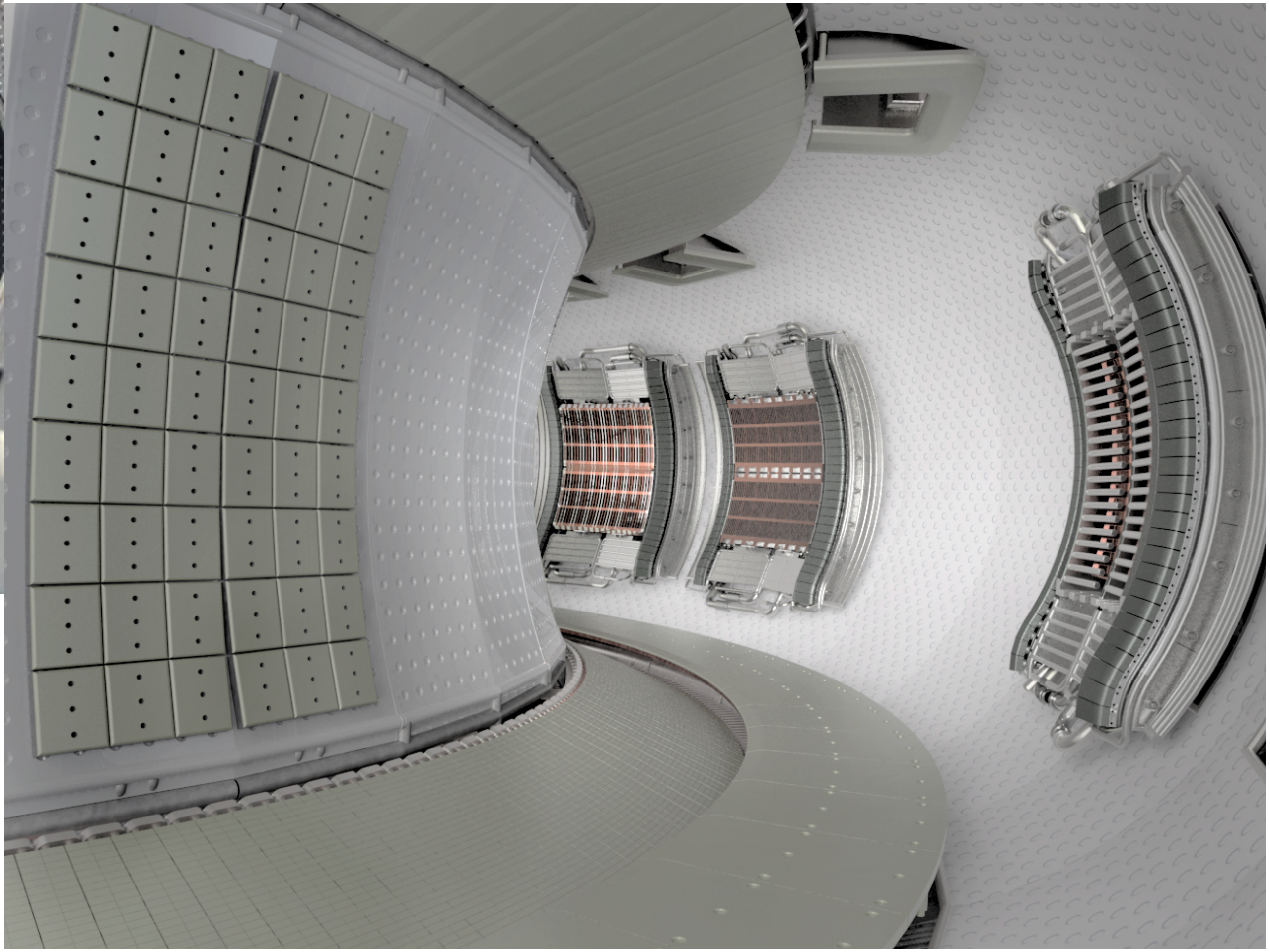
MODELING OF TRAPPING/DETRAPPING OF HYDROGEN ISOTOPES IN TUNGSTEN MATERIALS

WHISCI modeling TEAM
(CS Becquart, R Bisson, N Fernandez, Y Ferro, C. Grisolia, E. Hodille, J Mougenot)

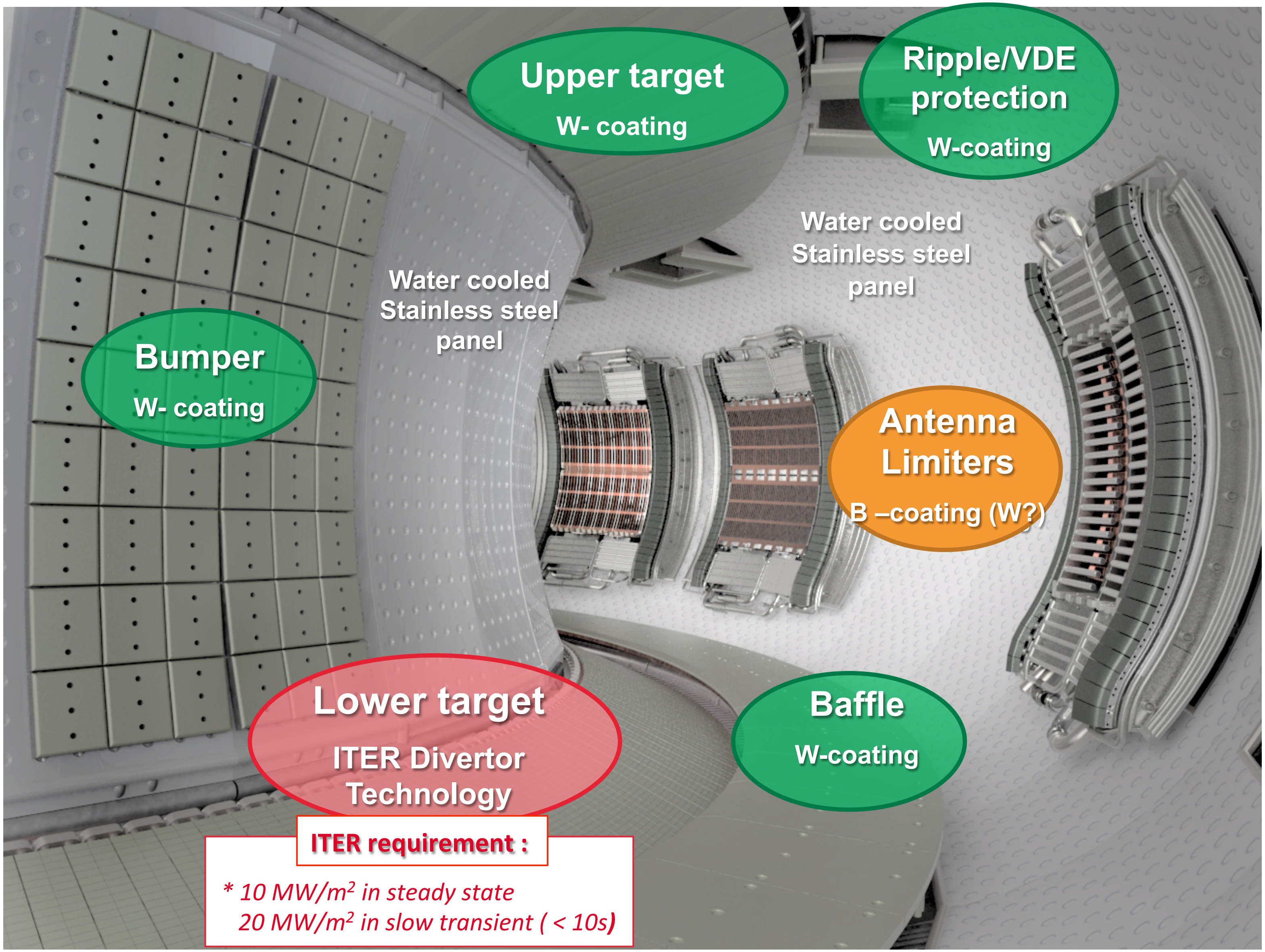
TORE SUPRA going WEST

CIEL configuration



WEST configuration

WEST Plasma Facing Components : full metallic actively cooled environment



ITER requirement :

* 10 MW/m² in steady state
20 MW/m² in slow transient (< 10s)

WEST plasma scenarios

- **H1 : testing ITER PFC**
  Long pulse 10-20 MW/m²
- **H3 : high fluence**
  ITER fluence in a few days of operation
- **H4 : high power**
  Shorter pulse towards hybrid scenarios

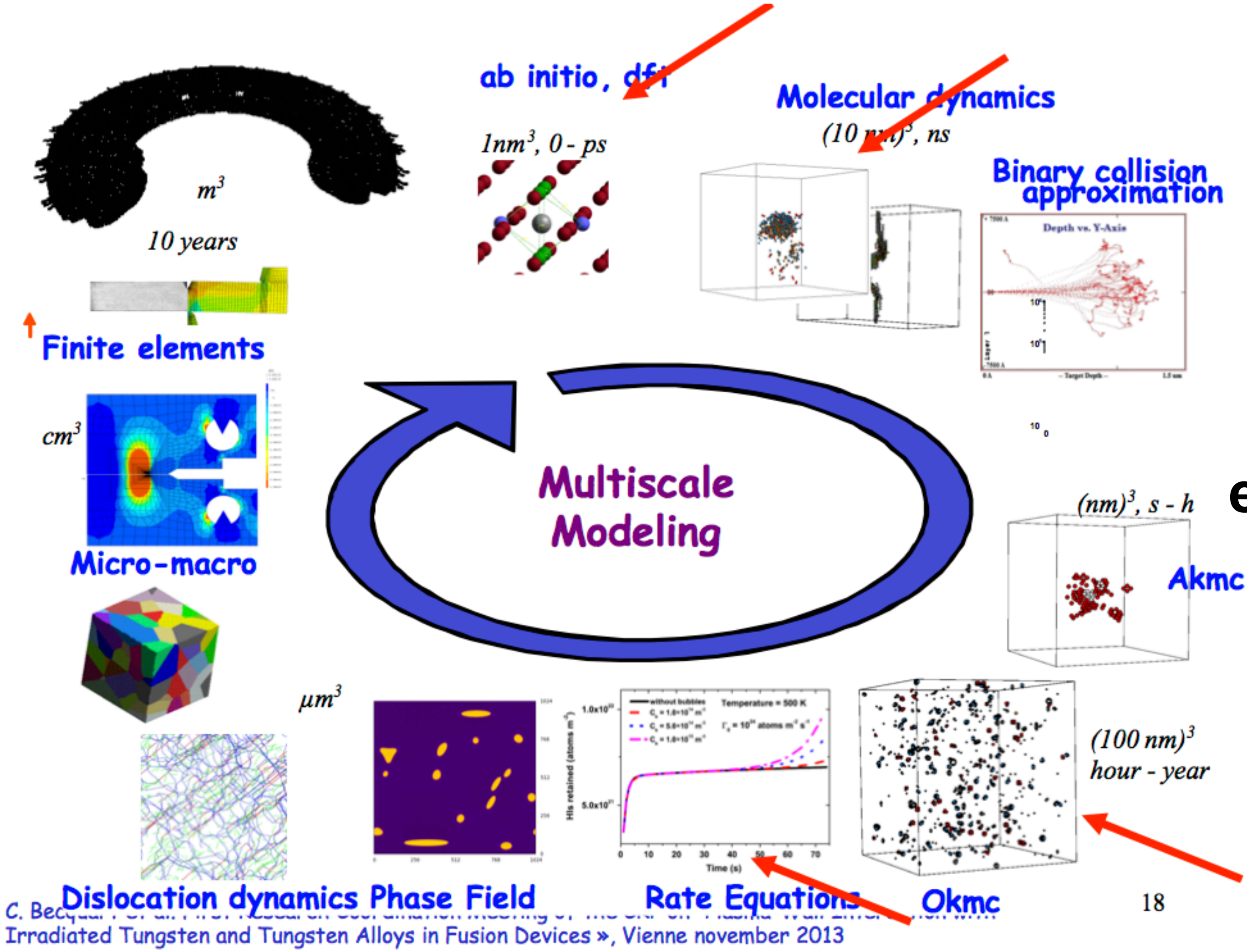
SCENARIO (3.7 T)	HIGH POWER H4	STANDARD H1	HIGH FLUENCE H3
Plasma current	**0.8 MA**	**0.6 MA**	**0.5 MA**
Plasma density	9 $10^{19} m^{-3}$	6 $10^{19} m^{-3}$	4 $10^{19} m^{-3}$
Total radiofrequency heating power	**15 MW**	**12 MW**	**10 MW**
Lower Hybrid Current Drive	6 MW	6 MW	7 MW
Ion Cyclotron Resonance Heating	9 MW	6 MW	3 MW
Plasma current flat-top duration	**30 s**	**60 s**	**1000 s**
Expected heat load*	**10 MW/m²**	**10-20 MW/m²**	**10-20 MW/m²**
Expected ELM frequency	59 Hz	76 Hz	77 Hz
Expected ELM load	40 kJ/m²	52 kJ/m²	74 kJ/m²
Expected operation time to reach one ITER pulse particle fluence	**~6 months**	**~2 months**	**~few days**

