UMET Cemhti LSPM PIIM CSNSM

Modeling and experimental validation of Hydrogen behaviour in tungsten for Tokamak

Institution: CNRS
M.F. Barthe CEMHTI (Orléans)
C.S. Becquart UMET (Lille)
Y. Ferro PIIM (Marseille)
X. Bonnin LSPM (Paris-13)
B. Décamps CSNSM (Orsay)
A. L. Thomann GREMI (Orléans)

Complementary to

Quantification of tritium implantation in tungsten-based fusion materials (C. Grisolia (CEA))

Conditions Extrêmes et Matériaux: Haute Température et Irradiation. Leader: C. Bessada

http://www.cemhti.cnrs-orleans.fr

~110 people: 28 scientists, 42 professionals, 10 postdocs, 21 phD

Materials Science / High temperature / Irradiation

- **Molten materials** glasses, ceramics, High Temperature processes
- **Local Structure** NMR, X-Ray synchrotrons, Neutrons
- **Optical Properties** IR, Raman, Brillouin, transmission, reflexion, emission
- **Defects in Solids** Nuclear Materials, electronics materials
- **Application of Ion/Particle Beams** Cyclotron, Van de Graff, Positons

Experimental tools for irradiation studies

- **Cyclotron**
  (H⁺, D⁺, ^{3}He, α -10-45 MeV)
- **Van de Graaff**
  (H⁺, D⁺, ^{3}He, α - 0.5-3 MeV)

→ Irradiations/implantations
nuclear Techniques of caracterization (IBA): chemical, microstructural analysis

Nuclear Reaction Analysis : ^{3}**He (d, p)** α

- **Positron Sources** → Positron annihilation Spectroscopy (PAS): **Nanostructure, vacancy defects**

Thin layers (1 µm in W) : ***Slow positron beam*** (0.1-25 keV)
Doppler broadening spectrometer (30-600K)

Thick samples (few 100 µm) : (^{22}Na) **fast positrons**
Lifetime and Doppler broadening spectrometers (20-600K)

Collaborations : LSI, CIRIL-GANIL, CSNSM, IPNL, LPS, CENBG

Institut Galilée cnrs LSPM Sorbonne Paris Cité Université Paris 13 Nord

Processes and Materials. Leader: K. Hassouni

Development, study and optimization of processes for materials synthesis and transformation

The study and comprehension of the evolution of the structural characteristics and properties of materials and their couplings

The integration of materials in systems, devices and processes

1. **PolyPhasic Media and Plasma Processes (MP4)**
2. Elaboration Processes for Advanced Materials (PEMA)
3. Thin Films, Functional Materials, and Nanostructures (FINANO)
4. Inorganic Nanomaterials (NINO)
5. High Pressure High Temperature Processes (HPHT)
6. Mechanics of Damage and Rupture of Materials (MER)
7. Plasticity, Anisotropy, Thermomechanic Behavior of Materials (PACTM)

7 research teams

64 scientists, 21 professionals, 46 PhD students, 7 post-docs

PolyPhasic Media and Plasma Processes (MP4)

RO: Treatment of gas pollutants by plasma-catalysis processes

RO: PLASMA-WALL INTERACTIONS

RO: Elaboration and characterization of mixed oxides by plasma processes

Development of reactors using non-thermal atmospheric pressure discharges (corona and DBD)
Characterization of gas pollutants and soot particles by chemical analysis
Expertise on treatment of particulates and PAHs
Expertise in plasma-catalysis processes
Modeling and optical diagnostics of streamer discharges and their reactive flows

Modeling of tokamak plasma edge flows and kinetics
Integrated modeling of plasma-wall interactions
Dust formation theory in tokamak edge conditions and other plasma systems
Experimental studies of properties of the dust obtained in plasma reactors
Study of the erosion of mixed materials targets
Staff: X. Bonnin, G. Lombardi, M. Redolfi, K. Hassouni, A. Michau
2 PhD students: K. Ouaras, C. Quirós

