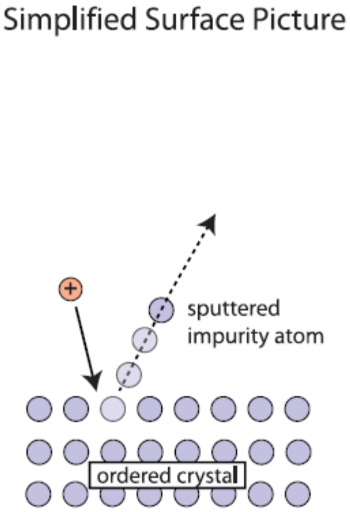
Many processes occur at the same time

→ Difficult to disentangle them

Context - the international fusion experiment ITER

Simulating plasma-wall interactions with beam-surface experiments





Wirth *et al.* MRS Bulletin (2011)

1. Pick only a single impinging gas species
2. Choose a simple material
3. Understand this specific interaction
4. Repeat for another combination…

fundamental approach

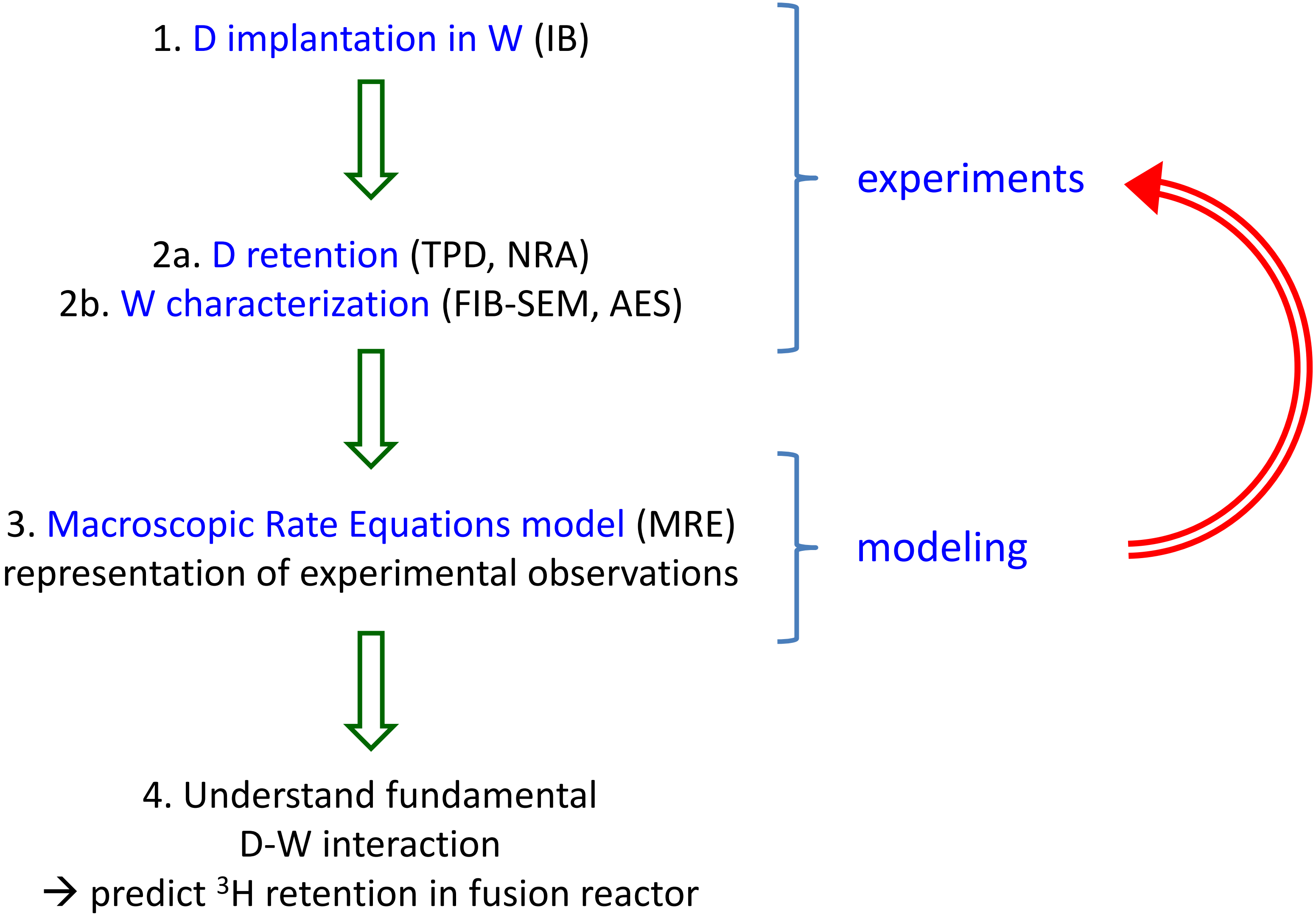
Beam experiments

Few processes occur at the same time

→ Easier to disentangle them (but time consuming)

simulating plasma-wall interactions with beam-surface experiments

D retention in W: fundamental approach



1. D implantation in W (IB)

2a. D retention (TPD, NRA)
2b. W characterization (FIB-SEM, AES)

3. Macroscopic Rate Equations model (MRE)
representation of experimental observations

4. Understand fundamental
D-W interaction
→ predict ^{3}H retention in fusion reactor

experiments

modeling

simulating plasma-wall interactions with beam-surface experiments

D retention in W: fundamental approach

1. D implantation in W (IB)

⇩

2a. D retention (TPD, NRA)

2b. W characterization (FIB-SEM, AES)

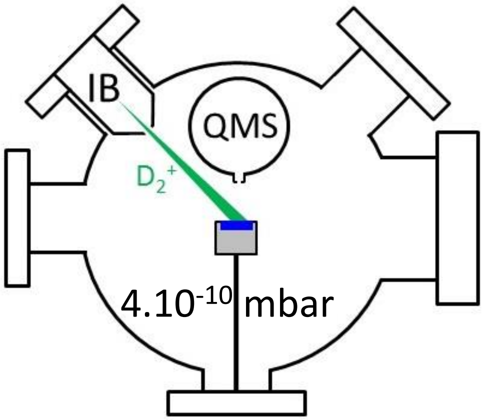
⇩

3. Macroscopic Rate Equations model (MRE)
representation of experimental observations

⇩

4. Understand fundamental
D-W interaction
→ predict ^3H retention in fusion reactor

1.