H2

- **H2 : long pulse H mode**
  Pre-requisite for the programme

Ion flux: 10^{22} 10^{23} D/s m²

CRP VIENNA 2013, PROPOSED APPROACH



+

crosscheck with experimental data

THE WHISCI PROJECT:
W/H INTERACTION STUDIES IN A COMPLETE AND INTEGRATED APPROACH

WHISCI – Predict and control Tritium/Deuterium trapping/degasing

Real/Complexity

Models	Experiments
macroscopic « Rate Equations (RE) + Finite Element Methods (FME)»	Realistic wall « ITER-WEST grade»
mesoscopic « Object Kinetic Monte Carlo (OKMC) »	Semi-realistic wall « polycrystals (controlled defects)»
microscopic « Density Functional Theory (DFT) »	Model wall « single crystals(controlled defects)»

Model/Understanding

Multi-scale modeling validated by well controlled laboratory experiments

Coordinator: Regis Bisson (PIIM Laboratory)

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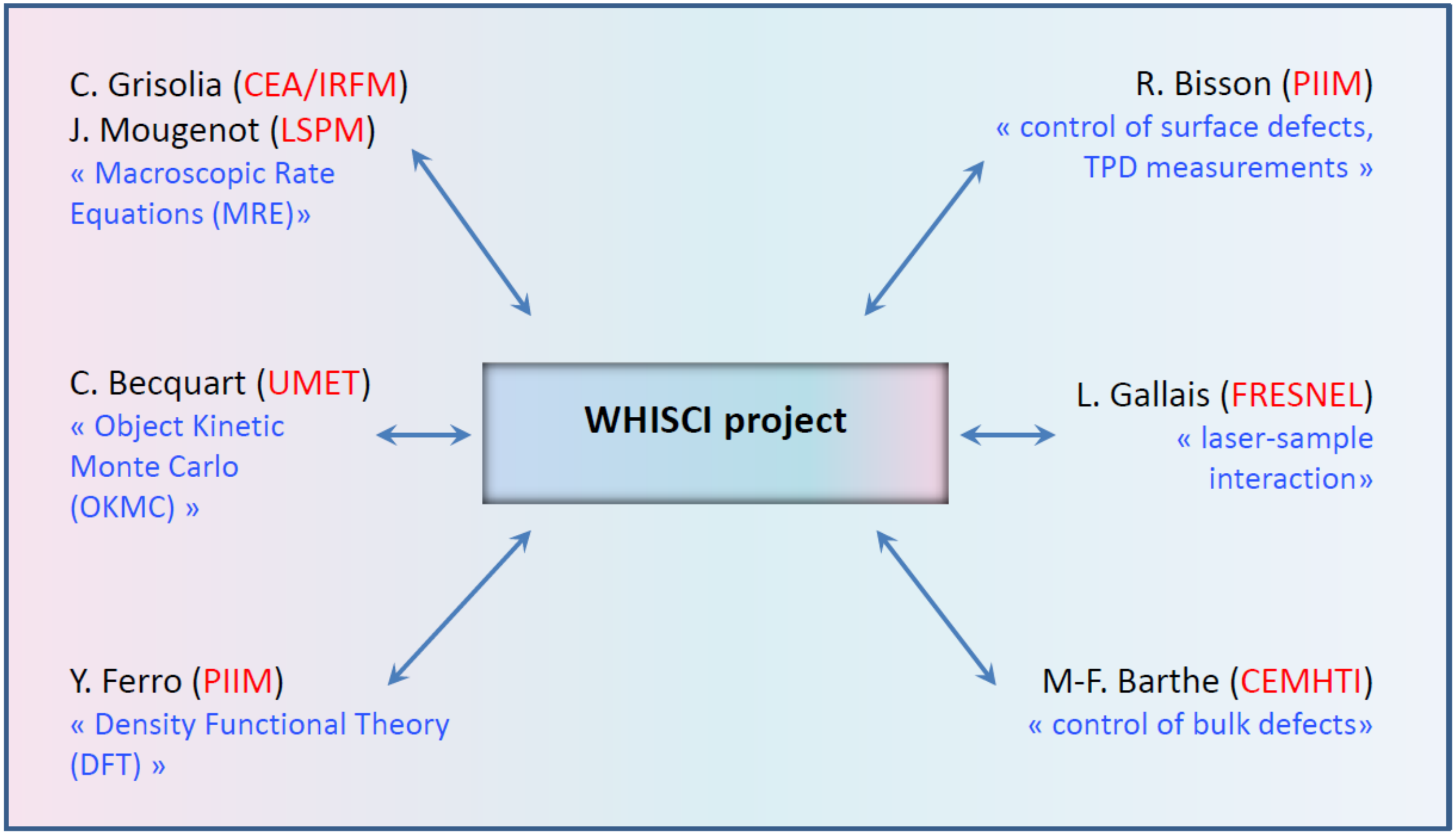

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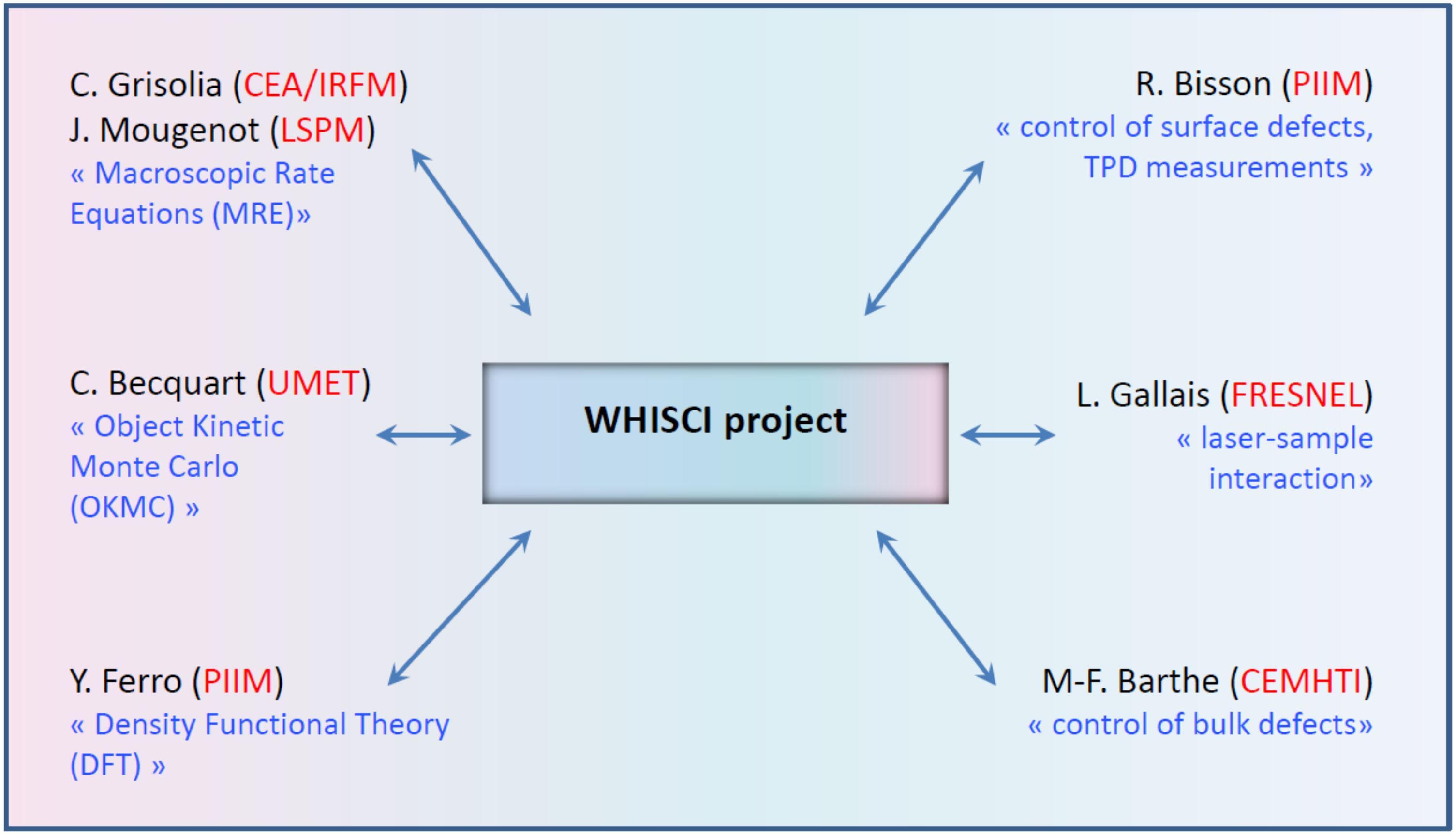

Strong and constant interactions in place
(starting 3 years ago)

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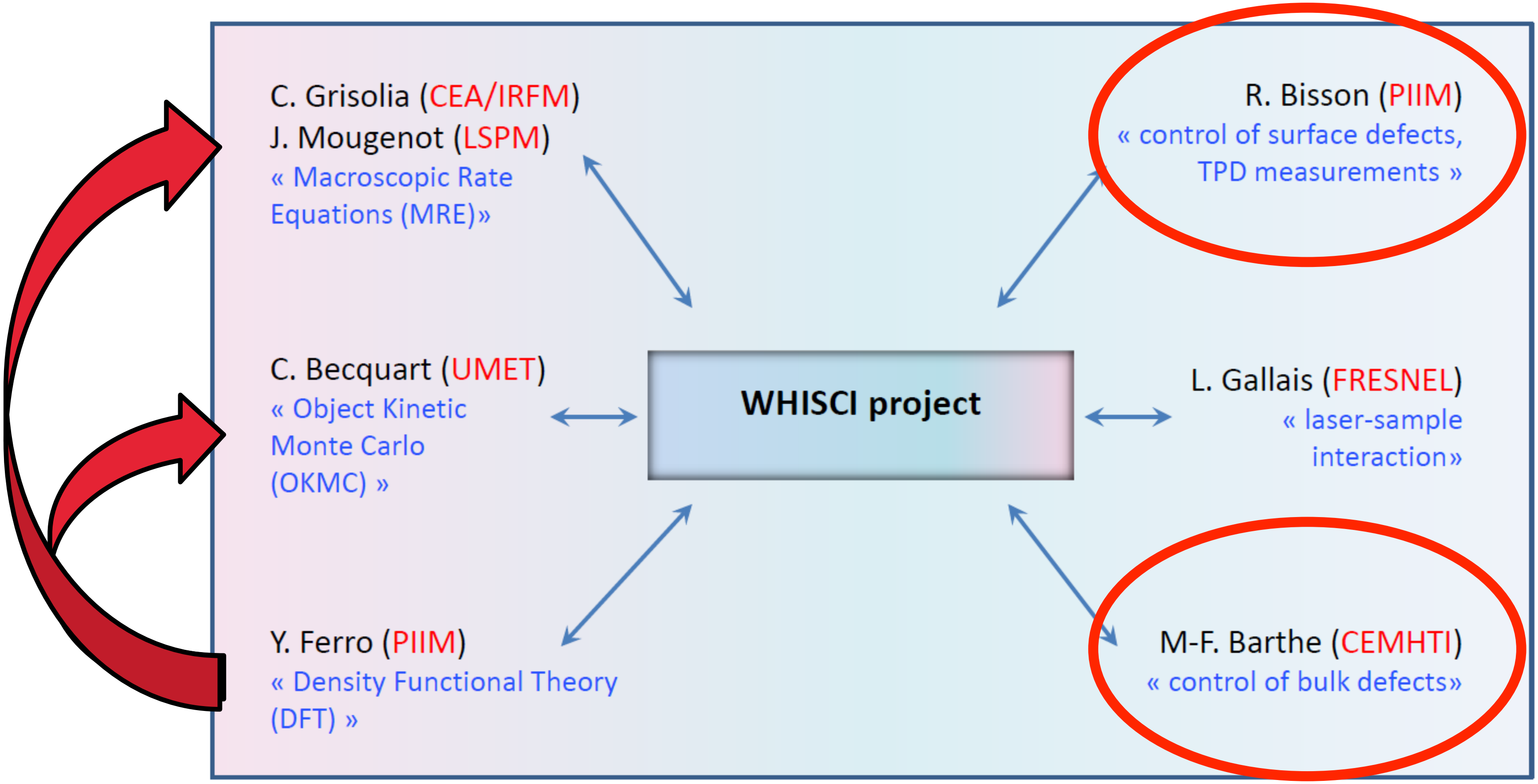