Development of plasma processes for the deposition of mixed oxides
Elaboration and characterization of thin films of ZnO and TiO_2 by plasma and sol-gel processes
Plasma processes for syngas fabrication and methane reforming
Implementation of global models for plasma reactors

PIIM Aix*Marseille université cnrs

Laboratory Physique des Interactions Ioniques et Moléculaires. Leader: Jean-Marc Layet

89 people – 34 Scientists

Teams and Topics

CIML – High resolution spectroscopy of confined ions in a Paul trap
DGP – Spectroscopic diagnostics in edge plasma
DSC – Characterization and control of turbulent transport in plasmas
TP – Physics of turbulent plasma: theoretical and experimental investigations
XPM – Experimental physics of magnetized plasmas
PS – Plasma-surface interaction on model Laboratory experiments
SDM – Atomistic modeling and experimental characterization of wall materials

UMET cnrs Chimie Lille Université Lille1

Unité Matériaux Et Transformations (Lille). Leader: A. Legris

http://umet.univ-lille1.fr/

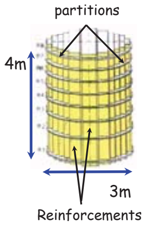
Molecular and therapeutic materials
Physical metallurgy
CENTRE COMMUN DE MICROSCOPIE
MATERIALS
Synthesis
Characterisations
Study of phase transformations
Mineral physics
Polymer systems engineering

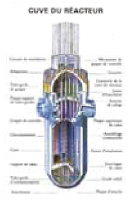
66 permanent scientist, 24 professionals, 7 post docs, 63 PhDs

Physical metallurgy modeling team

Multi-scale modeling of metallic materials close or far from equilibrium with or without external sollicitations (impacts, irradiation, mechanical stresses)

Permanents:
A. Legris
R. Besson
L. Thuinet
C. S. Becquart
Post doc:
A. De Backer
J. Boisse
J.B. Piochaud
PhD:
H. Rouchette
J. Kwon





-Zr alloys
-Ferritic and austenitic steels
-W
-NiAl

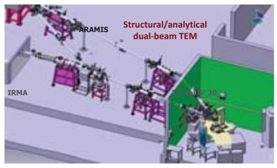
Centre de Sciences Nucléaires et de Sciences de la Matière (CSNSM)
Leader: Jean-Antoine Scarpaci

40 permanent scientists, 41 professionals

Multidisciplinary laboratories:

- **Astrophysique nucléaire**
- **Astrophysique du solide**
- **Physico-chimie de l'irradiation**
- **Physique du Solide**
- **Structure du Noyau**

JANNuS (Joint Accelerators for Nanoscience and Nuclear Simulation) PLATFORM (EMIR network)



Question: how will the wall behave during plasma operation (including neutrons)?

What is needed: a proper description of the D interaction with the wall for global tokamak modeling

How: a multi-scale modelling approach supported by corresponding data obtained by well controlled "separated effects" experiments

Modeling coupled to experimental validation: approach used before in european projects: Perfect, Perform-60, Getmat ...

Here ==> from single crystal without defects to complex case of a polycrystal with defects induced by irradiation with protons and high energy tungsten ions

Final goal: propose a model of the deuterium interaction with a polycrystal in a state resulting from neutron irradiation (i.e. with multiple point and extended defects).

www.perform60.net
http://nuklear-server.ka.fzk.de/getmat/

Experimental facilities

- **Positron annihilation spectroscopy**: fast positron spectrometers and slow positron beams (built by and at CEMHTI) ➔ vacancies/dislocations measurements

- **Irradiation and implantation facilities** (cyclotron: high energy light ions and neutrons ; pelletron from NEC company 0.4 to 3 MeV light ions) (CEMHTI) + **Jannus**

- **T infusion** (see C Grisolia CRP)

- **Ion beam analysis** (**NRA**, ERDA, RBS/C installed by CEMHTI on the Pelletron beamlines) (CEMHTI)

- **TEM ex-situ** in Orleans and **in-situ** Jannus platform Orsay : collaboration with B Decamps and R Schaublin - EPFL)

- **TDS** to measure H release (total quantity + modelling) (PIIM, CEA-IRFM)

- **LEED (Low Energy Electrons Diffraction) and XPS, Auger Electron Spectroscopy for surface analysis** (PIIM)

Procedure to be followed

Samples prepared and microscopically characterized by **one expert** before any experimental investigations by other partners.