IB: ion beam
D_2^+ (250 eV/D) – 45° incidence angle

simulating plasma-wall interactions with beam-surface experiments

D retention in W: fundamental approach

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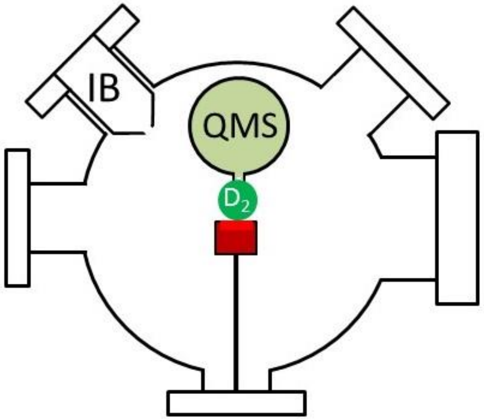
D-W interaction
→ predict ^{3}H retention in fusion reactor

detrapping
energetics

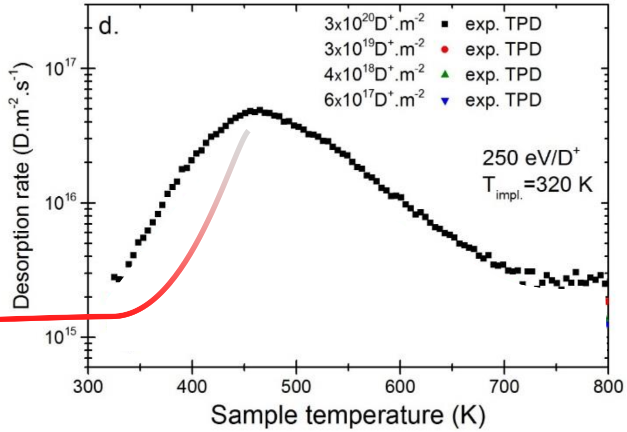
2a.



oven: 300 – 1350 K, increased linearly

QMS: mass spectrometer

oven + QMS: TPD (1 K.s^{-1})



TPD: Temperature Programmed Desorption

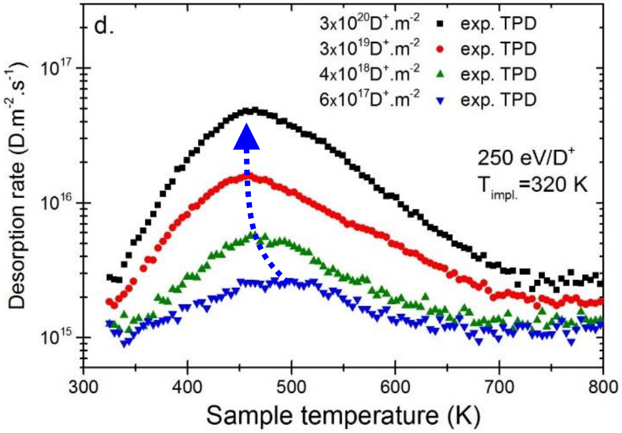
Deuterium retention in tungsten
Part 1 : Poly-W – building the experimental dataset

1. D implantation (IB)

2a. D retention (TPD,NRA)
2b. W characterization

3. MRE modeling

4. D – W interaction



Deuterium retention in recrystallized polycristalline W one TPD peak which temperature position depends on D ion fluence

Bisson *et al.*, Journal of Nuclear Materials **476** (2015) 432

Deuterium retention in tungsten

Part 1 : Poly-W – building the experimental dataset

1. D implantation (IB)

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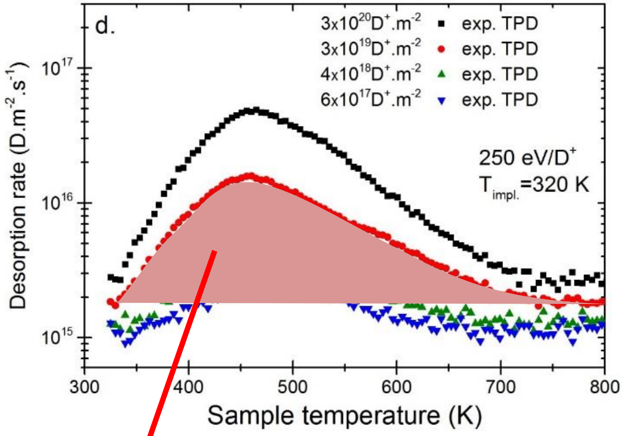
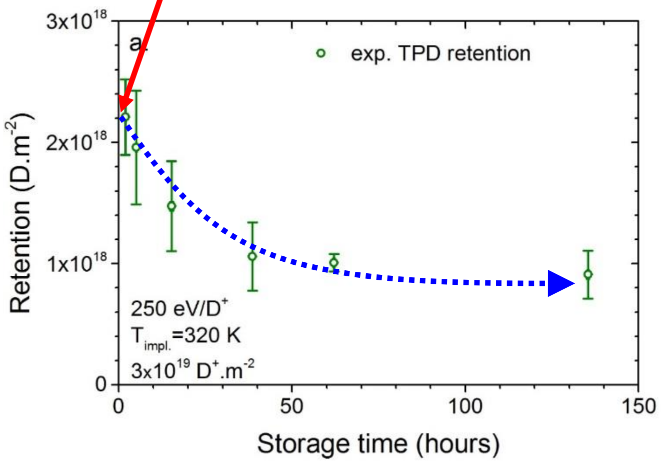


Deuterium retention depends on the storage time between implantation and TPD: deuterium is released from W at 300 K on the timescale of 2 days

Bisson *et al.*, Journal of Nuclear Materials **476** (2015) 432



Deuterium retention in tungsten

Part 1 : Poly-W – building the experimental dataset

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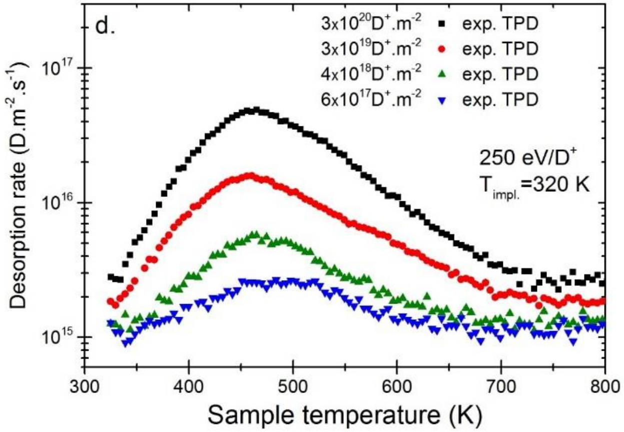
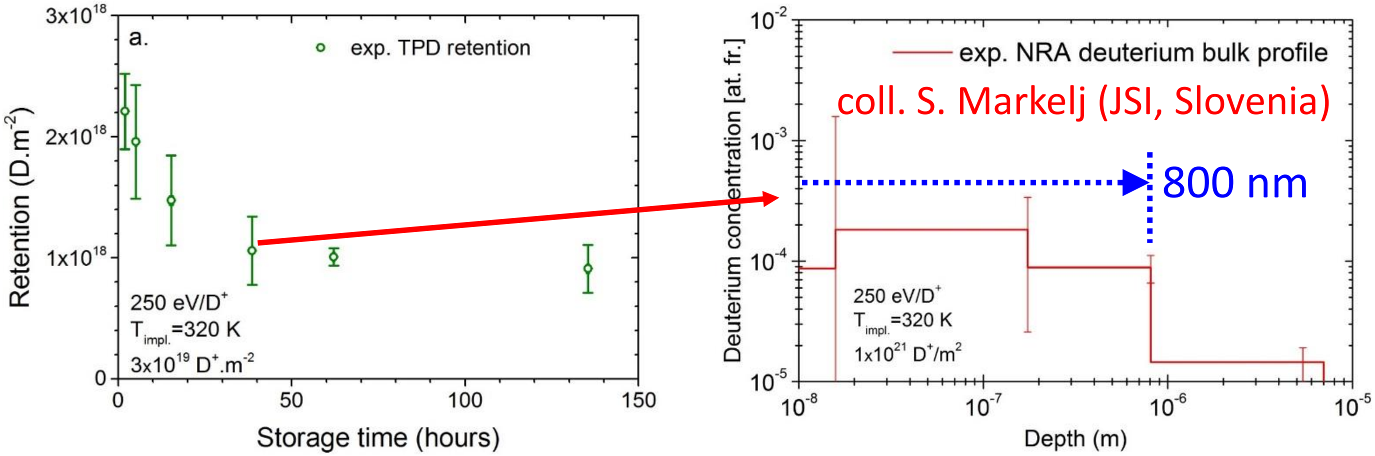


deuterium diffuses up to 800 nm deep within 40 hours at 300 K



coll. S. Markelj (JSI, Slovenia)