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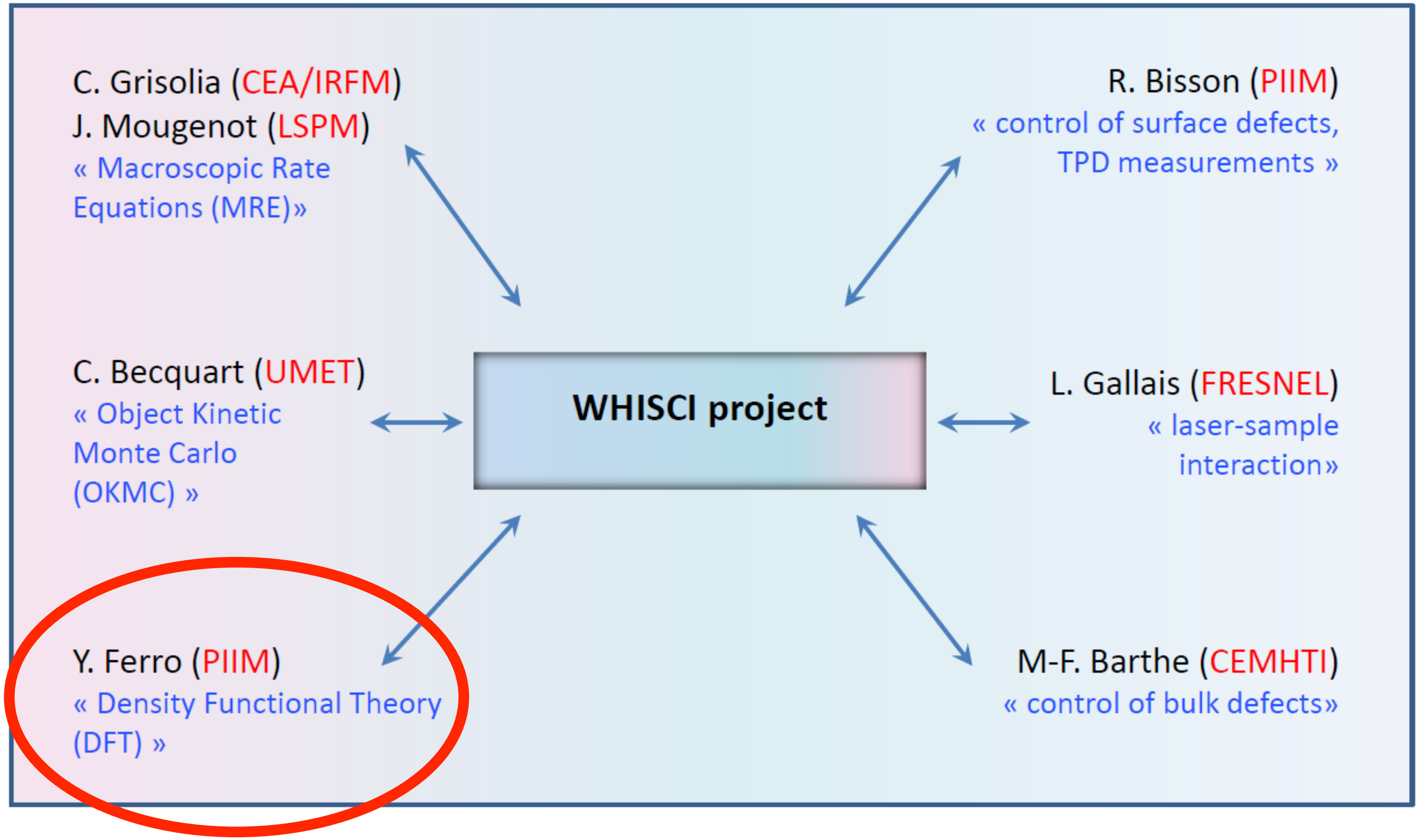


DFT: H TRAPPING IN VACANCIES

DFT results presented here are deeply detailed in:

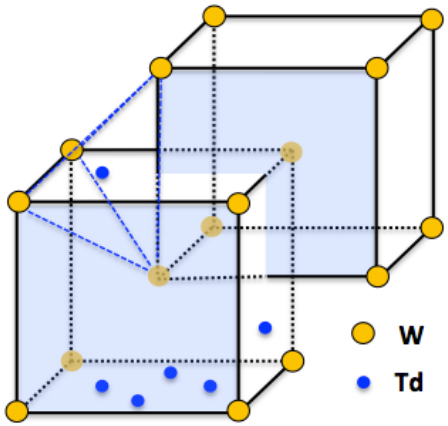
"**Hydrogen diffusion and vacancies formation in W: Density Functional Theory calculations and statistical models**", N Fernandez, Y Ferro, D Kato,
Acta Materialia, 94 (2015) 307

Small number of atoms (54 atoms)

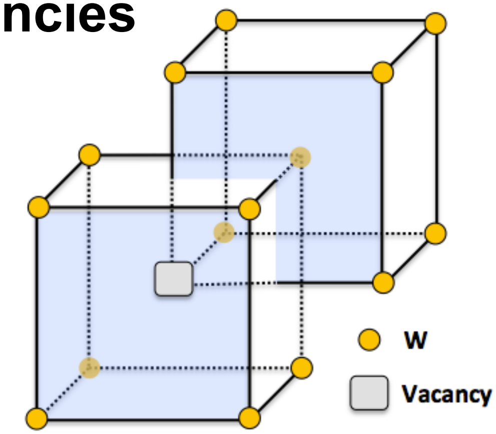
Pure Single Crystal (where vacancies can be introduced)

Up to now, no surface effects (implementation in progress)

H interstitial as solute

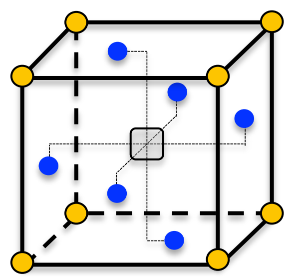


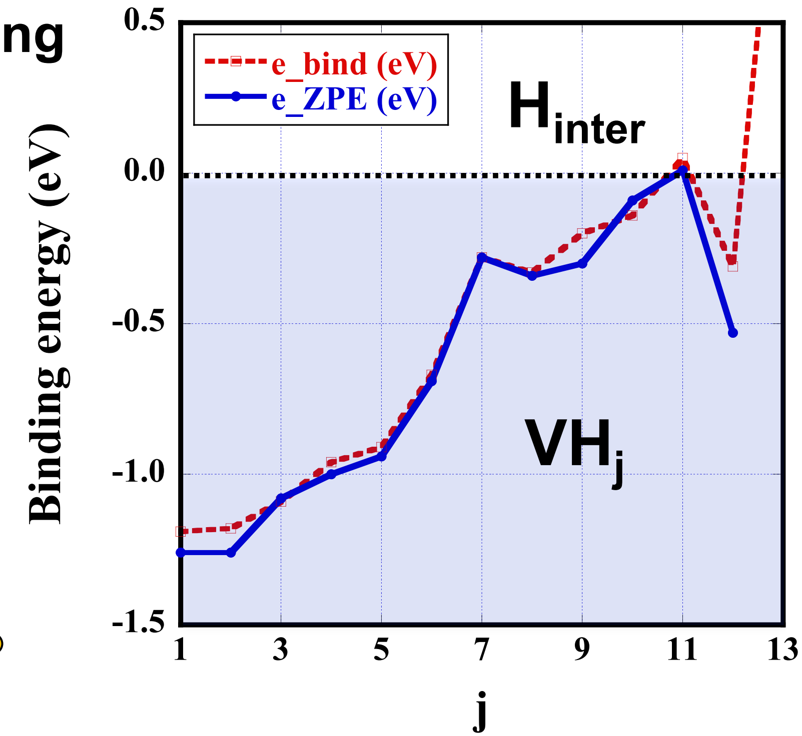
Vacancies



Multi-trapping

VH_6





Up to 12 H atoms in a vacancy

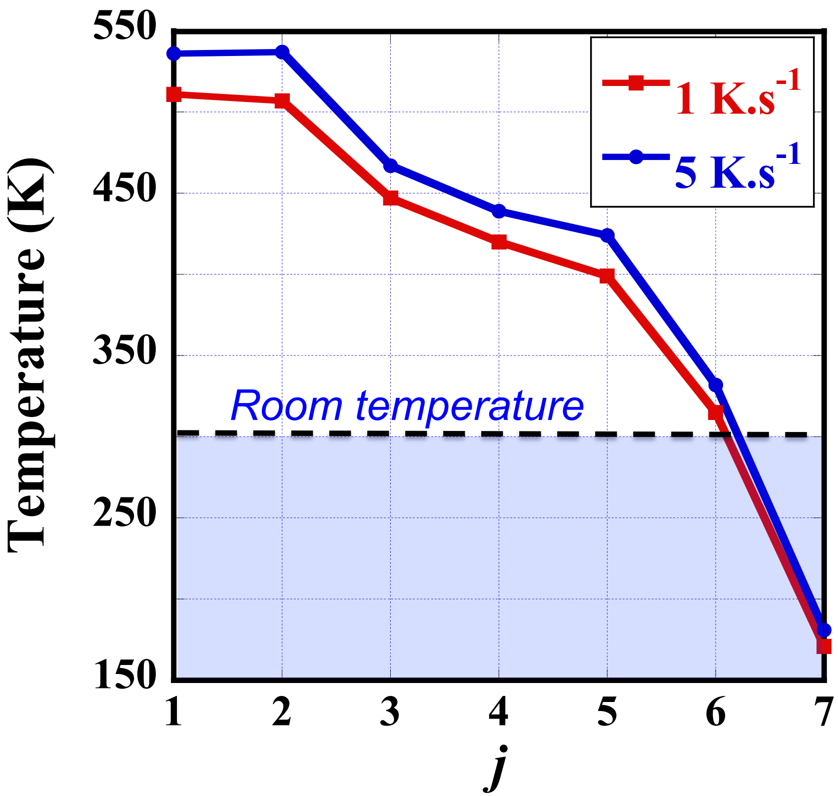
DFT: FILLING LEVEL AT ROOM TEMPERATURE

DFT results obtained at 0K

Using kinetic modeling, it can be also shown that during a Thermo-desorption experiment:

Desorption T at peak maximum

$\beta = 1Ks^{-1}$	6H	5H	4H	3H	2H	1H
E^{des} (eV)	0.86	1.11	1.17	1.25	1.42	1.43
T_{max} (K)	311	399	420	447	507	511

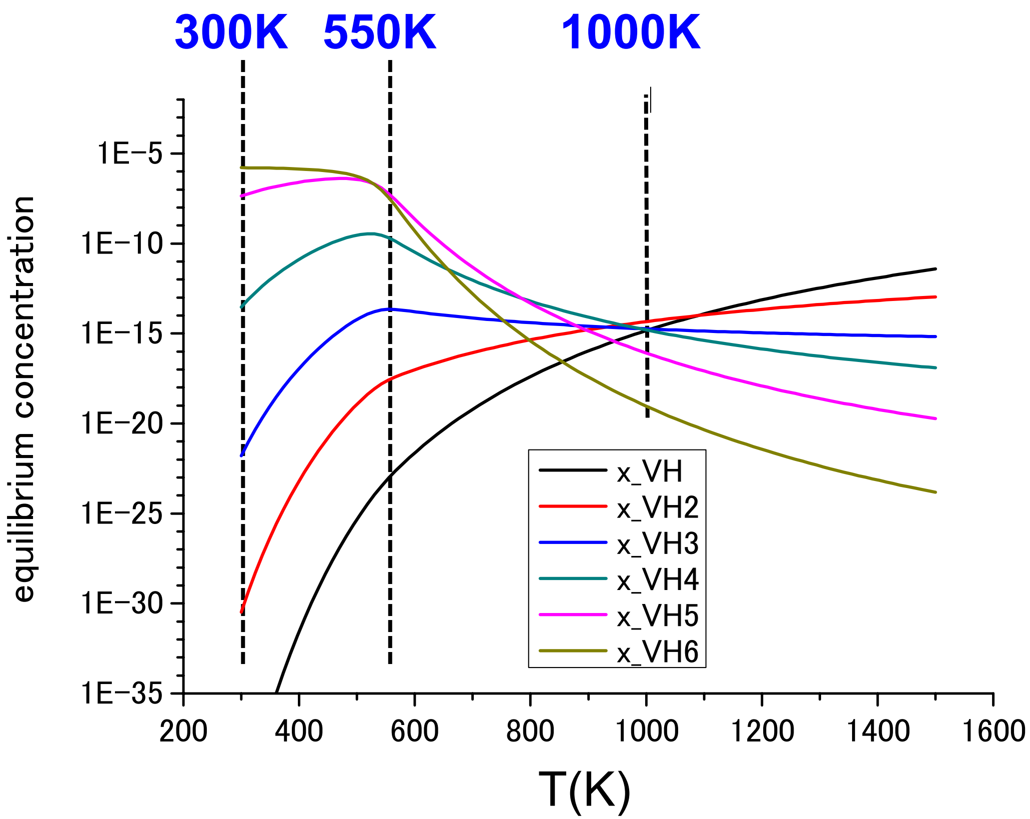


Filling level at RT: VH6

DFT: VHj VACANCIES FRACTION

Perfect crystal submitted to a H flux up to H concentration: 10^{-5} (≅10^{22} D m^2/s)

➔ **VH_j fractions at Thermo Equilibrium**



VHj fractions

- 300K<T<550K – **VH_6**
- 550K<T<1000K – **pop. Inverted**
- T>1000K – vacancies depopulated

DFT: MODELLING THERMO-DESORPTION WITH A CRUDE MODEL

Simple kinetic model:

- diffusion is neglected (0.2eV)
- the surface of the sample is neglected
- hydrogen is assumed to desorbed as released from a vacancy type VH_j
- kinetics of order one are assumed

