# MoD-PMI 2015


# PROGRAM and ABSTRACT BOOKLET

## Aix-Marseille University

*3 place Victor Hugo, 13001 Marseille, France*

*25-27 May 2015*

## Invited Speakers

| | |
|---|---|
| **Tommy Ahlgren** | *University of Helsinki* |
| **Marie-France Barthe**, | *CNRS Orléans* |
| **Charlotte Becquart** | *Université de Lille* |
| **Bas Braams** | *IAEA Vienna* |
| **María José Caturla** | *Universidad de Alicante* |
| **Michele Ceriotti** | *EPFL* |
| **Huiqiu Deng** | *Hunan University* |
| **Gregory de Temmerman** | *ITER Organization* |
| **Christian Grisolia** | *CEA Cadarache* |
| **Kalle Heinola** | *CCFE & University of Helsinki* |
| **Atsushi M. Itoh** | *NIFS* |
| **Jorge J. Kohanoff** | *University of Belfast* |
| **Heun-Tae Lee** | *Osaka University* |
| **Jörg Neugebauer** | *MPI für Eisenforschung* |
| **Olga Ogorodnikova** | *NRNU MEPhI* |
| **Kazuhito Ohsawa** | *Kyushu University* |
| **Anthony Paxton** | *King's College London* |
| **Klaus Schmid** | *IPP Garching* |
| **Toshiyuki Takayanagi** | *Saitama University* |
| **Pavel Vladimirov** | *Karlsruhe Institute of Technology* |

## Scientific Committee

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|---|---|
| **Yves Ferro** (Chair) | *Aix-Marseille Univsersity* |
| **Bas Braams** | *IAEA Vienne* |
| **Jean-Paul Allain** | *University of Illinois* |
| **Gregory de Temmerman** | *ITER Organization* |
| **Maria Ganchenkova**, | *MEPhI* |
| **Daiji Kato** | *NIFS* |
| **Predrag Krstic** | *Stony Brook University* |
| **Christian Linsmeier** | *FZ Jülich* |
| **Duc Nguyen-Manh** | *CCFE Culham* |
| **Kai Nordlund** | *University of Helsinki* |
| **Takuji Oda** | *Seoul National University* |
| **Klaus Schmid** | *IPP Garching* |