800 nm

Deuterium retention in tungsten

Part 1 : Poly-W – building a MRE model

1. D implantation (IB)

2a. D retention (TPD,NRA)
2b. W characterization

3. MRE modeling

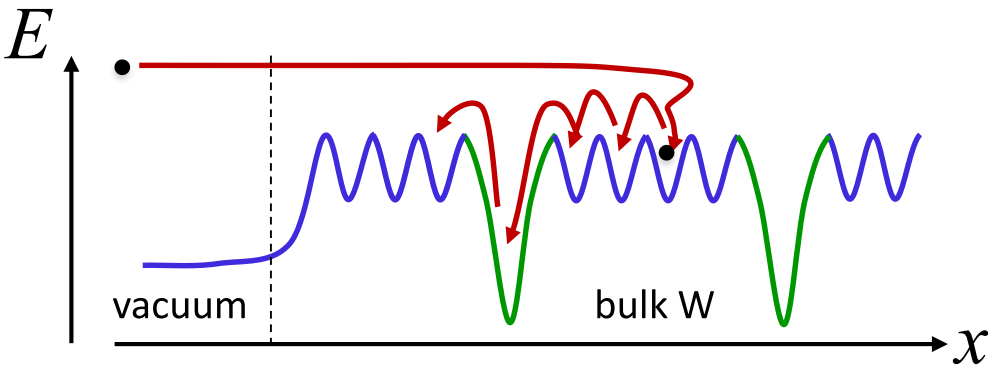
4. D – W interaction

1D MRE model – MHIMS code: Hodille *et al.*, J. Nuc. Mater. **467** (2015) 424
Hodille *et al.*, Phys. Scr. **T167** (2016) 014011

implantation bulk diffusion (de)trapping

$$\partial c_m/\partial t = \varphi \cdot (1 - r) \cdot f(z) + \nu_{diff} \cdot \partial^2 c_m/\partial z^2 - \partial c_t/\partial t \qquad (1)$$

$$\partial c_t/\partial t = \nu_{trap} \cdot (c_m/n_m) \cdot (n_t - c_t) - \nu_{detrap} \cdot c_t \qquad (2)$$



Deuterium retention in tungsten

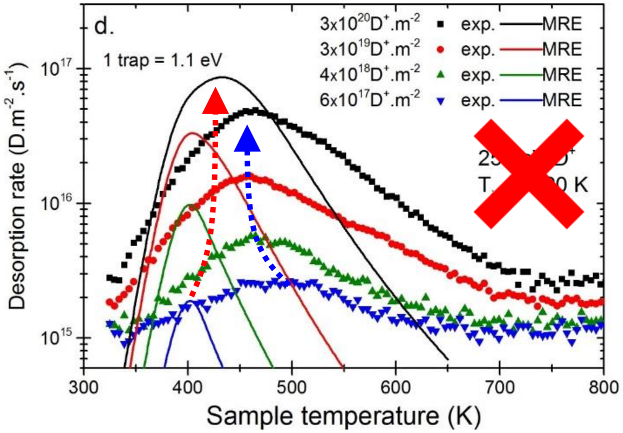
Part 1 : Poly-W – testing an ad-hoc MRE model

1. D implantation (IB)

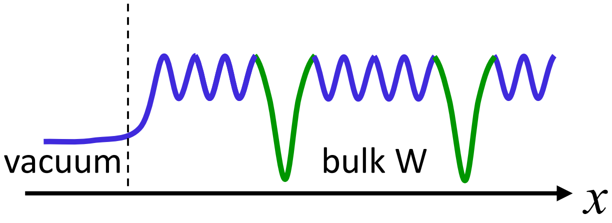
2a. D retention (TPD,NRA)
2b. W characterization

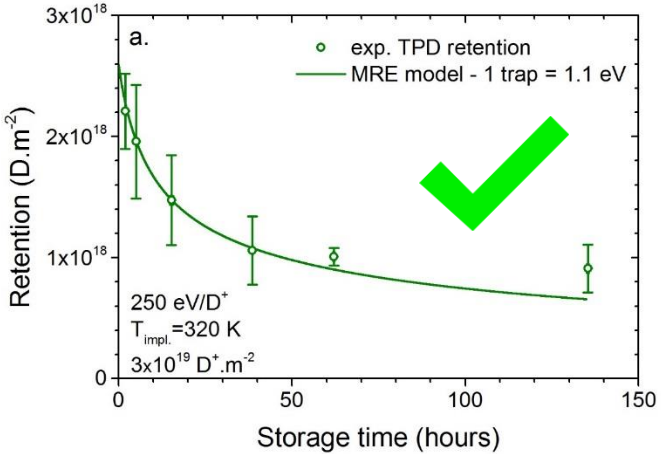
3. MRE modeling
(ad-hoc)

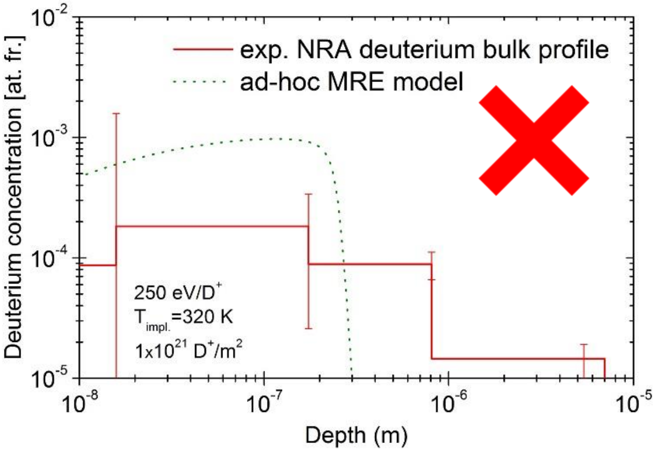
4. D – W interaction



1 TPD peak
1 defect type
2 free parameters
(detrapping energy + density)







Deuterium retention in tungsten

Part 1 : Poly-W – completing the experimental dataset / constraining the model

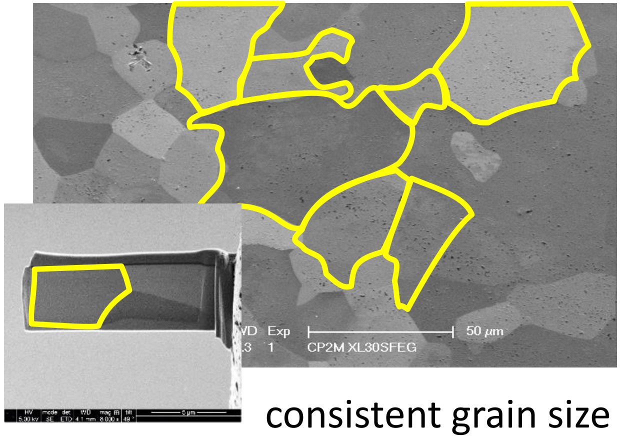
1. D implantation (IB)