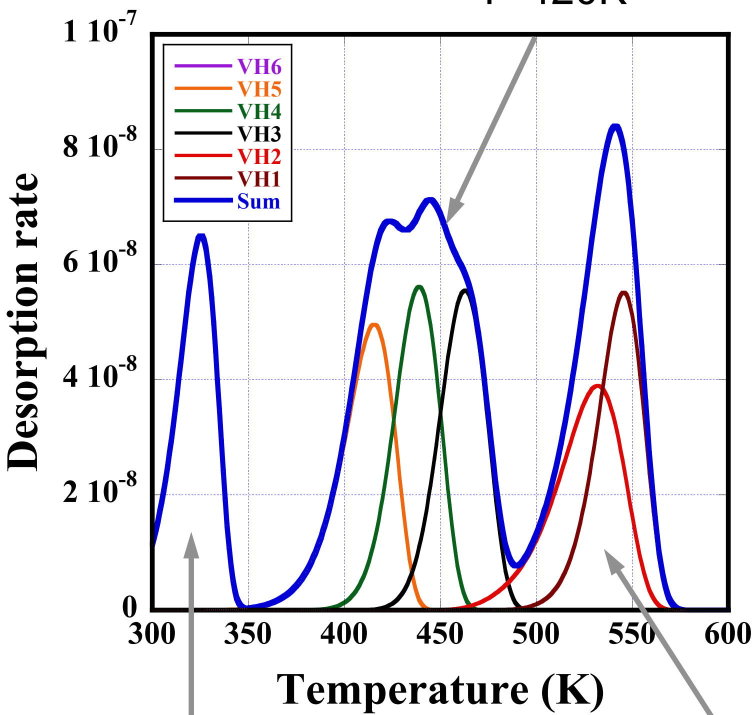
TDS conditions:

- H implantation T=300K
- VH_j fraction from stat. model
- β=5Ks^{-1}
- 0.85 10^{13} Hz < ν < 1.45 10^{13} Hz

DFT: MODELLING THERMO-DESORPTION WITH A CRUDE MODEL

Low temperature peaks

VH3-5
T=420K



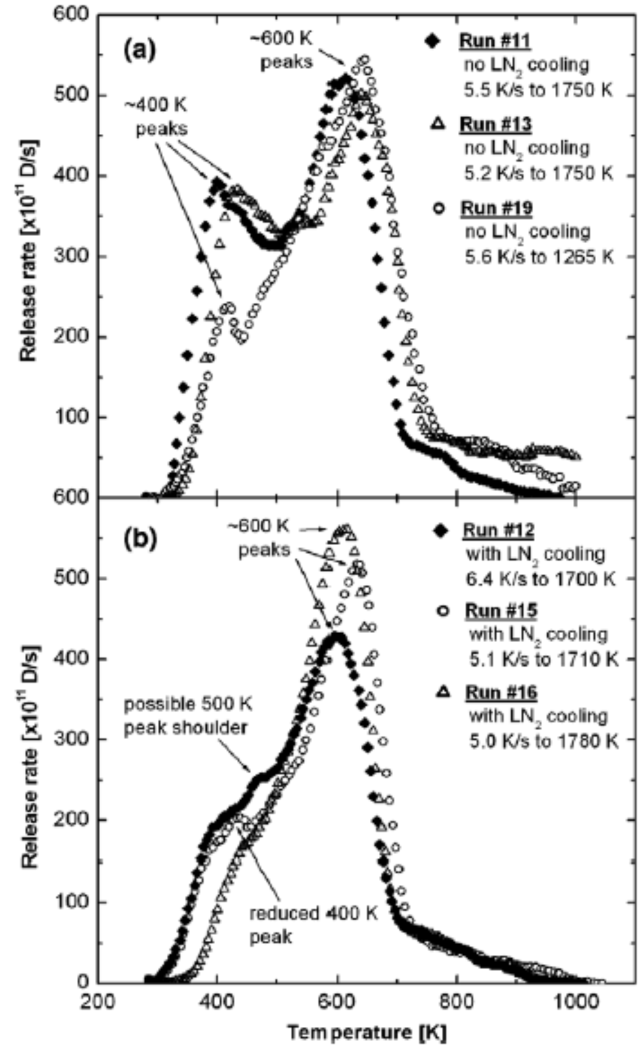
VH6
Not observed
Already desorbed

High temperature peaks

VH1,2
T=540K

Exp.

TDS peaks include desorption from multiple VH_j traps



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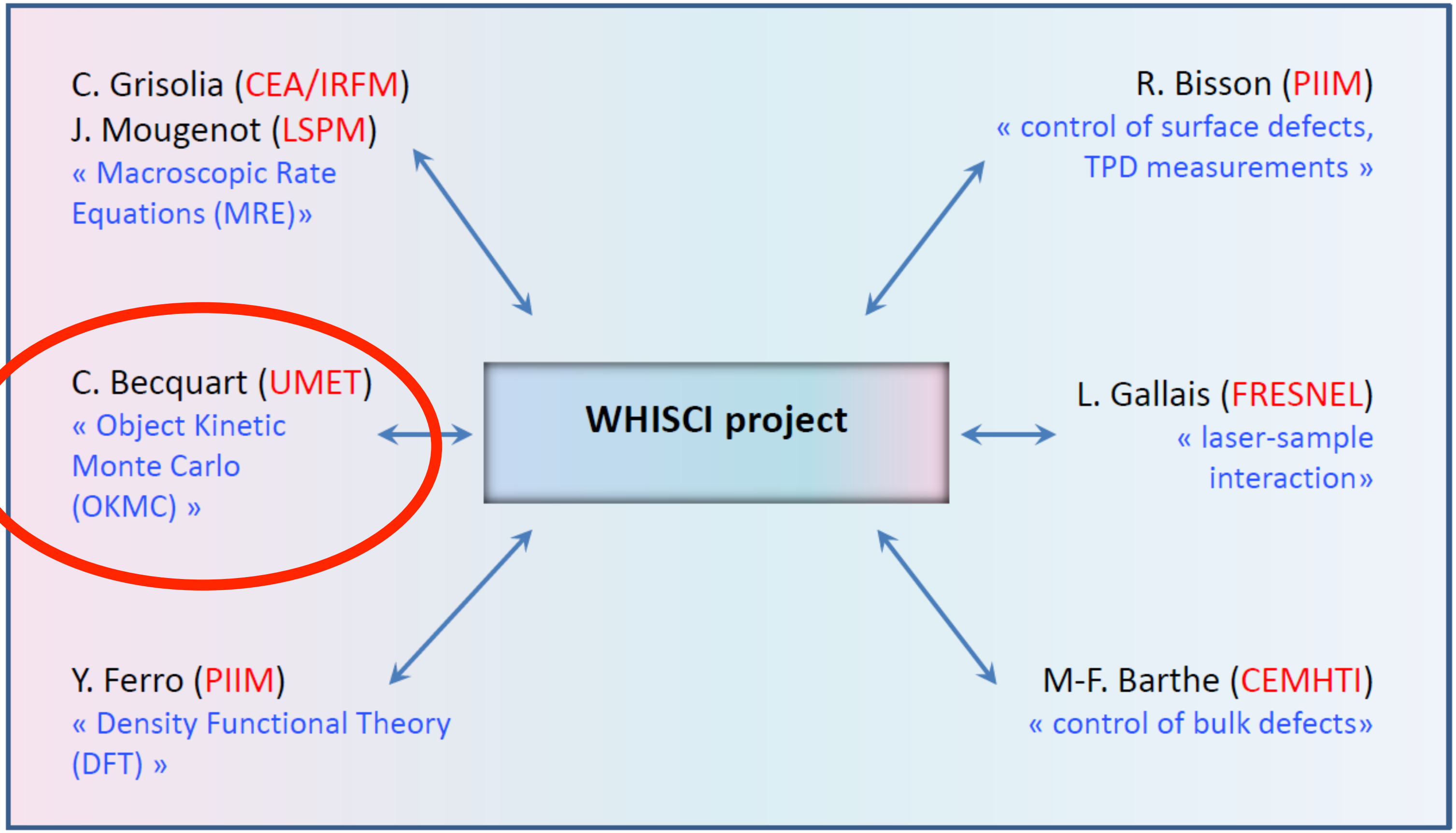
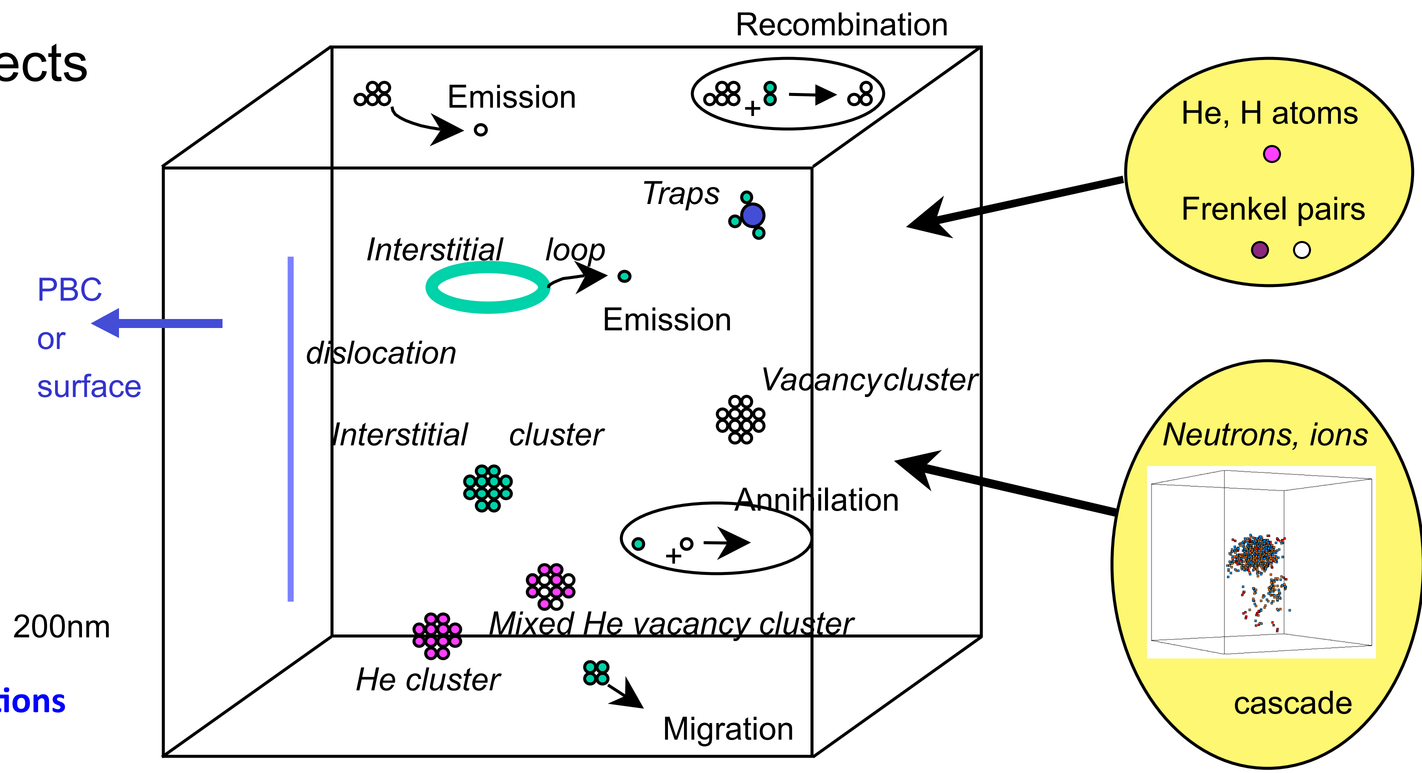
Multi-scale modeling validated by well controlled laboratory experiments



Object Kinetic Monte Carlo

Microstructure = objects defined by:

- type
- centre-of-mass position
- reaction radius
- possible reactions



PBC : periodic boundary conditions

Large box: 330nm of depth (see end of presentation)