Complementarity in terms of defects size characterization of well-established techniques (PA and TEM).

TDS very carefully **validated** using well characterized samples with a known D implantation + Crosschecked with IBA.

Implantation plasma to be carefully **assessed** concerning the ions energy, flux and fluence.

Study of the interaction of deuterium atoms and ions with a single crystal (SC) with no defects

- Study of the interaction of low energy D ions (<100eV) with a SC without defects.

- Study of the interaction of D atoms with a SC surface. SC orientation (111) and (110)

- Defects induced by W ions in W (effect of dpa and temperature) : vacancy defects , loops…(PAS and first TEM observations)

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Study of the interaction of deuterium with points defects in SC and PC

- Study of the interaction of low energy D ions (<100eV) with a SC and a Polycrystal (PC) containing mono vacancies (D/V).

- Defects induced by W ions in W (effect of dpa and temperature): vacancy defects , loops…(PAS and TEM observations) following

- Study of the interaction of D with a SC and a PC containing multi vacancies.

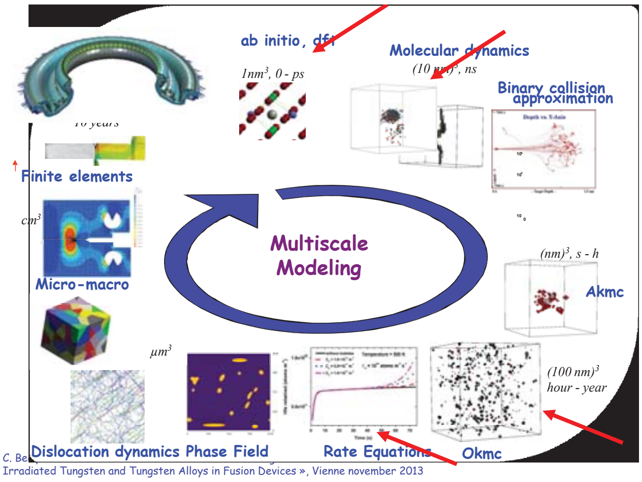
Study of the interaction of deuterium with extended defects (grain boundaries, dislocation, D/Vn)

- Study of the interaction of low energy D ions (<100eV) with a PC containing only grain boundary defects.

- Study of the interaction of low energy D ions (<100eV) with a SC and a PC containing dislocations.

- Study of the interaction of low energy D ions (<100eV) with a SC and a PC containing multiple vacancies and extended defects (D/Vn, dislocations, …): effect of dpa.

- Study of the interaction of helium on the D retention in W.



DFT calculations – H trapping in a W vacancy

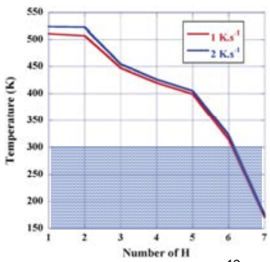
- H trapping energies are computed by **DFT at 0K**
- **Temperature dependency** is further added thanks to **thermodynamic**
- Trapping and de-trapping activation energies are determined
- Pre-factors are computed

$$\nu = \frac{k_B T}{h} \exp\left(\frac{S^{des}}{k_B}\right) \exp\left(-\frac{H^{des}_{vib}}{k_B T}\right)$$

- De-trapping temperature

$$\nu \exp\left(-\frac{E^{des}}{k_B T}\right) = \frac{k_B T}{h} \exp\left(-\frac{G^{des}}{k_B T}\right)$$