2a. D retention (TPD,NRA)

2b. W characterization (FIB-SEM,AES)

3. MRE modeling

4. D – W interaction



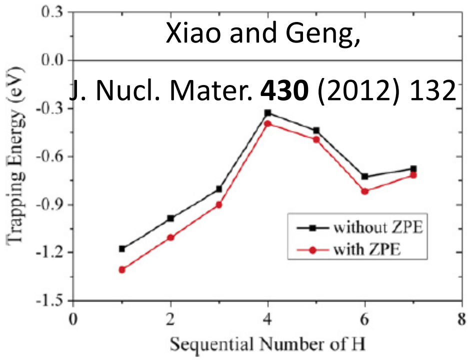
consistent grain size from bulk to surface (FIB-SEM)

↓

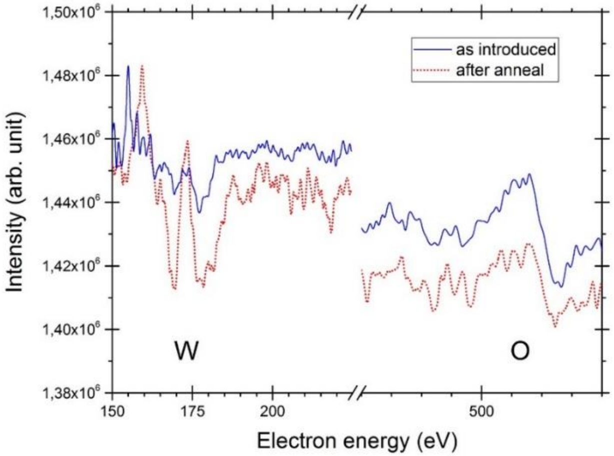
homogen. grain boundary density

↓

grain boundary (de)trapping E_a: DFT



Xiao and Geng, J. Nucl. Mater. **430** (2012) 132

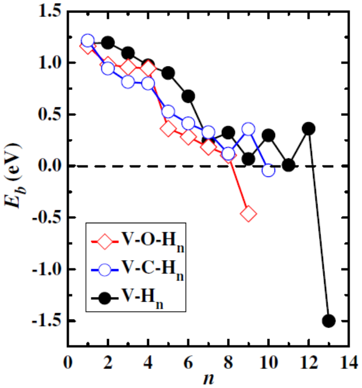


chemical analysis (AES,FIB-SEM):

native oxide layer at surface (<5 nm)

↓

Vacancy-oxygen cluster detrapping energetics from DFT



Kong *et al.*, J. Nucl. Mater. **433** (2013) 357

Deuterium retention in tungsten

Part 1 : Poly-W – testing the more complete DFT-MRE model

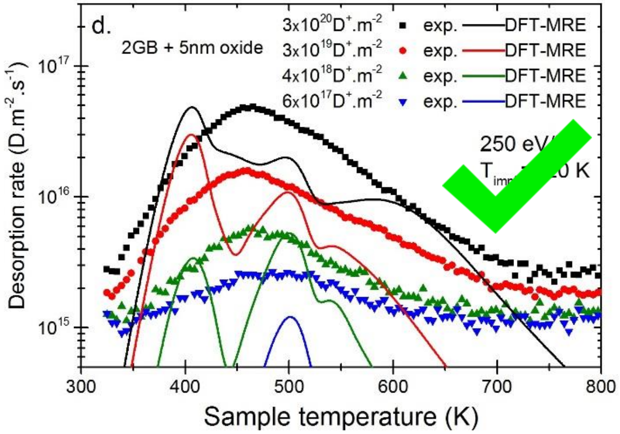
1. D implantation (IB)

2a. D retention (TPD,NRA)

2b. W characterization (FIB-SEM,AES)

3. DFT-MRE modeling (GB + oxide)

4. D – W interaction

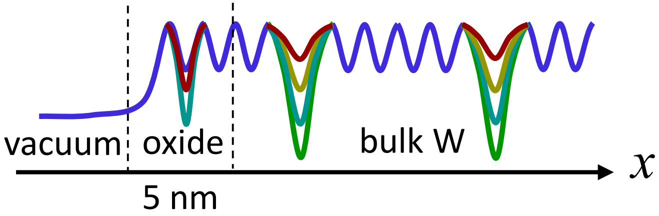


2 defect types

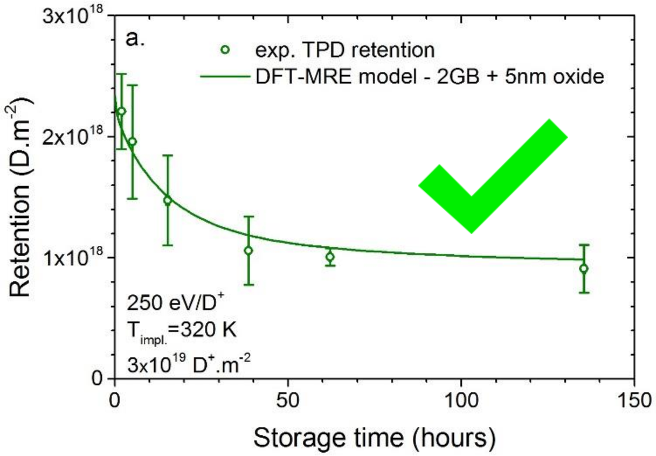
DFT detrapping energies

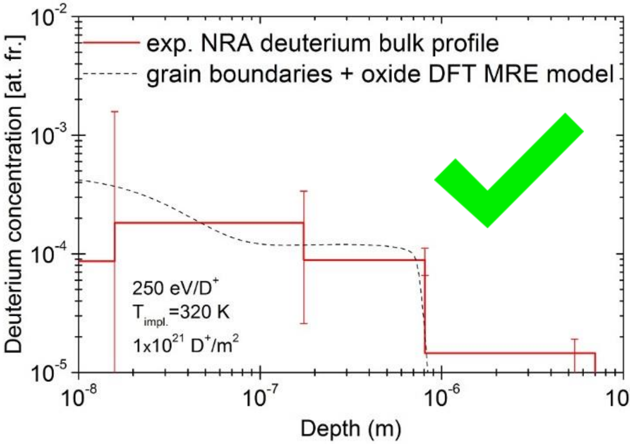
2 free parameters

(GB + oxide densities)



Hodille *et al.*, Nuclear Fusion **57** (2017) 076019





Deuterium retention in tungsten

Part 1 : Poly-W – Summary

Recrystallized polycristalline tungsten (Poly-W):

- ➢ 2 rate limiting steps should co-exist for D release (even though one TPD peak)
- ➢ Grain boundaries + oxide layer

However:

- ❖ No direct evidence for 2 rate limiting steps (inference from exp. vs model.)