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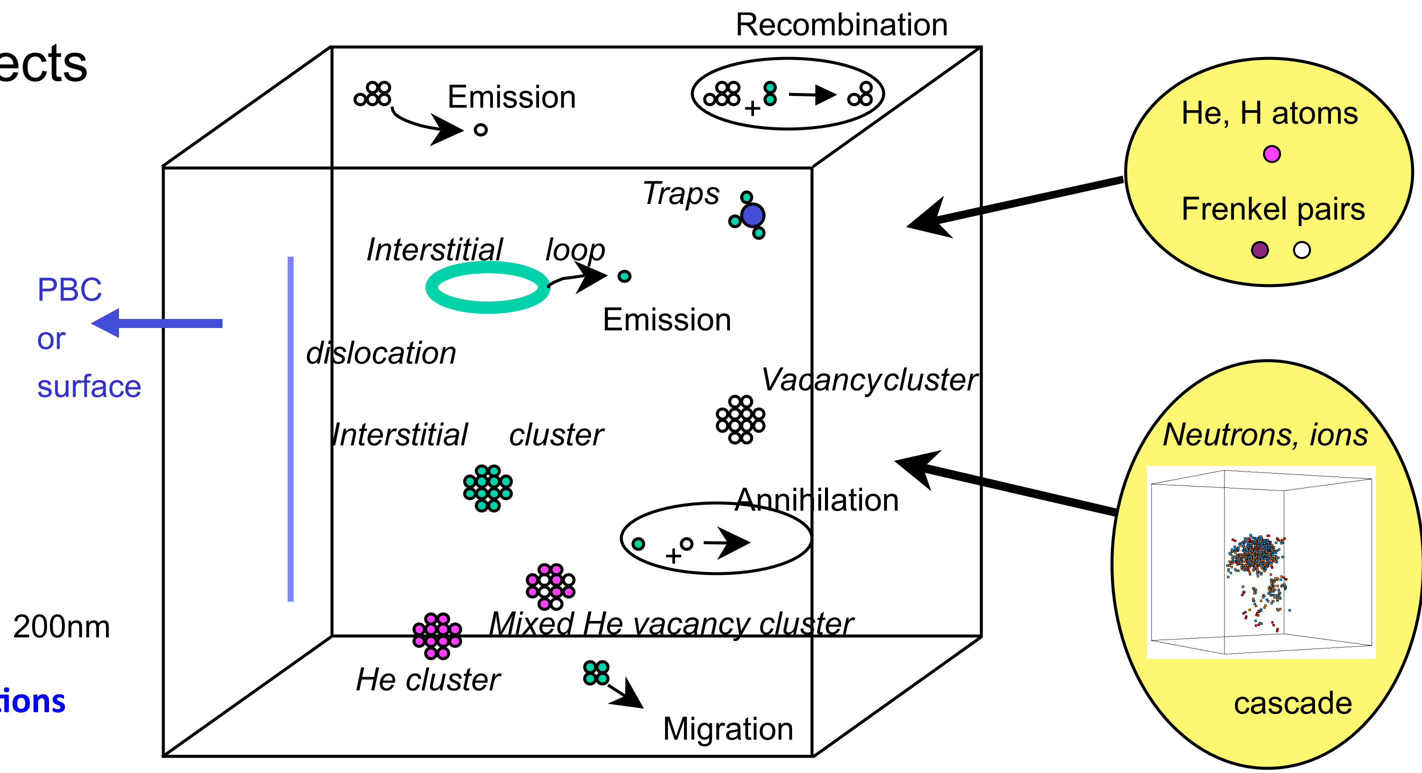

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Internal events: migration of the objects, emission from the objects or capture

External events: H / He implantation, neutron irradiation…

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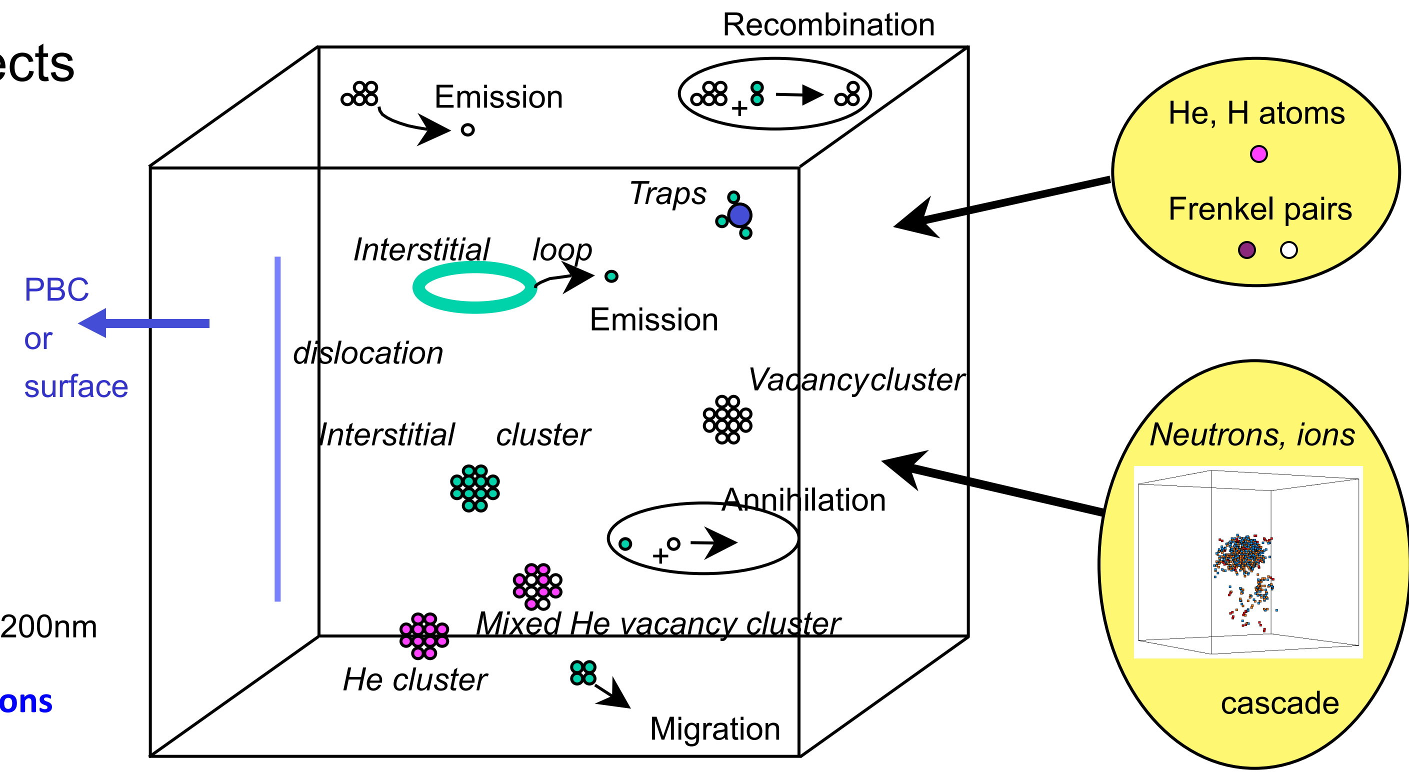

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Internal events: migration of the objects, emission from the objects or capture

External events: H / He implantation, neutron irradiation…

Objects that we can encounter in the OKMC box:
- vacancies, intersitials, impurities, dislocations, grain boundaries, helium atoms, ...
- If they can form clusters, these clusters are a different object: i.e. a cluster which contains 3 vacancies and one H atom is an object.

Object Kinetic Monte Carlo

What can we obtain ?

A description of the microstructure in terms of positions of the objects in the volume and concentration

So we can model a desorption experiment for instance

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For all the objects that can move, we need their diffusion coefficient:

activation energy/migration barrier : Emig

How can we obtain them ?

- **Emig** from **DFT**, from experimental results, … tuning parameters adjusted on experimental data one this is possible. So we need the diffusion coefficient of the mono-vacancy, the di-vacancy, the tri-vacancy and so on ……

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For all the objects that can emit:

a di-vacancy can emit a vacancy, a tri-vacancy containing 2 hydrogen atoms can emit either a vacancy or an hydrogen atom, a grain boundary can trap an intersitial or an hydrogen atom and re-emit it, etc…)

we need the **binding energy** of the emitted species with the object.

How can we obtain them ?

From **DFT** for small objects, from experimental results, … tuning parameters adjusted on experimental data one this is possible

Object Kinetic Monte Carlo

OKMC is a tool that can be used to « check » the data obtained from DFT.
For instance if DFT predicts that H migration energy is XXX eV, we plug this value into OKMC and see whether H desorption takes place at the right temperature …

I will come back to code comparaison at the end of this presentation

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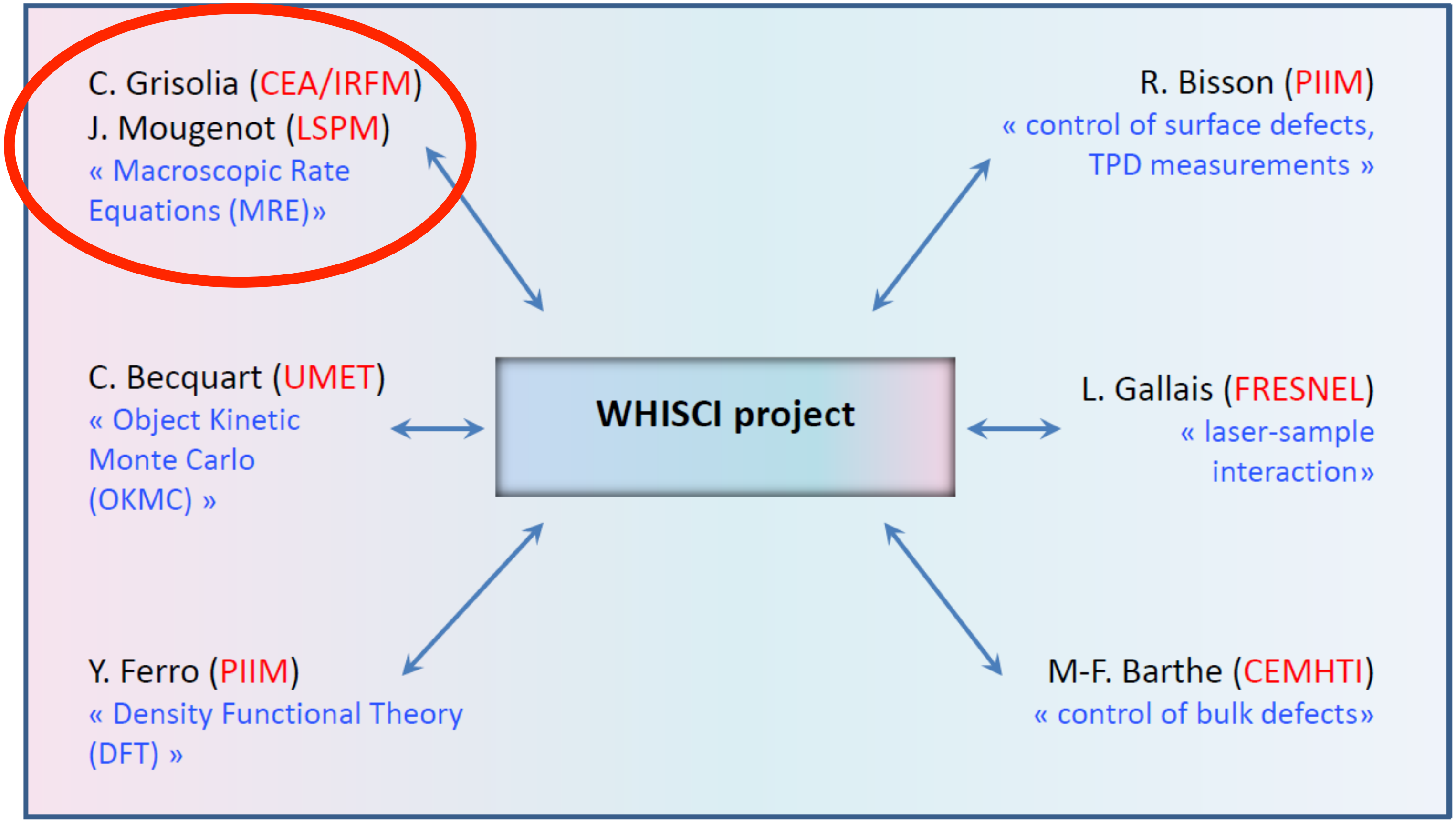

MACROSCOPIC RATE EQUATION (MRE) APPROACHES

MRE

- Usual one
- developed to fit experimental data coming from polycrystal experimental studies
- Check parameters, … without any link with physical processes
- Approach is an "engineer" one

MHIMS code

(Migration of Hydrogen Isotopes in MetalS)

- New one
- Linked to the DFT approach
  - Used to integrated the DFT outcomes
- Up to now, fit single crystal experimental data

MHIMS-reservoir

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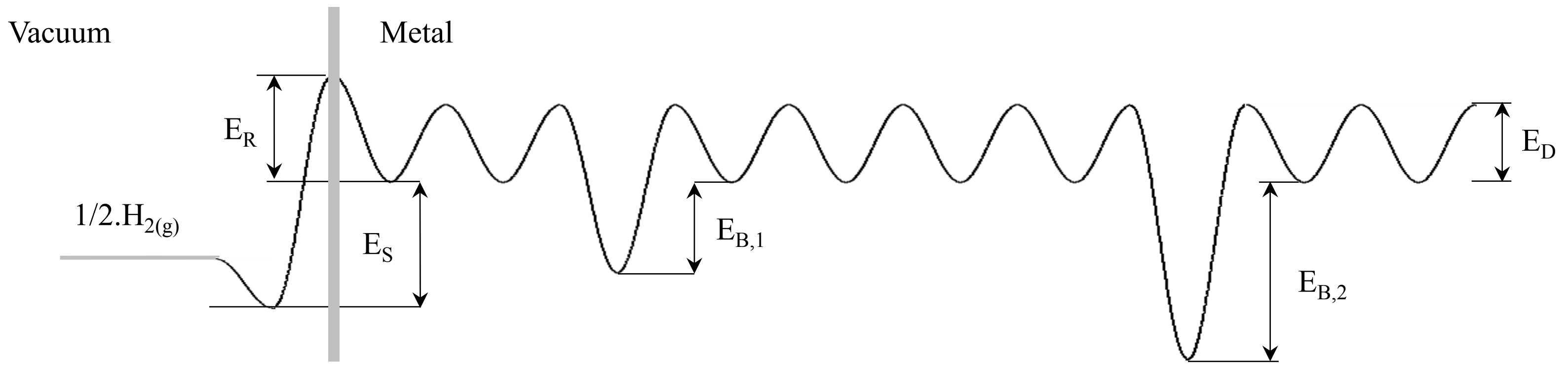
USUAL MRE APPROACH