Desorption Temperature



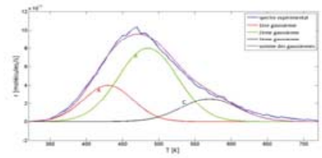
The maximum number of H in a mono-vacancy is 5-6 at room temperature

DFT *vs* Experiment

Thermal Desorption Spectroscopy

Temp(K) 430 470 570

Plasma Surface Team - PIIM Lab – JM Layet



Density Functional Theory

	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

Estimation of TDS profiles from DFT

Experimental and Theoretical results are consistent

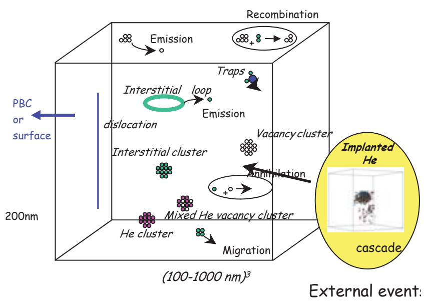
OKMC: LAKIMOCA

- Implantation: slowed down ion + its displacement cascade

- Point defects (SIA and vacancies) and He are mobile
- Pure or mixed clusters may be formed

- Instantaneous reactions submitted to a distance criteria
  $d_{ij} < R_i + R_j$

- Diffusion and emission thermally activated
  $\rightarrow \Gamma = \nu_0 \times e^{(-Ea/KT)}$



External event:

- Residence time algorithm: $\Delta t = 1/\Sigma_i \Gamma_i$

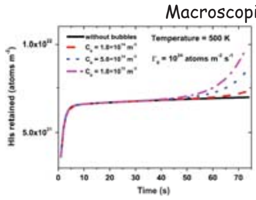
Approach used successfully to understand the role of the He atoms on the formation of nanocavities

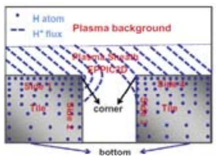
-Implantation of 800 keV ^{3}He with fluence from 10^{16} to 5×10^{20} ions m^{-2} at 300 K

-Isochronal annealing from 300 K to 1500 K

- Formation of cavities above 500 K
- At 900 K, the higher the fluence, the smaller the nanocavities

Macroscopic Rate Equation modeling





- Diffusion-trapping transport equations for hydrogen in tungsten
- Recombination at the surfaces
- Trapping energies provided by finer scale calculations shown before
- Additional term for bubble growth:
  - Chemical potential balance : H_2 molecules in bubble and HI solute in bulk
  - Bubble size determined by internal pressure and sample temperature
- Coupling to PIC sheath code for computation of incident fluxes (application to tile gaps)

C. Sang, J. Sun, X. Bonnin, S. Liu and D. Wang, *Numerical simulation of the bubble growth due to hydrogen isotopes inventory processes in plasma-irradiated tungsten*, Journal of Nuclear Materials **443** (1-3), 403-408 (2013).
C. Sang, X. Bonnin, M. Warrier, A. Rai, R. Schneider, J. Sun and D. Wang, *Modeling of hydrogen isotope inventory in mixed materials including porous deposited layers in fusion devices*, Nuclear Fusion **52** (4), 043003 (2012).

Codes:

-Density Functional Theory: VASP, QUANTUM ESPRESSO

-Molecular Dynamics: DYMOKA

-Object Kinetic Monte Carlo: LAKIMOCA

-Macroscopic Rate Equation modeling: HIIPC (Hydrogen Isotope Inventory Processes Code)

conclusions:

- Published results on:
  - He trapping in W (experiment and modeling)
  - H trapping in C, C/B, Be (experiment and modeling)

- Ongoing work on H trapping in W (SC, PC and perturbed SC and PC) with a well defined procedure:
  - Addressing all the significant parameters:
    - type of defects,
    - plasma,
    - Irradiation damage induced microstructure
  - Using a large set of modeling approaches
  - Coupling strongly modeling and experiments