➢ Need to find a way to disentangle these rate-limiting steps

Bisson *et al.*, Journal of Nuclear Materials **476** (2015) 432

Hodille *et al.*, Nuclear Fusion **57** (2017) 076019

Ghiorghiu *et al.*, Nuclear Instruments & Methods B **461** (2019) 159

Deuterium retention in tungsten

Part 2 : disentangling the two rate-limiting steps

Redhead, Vacuum **12** (1962) 203

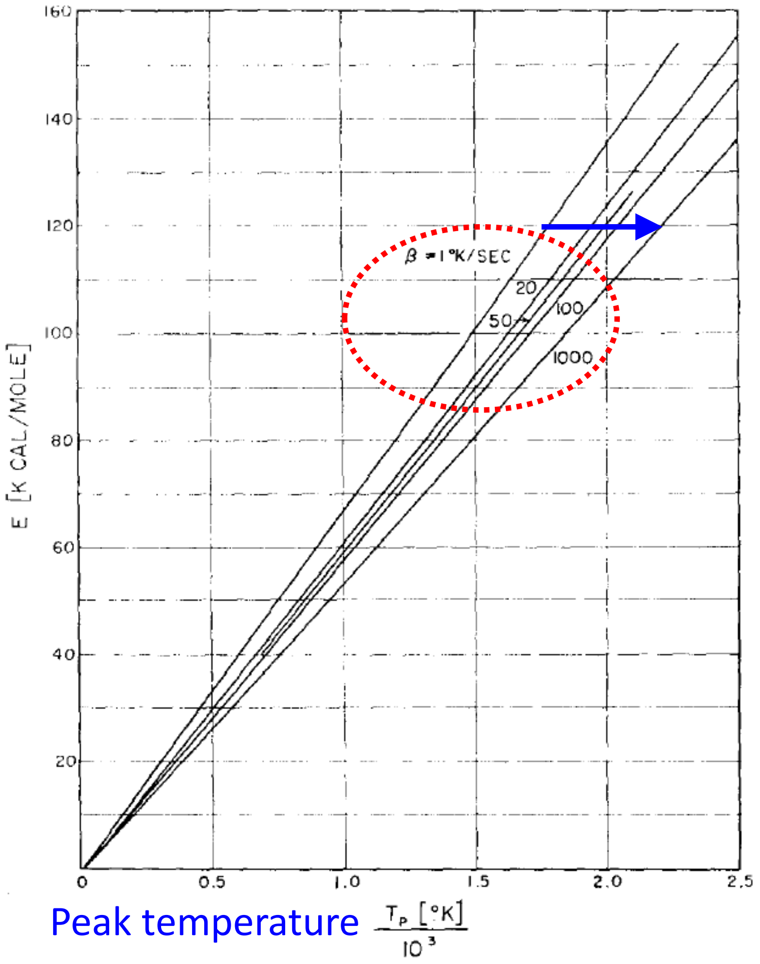


FIG. 3. Activation energy of desorption (E) as a function of T_p for a first-order reaction and a linear temperature sweep ($T = T_0 + \beta t$) taking $\nu_1 = 10^{13}$ sec^{-1}.

during TPD evaluation of D retention/release, the sample temperature varies with the heating rate $\beta = \frac{dT}{dt}$

kinetics of trapped D (c_t) release depends on β

$$\frac{dc_t}{dT} = -\frac{c_t}{\beta} \times \nu_0 \times e^{\left(-\frac{E_a}{k_b T}\right)}$$

increasing β shifts to higher temperature the peak of D release rate (Tp)

Deuterium retention in tungsten

Part 2 : disentangling the two rate-limiting steps

Redhead, Vacuum **12** (1962) 203

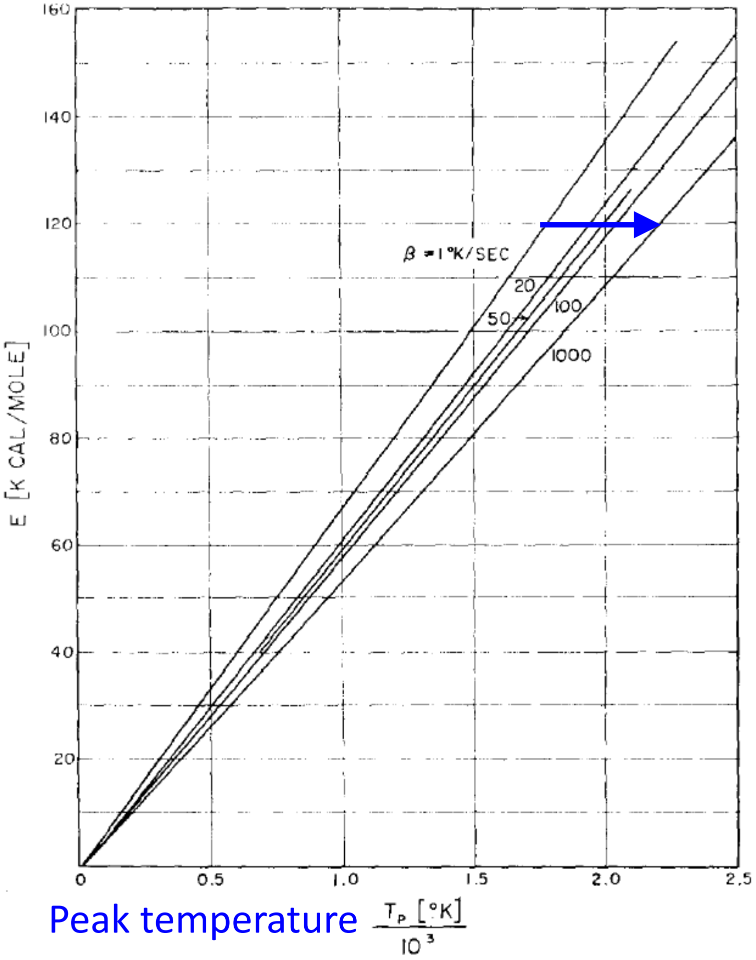
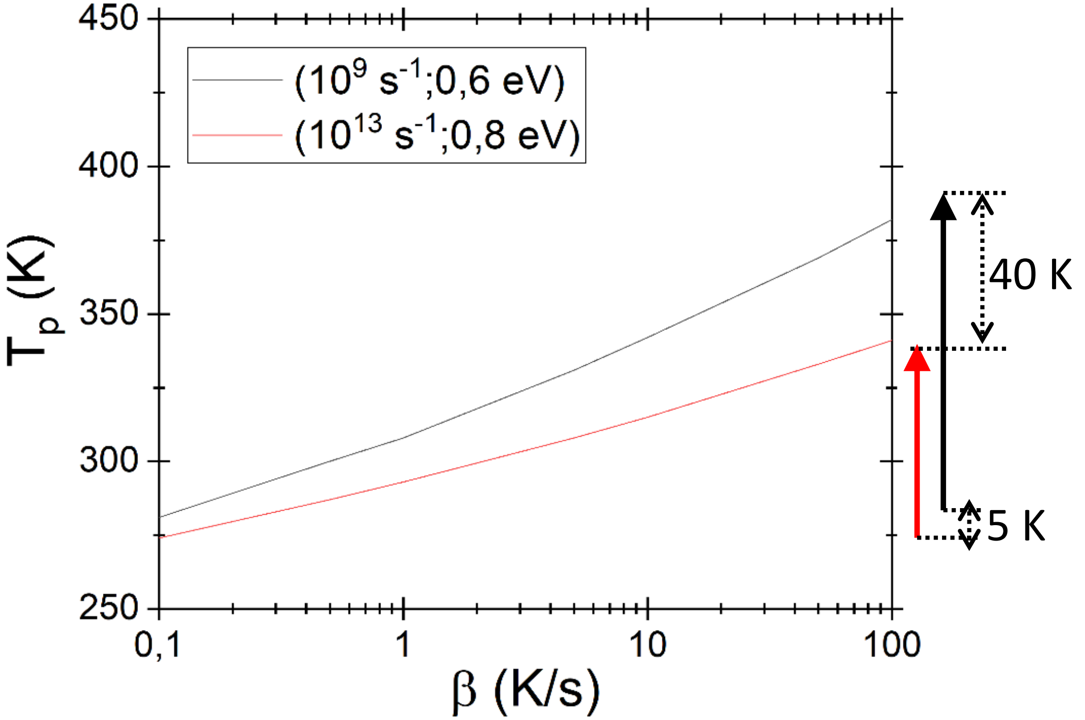