Energy diagram of HIs in tungsten (W)

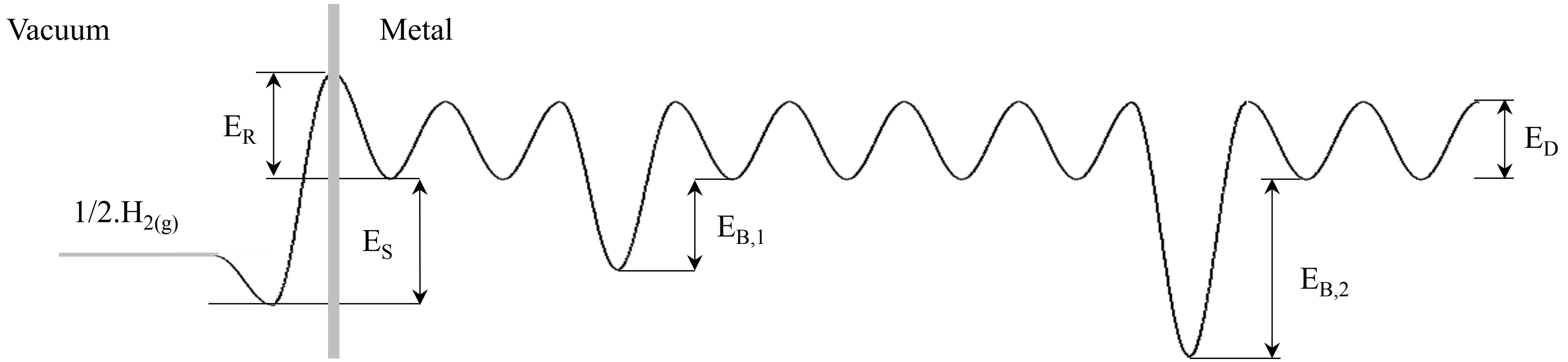


- E_S = solubility activation energy
- E_D = Diffusion activation energy
- $E_{T,i} = E_{B,i} + E_D$ detrapping activation energy. Trap = vacancies, grain boundaries …
- E_R = recombination activation energy

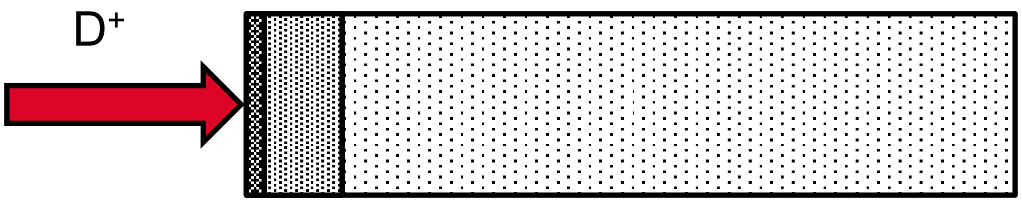
One trap of E_B trapping energy contents one H atom

USUAL MRE APPROACH

Energy diagram of HIs in tungsten (W)



Concentration and types of traps (from IBA)



<u>Induced traps</u>

- **In stopping zone: high concentration, due to collisions**
- **Up to 1μm, relatively high concentration due plastic deformations, vacancies diffusion ,…**

<u>Intrinsic traps</u>

In the bulk,
Low concentration

USUAL MRE: MODEL DESCRIPTION

MRE 1D modeling

$$\frac{\partial C_{t,i}}{\partial t} = -C_{t,i} \cdot \nu_i(T) + \nu_m(T) \cdot C_m \cdot \left(1 - \frac{C_{t,i}}{n_i}\right)$$

$$\frac{\partial C_m}{\partial t} = \mathrm{D}(T) \cdot \frac{\partial^2 C_m}{\partial x^2} - \sum \frac{\partial C_{t,i}}{\partial t} + S_{ext}$$

trapped particles ⇔ **mobile particles**

- ***n_i*:** trap density (intrinsic and created by incident ions)
- **D(T)**: diffusion coefficient (m²/s)
- $\nu_i(\mathrm{T})$: detrapping attempt frequency $\nu_0 = 10^{13}\ s^{-1}$
- $\nu_m(\mathrm{T})$**:** trapping attempt frequency. $\nu_m \propto D(T).n_i$
- ***S_{ext}*** = particles source by implantation

$$S_{ext} = (1-r).\varphi.f(x)$$

r: reflexion coefficient of HI on W, *f(x):* ions stopping range (both given by TRIM)
φ: incident ion flux

USUAL MRE: MODEL DESCRIPTION

Boundary conditions

- **Desorption no limited by recombination:**

$$C_m(x = 0, L) = 0$$

Experimental evidence of a desorption non limited by recombination [1, 2]

[1] R. A. Causey, J. Nucl. Mater. (2002)

[2] R. Bisson et al., J. Nucl. Mater. (2015)

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TDS simulation in 3 phases

- Implantation (initially empty): T_{imp}, E_{imp}, φ
- *"resting"* phase: T_{rest}, t_{rest}
- TDS phase: $T(t) = T_{rest} + \beta . t$ β: heating ramp (K/s)

MHIMS Code (Migration of Hydrogen Isotopes in Metals)

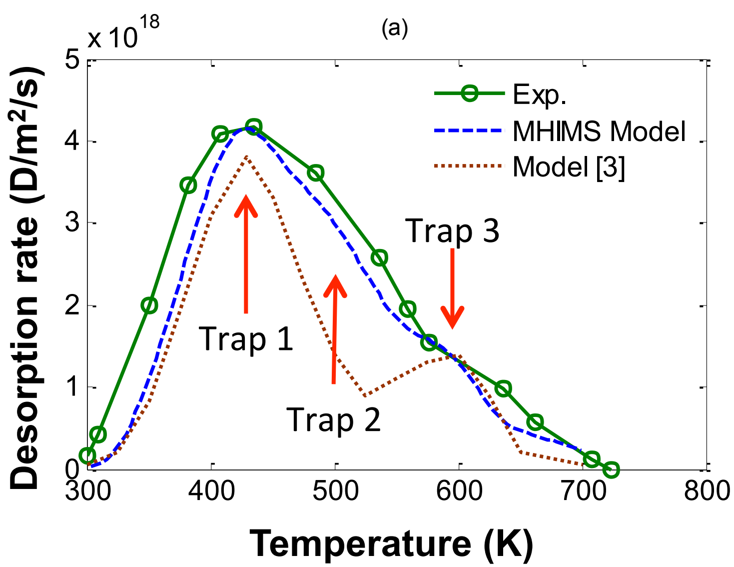
"Macroscopic rate equation modeling of trapping/detrapping of hydrogen isotopes in tungsten materials", E Hodille et al, JNM, 2015, doi:10.1016/j.jnucmat.2015.06.041

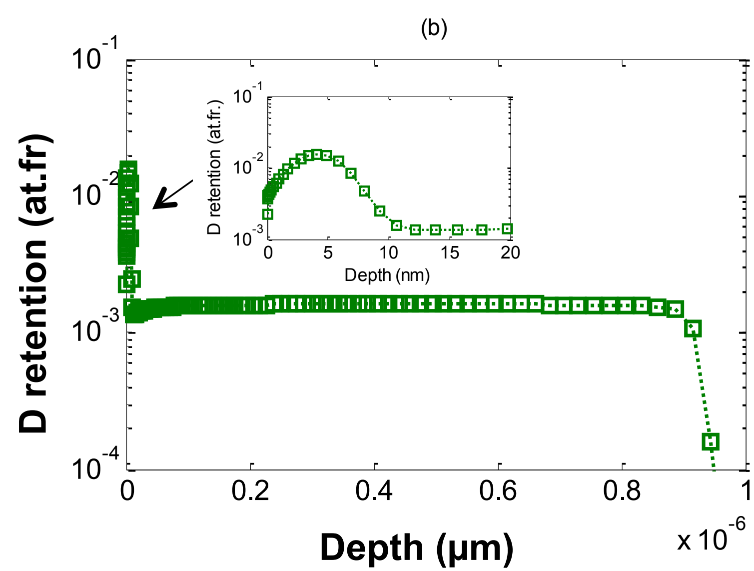
FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL

Fit of experimental TDS data

- **Input implantation and TDS parameters:**
  - E_{imp} **= 200 eV/D (r = 0,56),**
  - φ **= 2,5×10^{19} D.m^{-2}.s^{-1},**
  - $T_{imp} = T_{rest}$ **= 300 K,**
  - ***fluence*** **= 10^{22} D.m^{-2},**
  - t_{rest} **= 50 s,**
  - β **= 8 K/s.**

- **Input trapping parameters with $\nu_0 = 10^{13}$ s^{-1}:**
  - **trap 1 (intrinsic): $E_{T,1}$ = 0.87 eV (0,85), $n_1 = 1\times10^{-3}$**
  - **trap 2 (intrinsic): $E_{T,2}$ = 1.00 eV, $n_2 = 4\times10^{-4}$**
  - **trap 3 (extrinsic): $E_{T,3}$ = 1.5 eV (1.45) n_{3max}= 2x10^{-2}**
    Irradiation induced trap (∝ fluence)

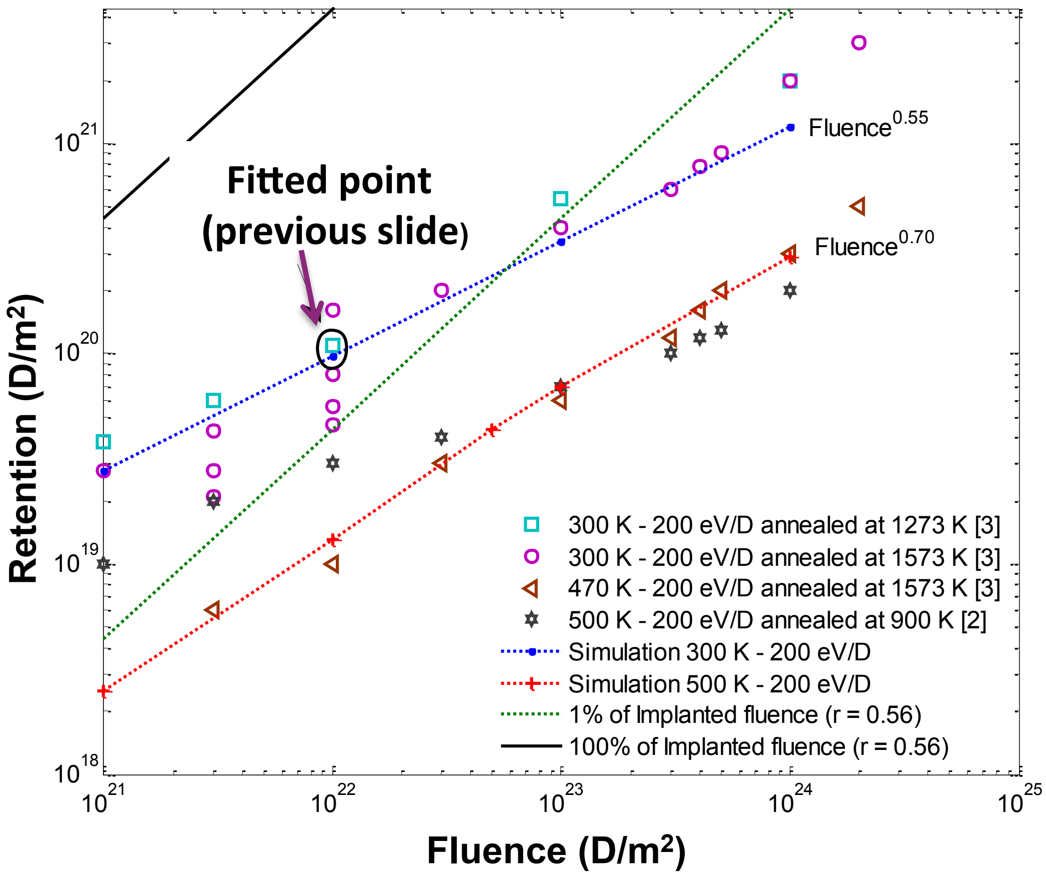




O.V. Ogorodnikova et al., J. Nucl. Mater. (2003)

FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL

Retention versus fluence at 2 implantation temperatures



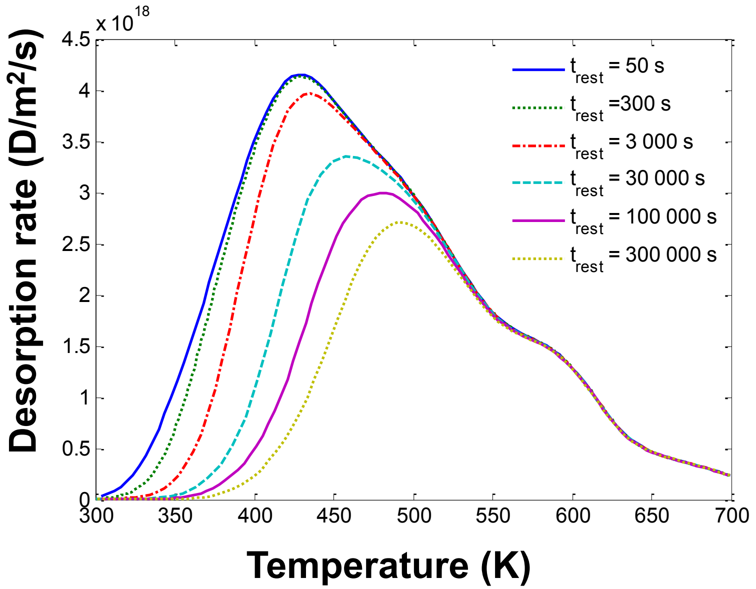
- **At 300 K: Retention ~ fluence$^{0.5}$ => diffusion limited**
- **At 500 K: Retention ~ fluence$^{0.7}$ => trap creation limited**