## Local Organizers

**Ferro Yves** (chair)
**Addab Younes**
**Cannuccia Elena**
**Ferry Laura**
**Khamchanh Régis**

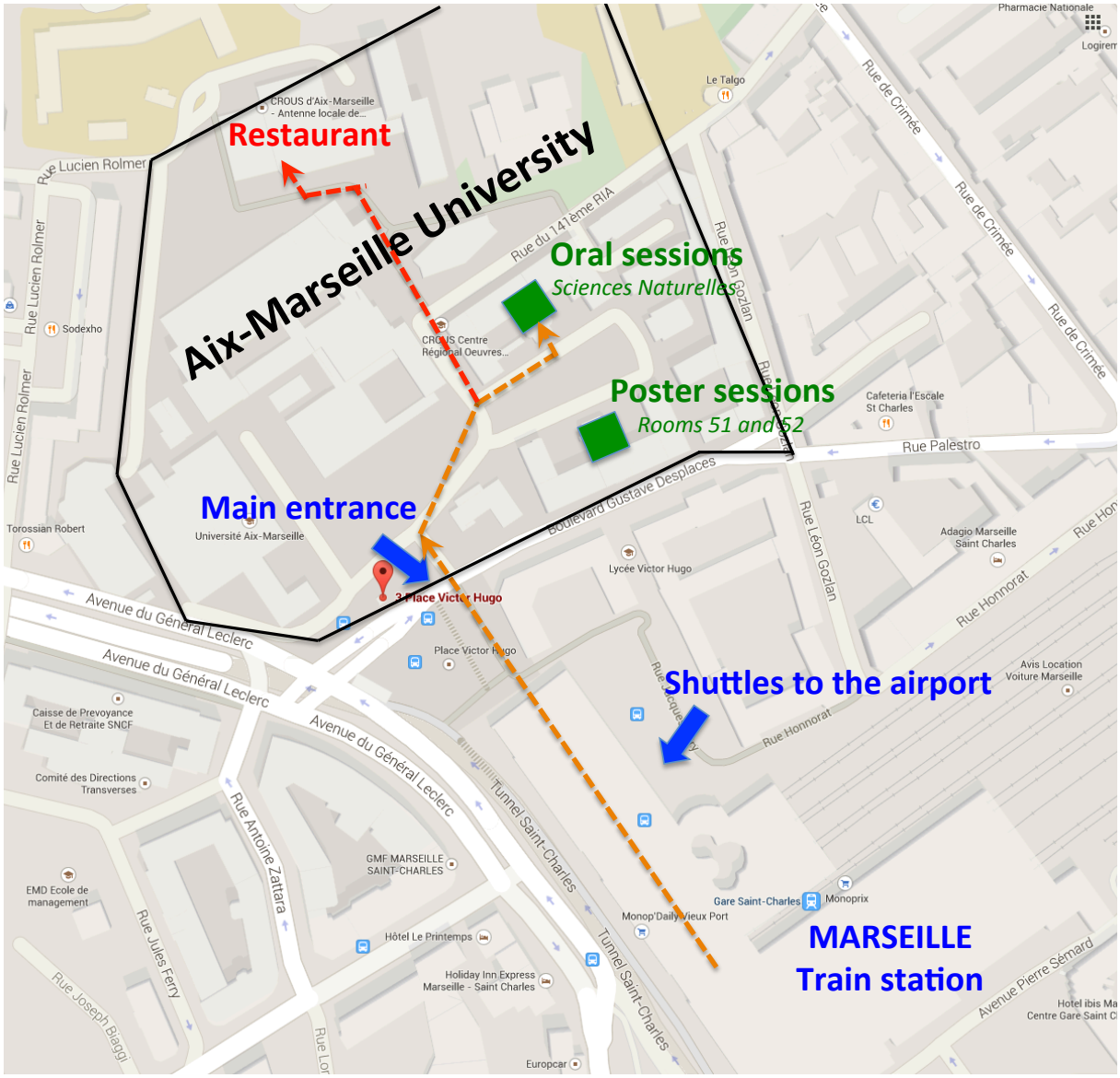
# How to come

The Saint-Charles campus of Aix-Marseille University is next to the train station.

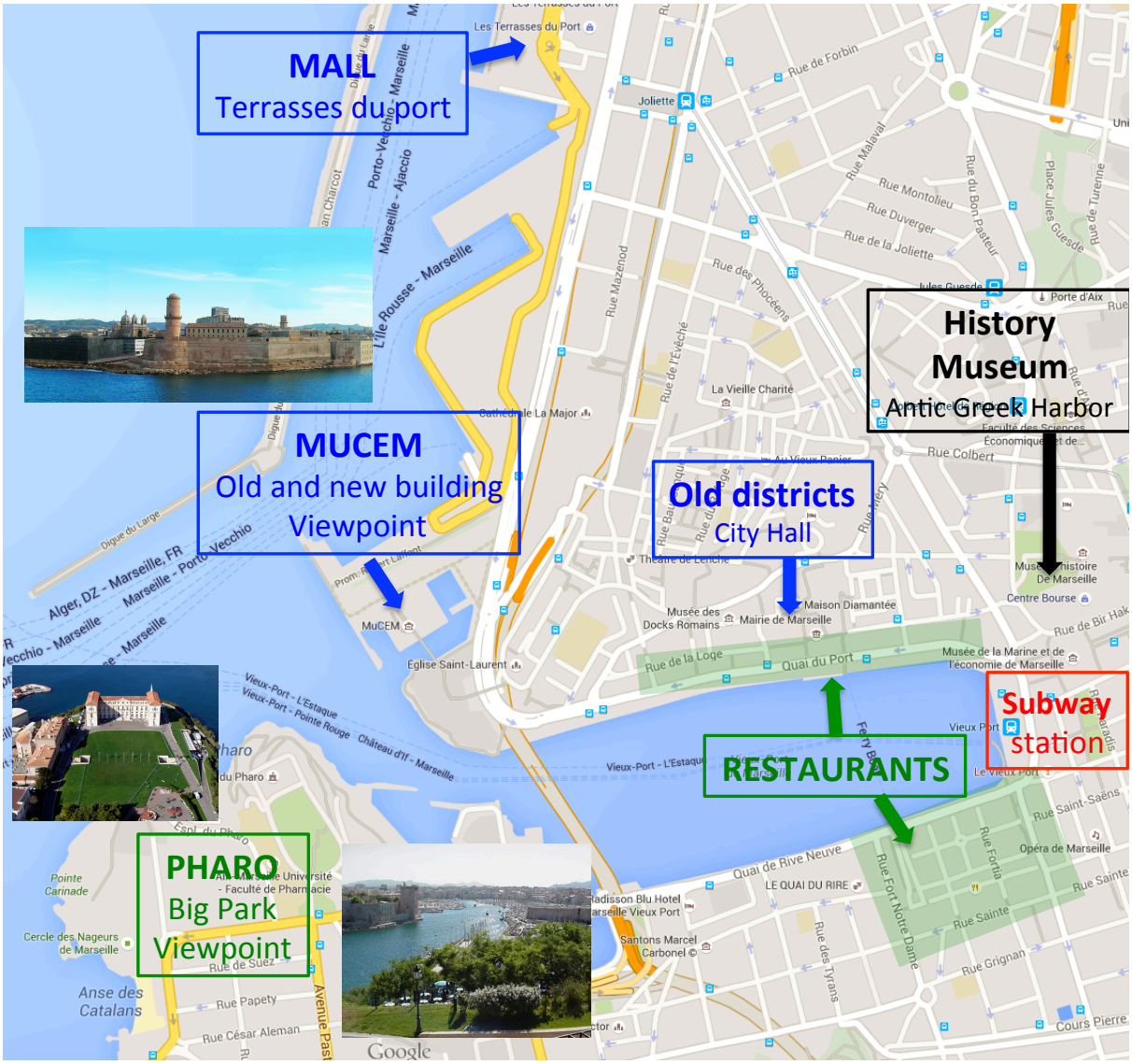
Shuttles are joining the airport Marseille-Provence, Marignane, to the train station “Gare Saint-Charles”, Marseille. Shuttles can be booked in advance here: http://mpshuttle.fr/en/

Oral session will be held in the “Sciences Naturelles” amphitheater.