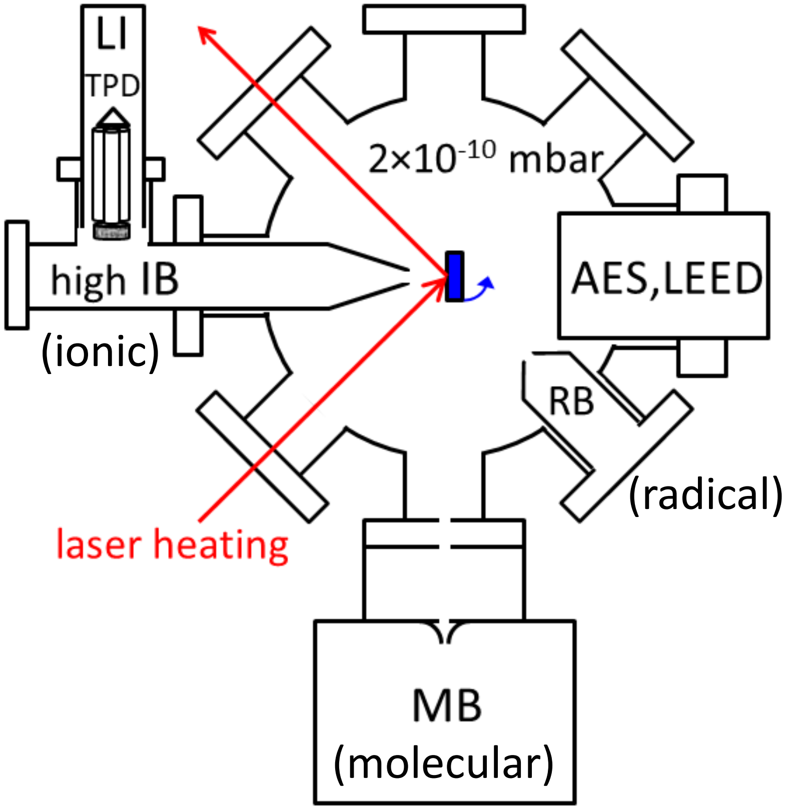
FIG. 3. Activation energy of desorption (E) as a function of T_p for a first-order reaction and a linear temperature sweep ($T = T_0 + \beta t$) taking $\nu_1 \approx 10^{13}$ sec^{-1}.

Two “merged” rate-limiting steps
with different kinetic parameters ($\nu_0^i; E_a^i$)
must be “separated in TPD”
when applying sufficient high heating rates

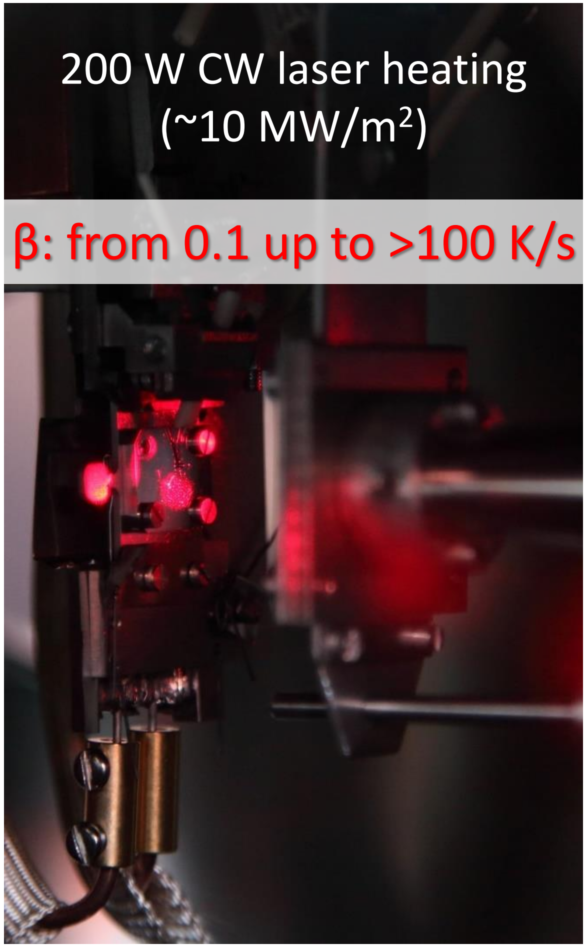


Deuterium retention in tungsten

Part 2 : disentangling the two rate-limiting steps



Advanced **MU**lti-beams experiment for
Plasma **S**urface **I**nteraction studies
(AMU-PSI)



200 W CW laser heating
(~10 MW/m^2)

β: from 0.1 up to >100 K/s

High IB: D_2^+ ion beam (250 eV/D)
LI TPD: Laser Induced TPD

Deuterium retention in tungsten

Part 2 : Poly-W vs Single-W – summary

Polycrystalline versus single crystal W study with Laser-Induced TPD:

- ✓ confirmation that Poly-W has 2 rate-limiting steps for D release
- ✓ grain boundaries + « native oxide » detrapping

However:

- ❖ « native oxide » cannot be modeled quantitatively (not shown here)

Ghiorghiu *et al.*, Nuclear Instruments & Methods B **461** (2019) 159

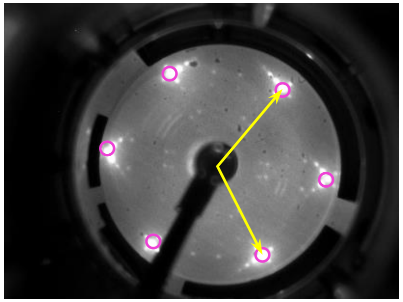
➢ Need to find a « cleaner » way to study the « native oxide » :

1. study « native oxide » retention of a single crystal (i.e. with no other defects)
2. remove the « native oxide » → study how D retention changes ?
3. study well-controlled oxide and try to model it quantitatively