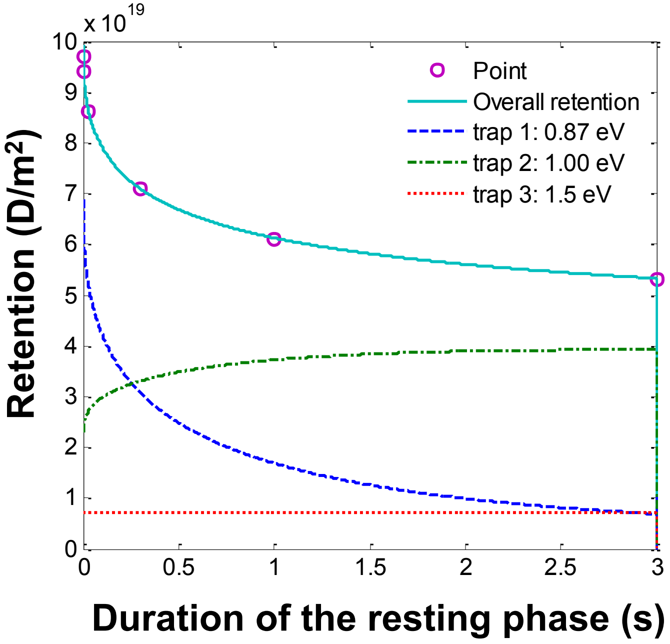
[2]: Tian, JNM, 2010
[3]: Ogorodnokiva, JNM 2003

FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL

Effect of the duration of the "resting" phase on retention

- **Implantation at 300 K (fluence = 10^{22} D.m^{-2}.s^{-1}): "resting" time varying from 50 s to 300 000 s (83 h)**





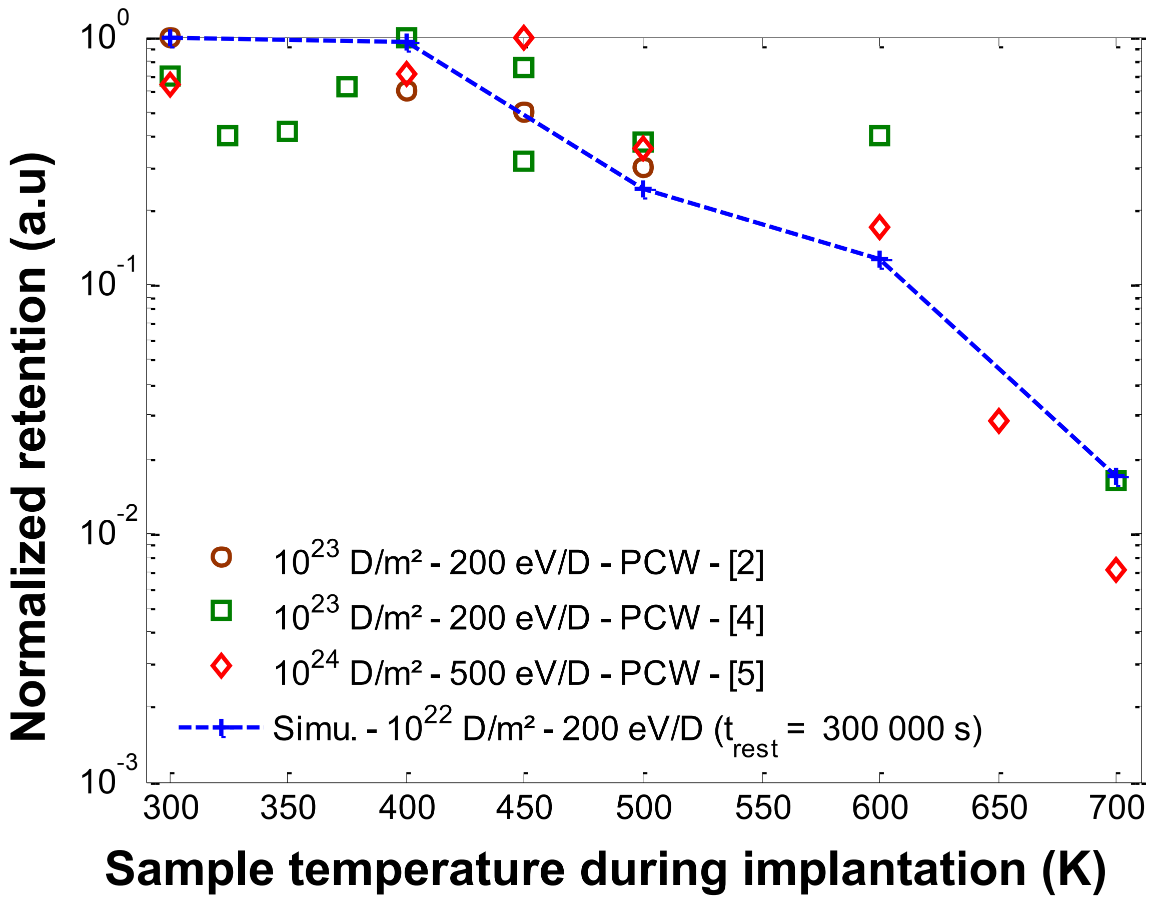
45 % of initial inventory lost in ~ 80 h (confirmed by experimental observations)

D twice deeper in the bulk

TDS spectra peak apparently shifted to high temperature

FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL

Evolution of retention with the sample temperature during ions implantation



FIT OF EXPERIMENTAL DATA WITH THE MIHMS MODEL

- **MHIMS model fits well the experimental data (PCW)**
- **No information of the fundamental trapping processes**
  (just an engineer approach)
- **This MHIMS code is in a crosschecked process using a test case to be fitted (Eurofusion approach) with two other codes:**
  - ✓ **HIIPC from LSPM, Paris**
  - ✓ **Klaus Schmidt code, Garching**

Good agreement observed

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trapped particles

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mobile particles

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- **trap 3 (extrinsic): $E_{T,3}$ = 1.5 eV (1.45) n3 = variable concentration**

Each trap containing one HIs

Different from DFT outcomes
From DFT, one vacancy can contain at RT up to 6 HIs

NEW APPROACH OF MACROSCOPIC RATE MODEL

Formalism

One single trap type (density N_t) can contain up to n HIs

- ***i−trap type,*** $N_i = density\ of$ ***i−trap*** $filled\ with\ 0 \leq i \leq n\ HIs,$
  - $N_t = \sum_{i=0}^{n} N_i$
- $C_{t,i} = concentration\ of\ particle\ in$ ***i−trap*** $trap = i \cdot N_i$

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Mechanisms & equations

i-trap type can be change into:

- ***i+1-trap type by trapping a solute particle***
- ***i-1-trap type by detrapping of a trapped particle from that trap***

$$for\ 0 < i < n, \frac{\partial N_i}{\partial t} = -\nu_m . C_m . N_i + \nu_m . C_m . N_{i-1} - \nu_i . N_i + \nu_{i+1} . N_{i+1}$$

And the mobile population is governed by :

$$\frac{\partial C_m}{\partial t} = D(T) . \frac{\partial^2 C_m}{\partial x^2} + \sum_{i=1}^{n} \frac{\partial C_{t,i}}{\partial t} + S_{ext}$$

Code MHIMS-reservoir

"Study of a multi trapping macroscopic rate equation model for hydrogen isotopes in tungsten materials", E Hodille et al, accepted for publication, Physica Scripta, 2015

MACROSCOPIC RATE EQUATION: NEW APPROACH

Boundary condition

- Desorption no limited by recombination:

$$C_m(x = 0, L) = 0$$

No Trap Creation

Trapping input

- Up to 6 atoms in a single vacancy at room temperature

TDS simulation in 3 phases

FIT OF EXPERIMENTAL DATA WITH MIHMS-RESERVOIR

Trapping in vacancy => Single crystal tungsten (SCW)

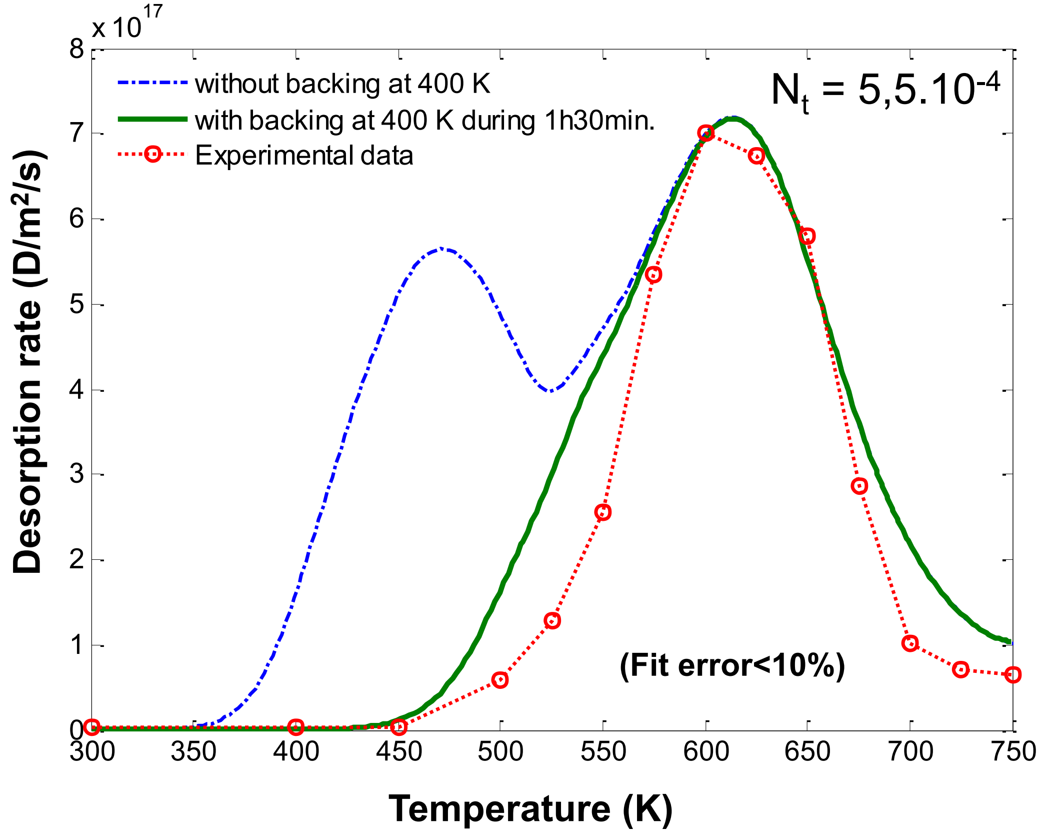
- Few data
  - Poon et al., JNM 2002:
    - fluence = $10^{21\text{-}22}$ D/m², flux = 10^{18} D/m²/s, 500 eV/D
    - Resting time ~ 8h – 72h + backing at 400 K during 1h30 min
    - Heating ramp = 4-6 K/s
  - Quastel et al, JNM 2006: (2)
    - fluence = 10^{23} D/m², flux = 10^{20} D/m²/s, 500 eV/D
    - well controlled resting time and backing
    - Heating ramp = 5,5 K/s
- Poon et al.: low flux and low fluence => **trap creation neglected** but **baking step** (sample at 400 K during 1h30 min before TDS and after the implantation)
- Quastel et al.: **Well defined experimental conditions** but high flux and fluence: **trap creation (different from vacancies)**?