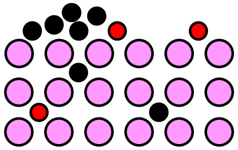
Deuterium retention in tungsten

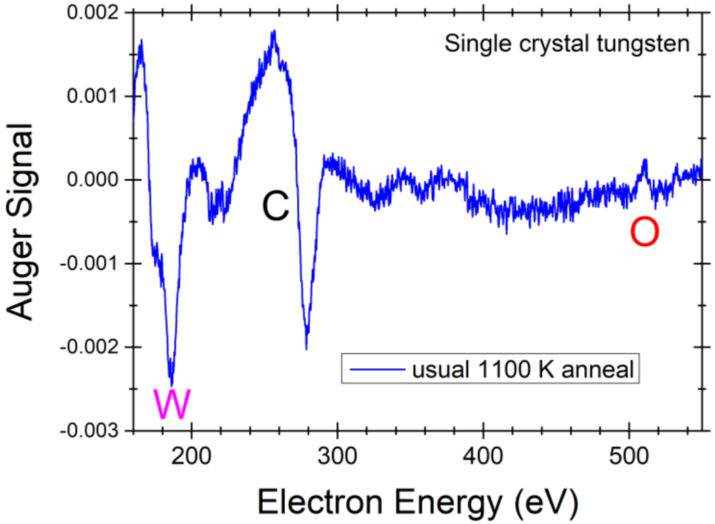
Part 3 : W(110) – the role of the native oxide

W(110):O_xC_y
"native oxide"



- LEED: several crystalline structures + an amorphous background
- AES: presence of C and O in the "native oxide"





Deuterium retention in tungsten

Part 3 : W(110) – the role of the native oxide

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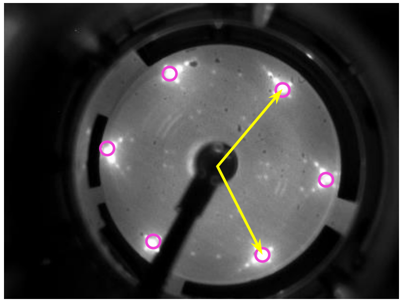

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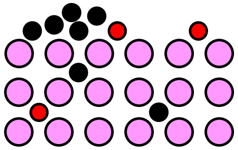

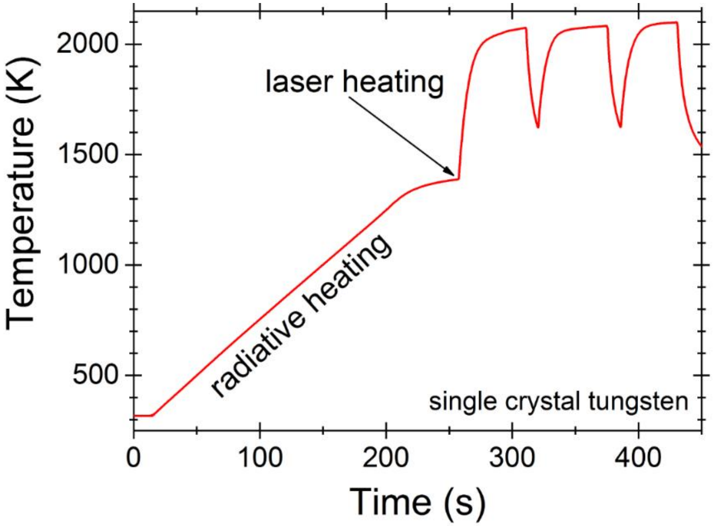

Deuterium retention in tungsten

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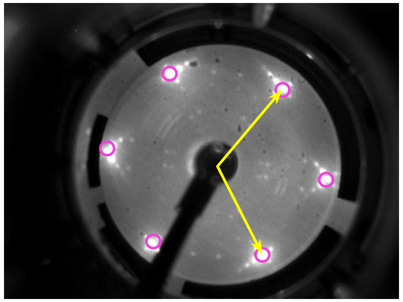

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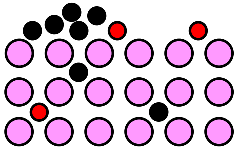
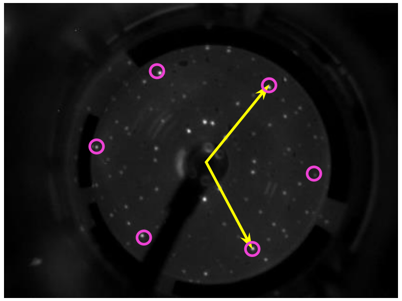
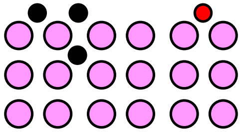
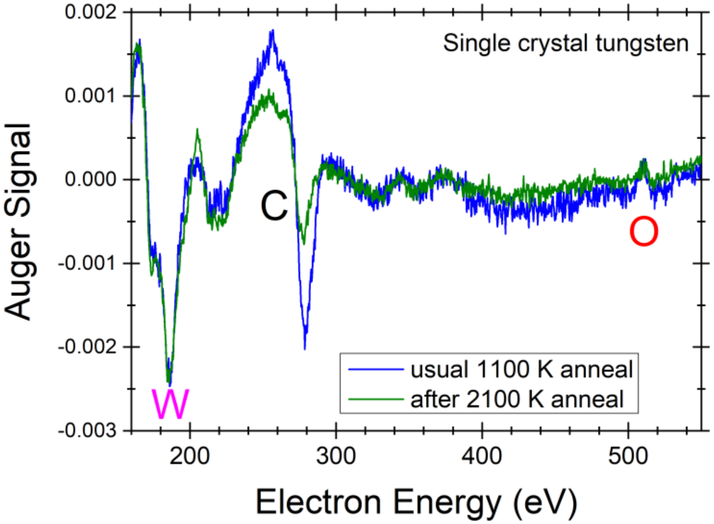


$W(110){:}O_\delta C_{\delta'}$
almost clean



- LEED: disappearance of amorphous background
- AES: still C and O





Deuterium retention in tungsten

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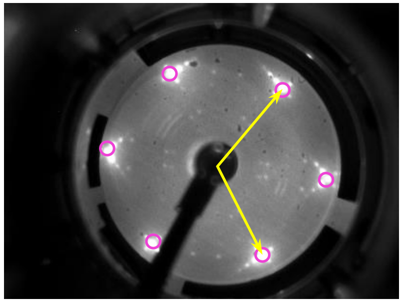

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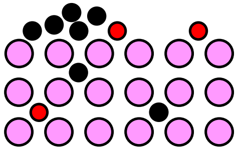

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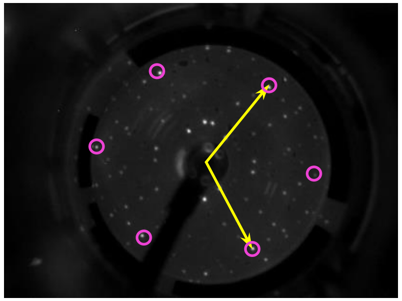

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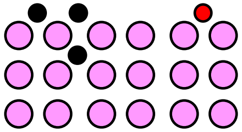
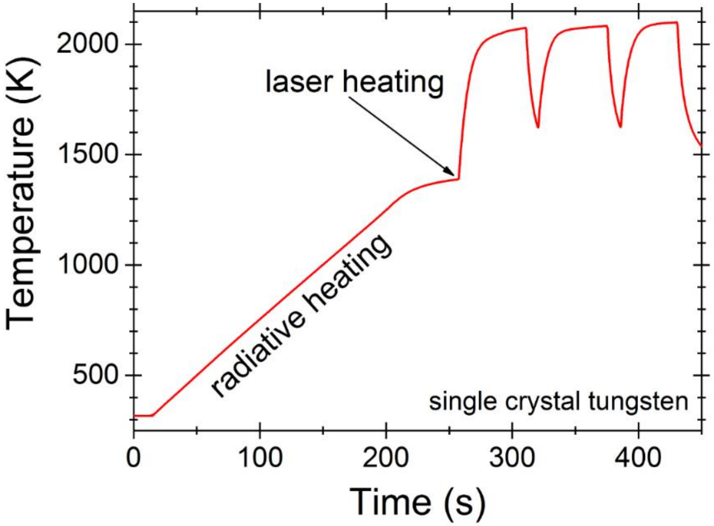
- AES: still C and O



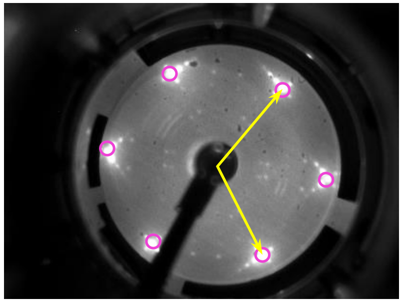


Repeat for a month
(using oxygen atmosphere)
…

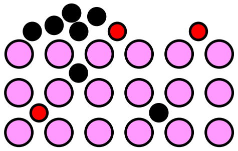
Deuterium retention in tungsten

Part 3 : W(110) – the role of the native oxide

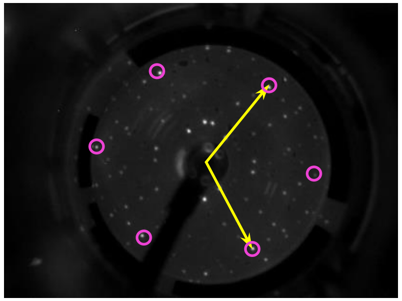
$W(110):O_xC_y$
“native oxide”



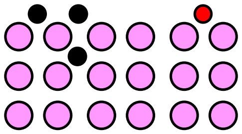
- LEED: several crystalline structures + an amorphous background
- AES: presence of C and O in the “native oxide”



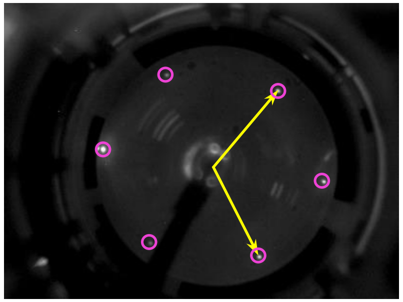
$W(110):O_\delta C_{\delta'}$
almost clean



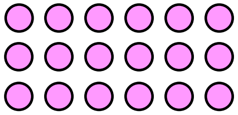
- LEED: disappearance of amorphous background
- AES: still C and O



W(110):clean
(1x1)



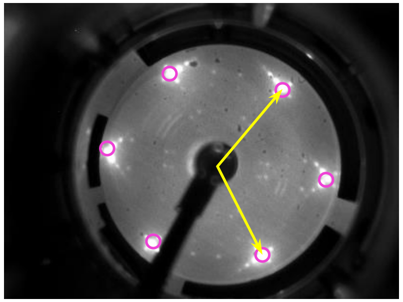
- LEED: 1x1 structure of clean W(110)
- AES: only W



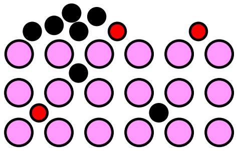
Deuterium retention in tungsten

Part 3 : W(110) – the role of the native oxide

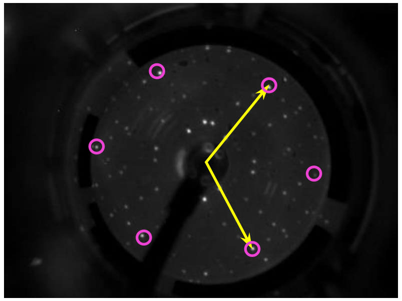
W(110):O_xC_y
“native oxide”



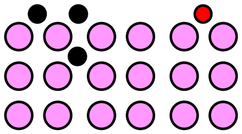
- LEED: several crystalline structures + an amorphous background
- AES: presence of C and O in the “native oxide”



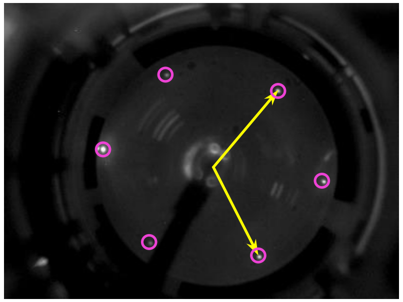
W(110):$O_\delta C_{\delta'}$
almost clean



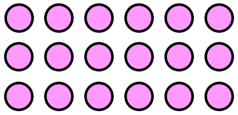
- LEED: disappearance of amorphous background
- AES: still C and O



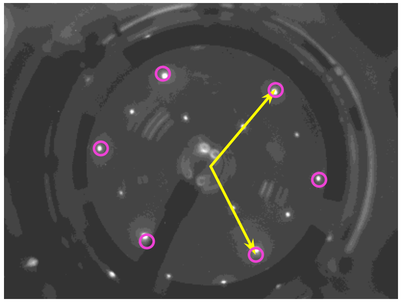
W(110):clean
(1x1)



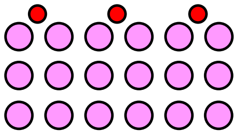
- LEED: 1x1 structure of clean W(110)
- AES: only W



W(110):$O_{0.5}$
(2x1)

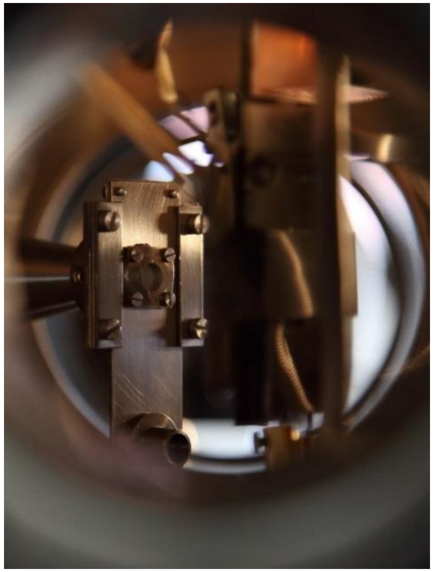


- LEED: 2x1 structure half-monolayer of oxygen
- AES: only W and O

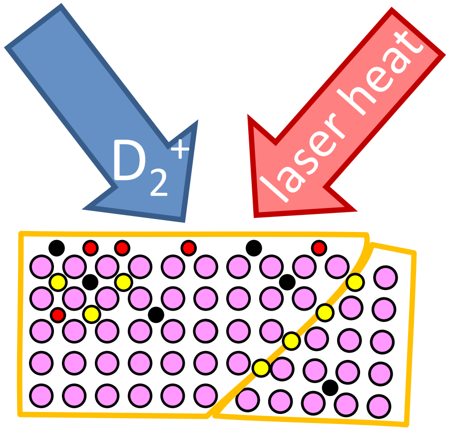


simulating plasma-wall interactions with beam-surface experiments

D retention in polycrystalline W: a fundamental approach



- ✓ 2 rate-limiting steps for D retention/release separated with fast laser heating
- ✓ grain boundaries trap D
- ✓ bulk impurities (O+C) trap D
- ✓ sub-monolayer O reduces D trapping at the surface
- ? What about D retention in pure thick tungsten oxides?
- ? What about D retention with C impurity (ubiquitous in bulk W + surface segregation) ?



thank you for your attention

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