FIT OF EXPERIMENTAL DATA WITH MIHMS-RESERVOIR: THE POON'S DATA

Parameters used in the simulation

- fluence = 10^{21} D/m², flux = 10^{18} D/m²/s, 500 eV/D, heating ramp = 5 K/s
- Resting time = 10 h and backing at 400 K during 1h30min just after the implantation (T of implantation = 300 K)

- Detrapping energy used (DFT values):
  - E_1 = 1,406 eV (1,43) (-2%)
  - E_2 = 1,402 eV (1,42) (-1%)
  - E_3 = 1,202 eV (1,25)
  - E_4 = 1,123 eV (1,17)
  - E_5 = 1,065 eV (1,10)
  - E_6 = 0,820 eV (0,86)



- **E_1 and E_2 in agreement with DFT**
- **Due to baking, no information at low temperature**

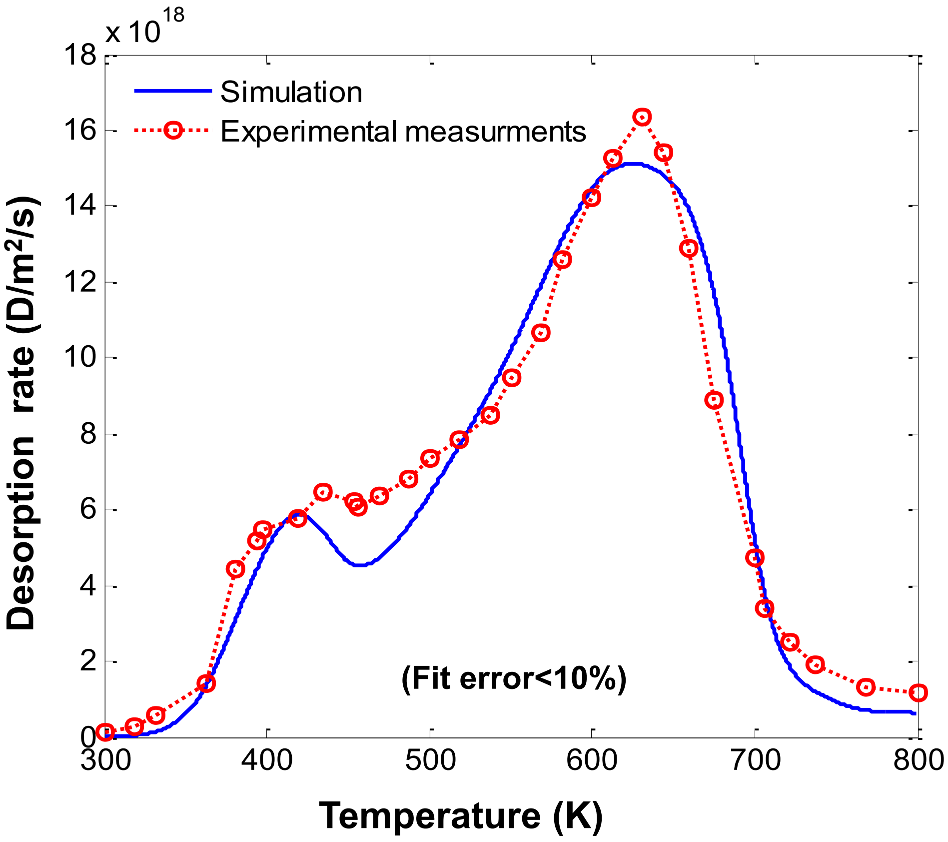
FIT OF EXPERIMENTAL DATA WITH MIHMS-RESERVOIR: THE QUASTEL'S DATA

Parameters used in the simulation

- fluence = 10^{23} D/m², flux = 10^{20} D/m²/s, 500 eV/D, heating ramp = 5,5 K/s
- Resting time = 0,42 h and no backing

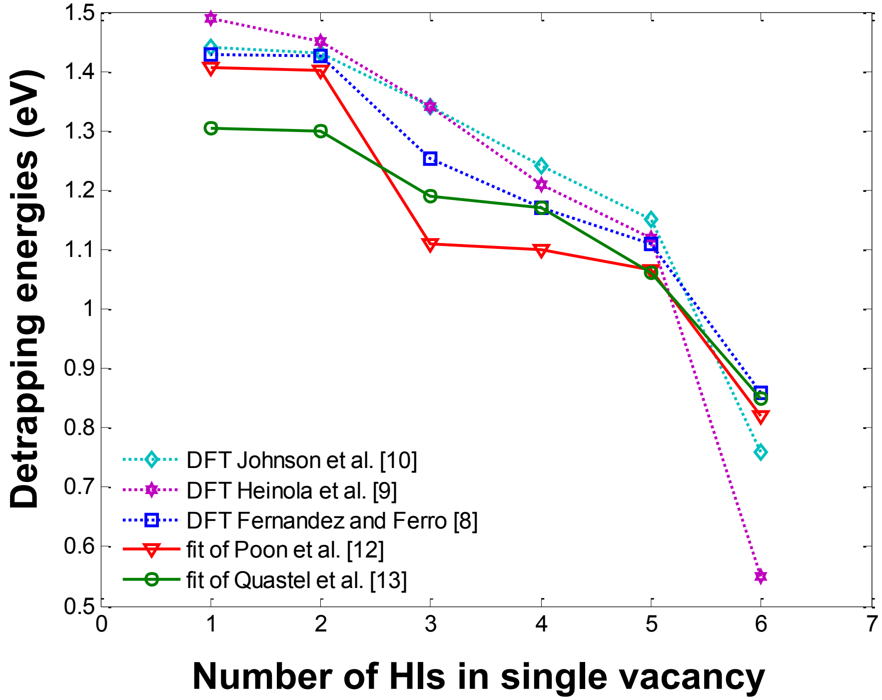
- The detrapping energy used (DFT values):
  - E_1 = 1,31 eV (1,43) (-8%)
  - E_2 = 1,30 eV (1,42) (-8%)
  - E_3 = 1,19 eV (1,25) (-5%)
  - E_4 = 1,17 eV (1,17) (0%)
  - E_5 = 1,06 eV (1,10) (-4%)
  - E_6 = 0,85 eV (0,86) (-1%)

- **E_1 to E_6 in agreement with DFT and with previous test**



THE MIMHS-RESERVOIR RESULTS

- MIHMS-reservoir able to fit TDS experimental data
- The detrapping energies obtained in agreement with DFT:



- Need of new experiment on very well characterized SCW samples
- Then, experiment with more complex crystal to discriminate between vacancies, Grain boundaries etc… : target of the WHISCI project

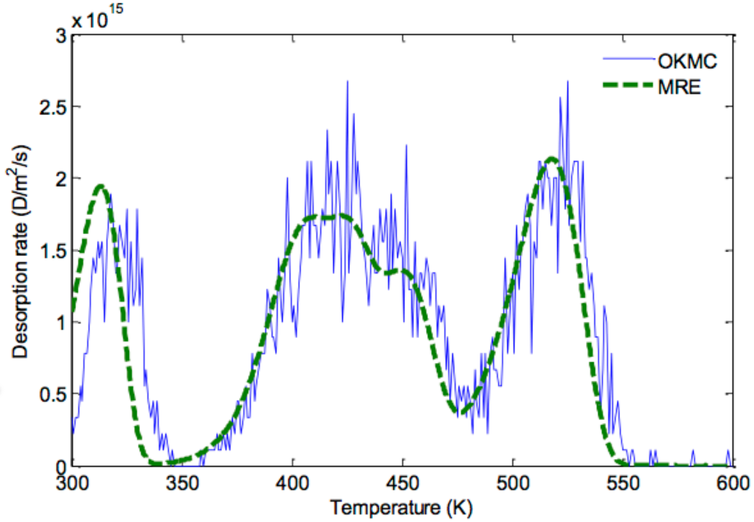
OKMC/MRE: MODELING THERMO-DESORPTION

Comparison between OKMC (LAKIMOCA) and MHIMS-reservoirs, based on DFT results

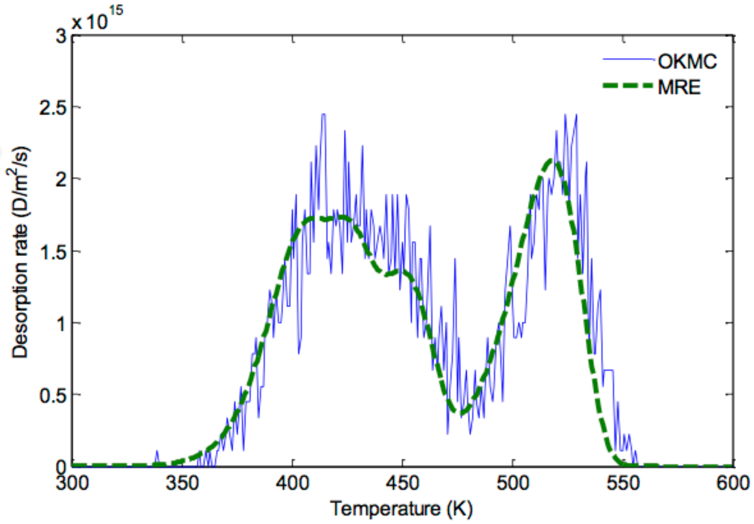
Conditions:`

- Sample of 300nm (1000W cells)
- Vacancies density: 2 10^{-6}
- At RT, vacancies filled by 6 H
- T ramp up: 1K/s

- TDS starts immediately (no resting time):
  - 3 peaks observed



- TDS starts after 1000s at 300K:
  - Disappearance of low temperature band



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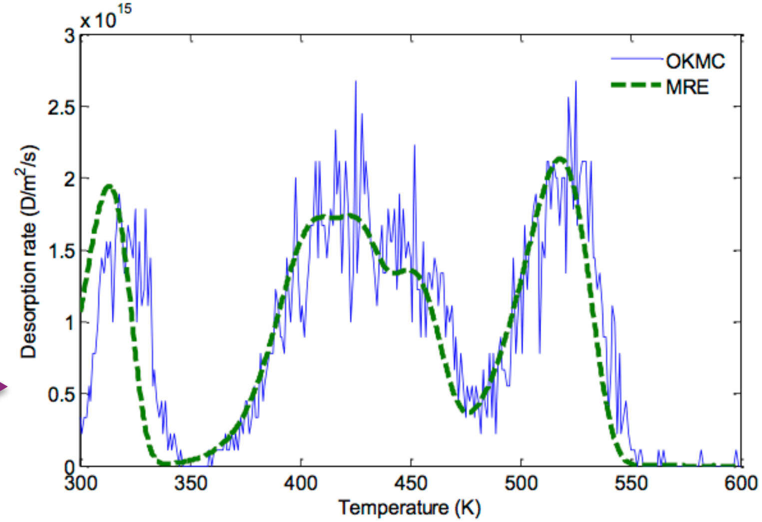

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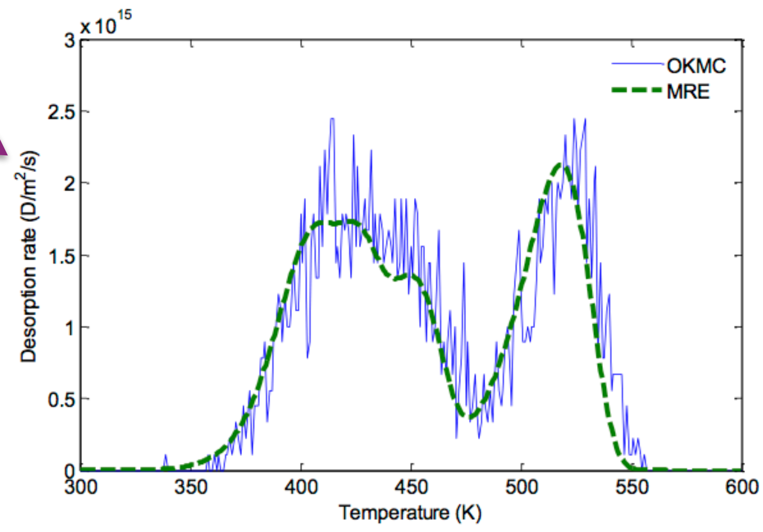

Same results obtained with both codes (confidence on MHIMS-reservoir)

CONCLUSIONS

- DFT predicts in SC:
  - H trapping energy, H migration energy, total concentration of vacancies,…

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- MHIMS Macroscopic Rate Equation Model:
  - Large number of parameters ☹
  - Some ad hoc hypothesis on the traps density ☹ but ok for low flux ☺
  - However,
    - ✓ good data fitting ☺
    - ✓ Good crosschecked with other macroscopic codes ☺
    - ✓ Valuable extrapolation for laboratory studies ☺
      - tokamak studies (role of impurity in the ion flux and on the surface properties) ☹

CONCLUSIONS

- DFT predicts in SC:
  - H trapping energy, H migration energy, total concentration of vacancies,…

- MHIMS Macroscopic Rate Equation Model:

- MHIMS-reservoir Rate Equation Model:
  - Reduced number of parameters ☺
  - Strong links with basic physics (DFT) ☺
  - Good data fitting for SCW ☺ but small numbers of experiment ☹
  - Extrapolation to PCW? ☹ and to tokamak ☹
    - ✓ The only way to proceed in order to address all the physical processes

CONCLUSIONS

- DFT predicts in SC:
  - H trapping energy, H migration energy, total concentration of vacancies,…
- MHIMS Macroscopic Rate Equation Model:
- MHIMS-reservoir Rate Equation Model:
- Comparison of OKMC/MRE modeling: excellent agreement ☺

CONCLUSIONS

- DFT predicts in SC:
  - H trapping energy, H migration energy, total concentration of vacancies,…
- MHIMS Macroscopic Rate Equation Model:
- MHIMS-reservoir Rate Equation Model:
- Comparison of OKMC/MRE modeling: excellent agreement ☺
- Future activities:
  - Improve data base of well characterized samples
    - On SCW and/or PCW
    - Well controlled surfaces + impurities effects
    - Well controlled implantation temperature and storage (down to 77K)
    - Neutrons simulation
    - Improving the MRE modeling
  - WEST application

This work has been carried out thanks to a partial support of the A*MIDEX project (n°ANR-11-IDEX-0001-02) funded by the "Investissements d'Avenir" French Government program, managed by the French National Research Agency (ANR)