Poster sessions will be held in rooms 51 and 52.



# Strolling around the “Vieux Port”




Here are some examples of what you can enjoy around the “Vieux Port”.

**How to join the conference site?**

The conference site is next to the subway station “Saint-Charles”
Line 1 join “Saint-Charles” to “Vieux Port” within 5 minutes; it is just three stations away.

# Program

## Monday 25 May 2015

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|---|---|
| 13:00 – 14:00 | Registration |
| 14:00 – 14:15 | Opening<br>***Yves Ferro*** |

### *Session 1 - Molecular Dynamics*

*Chair: Charlotte Becquart*

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|---|---|
| 14:15 – 14:50 | Self-trapping and trap mutation in bulk tungsten: a DFT and Molecular Dynamics investigation (I1)<br>***Charlotte Becquart*** |
| 14:50 – 15:25 | New interatomic potentials for studying the behavior of noble gas atoms in tungsten (I2)<br>***Huiqiu Deng*** |
| *Break* | |
| 15:50 – 16:25 | Tungsten Fuzzy Nanostructure Growth by Molecular Dynamics and Monte Carlo Hybrid Simulation (I3)<br>***Atsushi M Itoh*** |
| 16:25 – 17:00 | Modelling of Hydrogen Interactions with Beryllium Surfaces in Fusion Reactor (I4)<br>***Pavel Vladimirov*** |

### *Session 2*

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| *17:00 – 18:30* | *Poster session* |

## Tuesday 26 May 2015

### *Session 3* –*Quantum Effects In Molecular Dynamics*

*Chair: Bas Braams*

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| 8:40 – 9:15 | Modelling and Data Needs for Plasma-Material Interaction in Fusion Devices: Perspective from the IAEA Atomic and Molecular Data Unit (I5)<br>***Bas Braams*** |
| 9:15 – 9:50 | Time-*dependent* simulation of electronic stopping from first-principles (I6)<br>***Jorge J. Kohanoff*** |
| 9:50 – 10:25 | Quantum nuclei in materials: (when) do we need to worry? (I7)<br>***Michele Ceriotti*** |
| *Coffee break* | |
| 11:10 – 11:45 | Quantum theory of transport and trapping of hydrogen in iron (I8)<br>***Anthony Paxton*** |
| 11:45 – 12:20 | Nuclear quantum effects in tritium diffusion in $\alpha$-iron (I9)<br>***Toshiyukii Takayanagi*** |

*Lunch*

### *Session 4* – *Experimental Data for Modelling*

*Chair: Gregory de Temmerman*

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|---|---|
| 14:00 – 14:35 | The need for a better understanding of plasma-material interactions in ITER and the role of modelling (I10)<br>***Gregory de Temmerman*** |
| 14:35 – 15:10 | Vacancy defects studied in tungsten by using Positron annihilation spectroscopy (I11)<br>***Marie-France Barthe*** |
| 15:10 – 15:45 | Experimental studies of hydrogen transport parameters in tungsten (I12)<br>***Heun-Tae Lee*** |
| *Coffee break* | |
| 16:25 – 16:50 | Influence of aluminum oxide coating oxygen presence in plasma on deuterium retention in tungsten (O1)<br>***Leon Begrambekov*** |
| 16:50 – 17:15 | Deuterium retention in polycrystalline tungsten at low fluences (O2)<br>***Régis Bisson*** |

### *Summary and discussion*

17:15 – 18:00

## Wednesday 27 May 2015

### ***Session 5*** *– Multi-scale modelling 1: DFT and statistic methods*

*Chair: Joerg Neugebauer*

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|---|---|
| 8:40 – 9:15 | Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach (I13)<br>***Jörg Neugebauer*** |
| 9:15 – 9:50 | Setting up plasma pulse-scale simulations with electronic structure calculations (I14)<br>**Kalle *Heinola*** |
| 9:50 – 10:25 | Hydrogen recycling in tungsten during plasma pulse simulations with rate equations (I15)<br>***Tommy Ahlgren*** |

*Coffee break*

*Chair: Daiji Kato*

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|---|---|
| 11:05 – 11:40 | Multiscale modelling of radiation effects in materials: ion implantation versus neutron irradiation (I16)<br>***Maria José Caturla Terol*** |
| 11:40 – 12:05 | Hydrogen trapping at vacanciesand hydrogen impact on vacancy diffusion and self-diffusion in Ni (O3)<br>***Döme Tanguy*** |
| 12:05 – 12:30 | Vacancy nanoclusters in irradiated W and W alloys: First-principles assessments and multi-scale modelling (O4)<br>***Duc Nguyen-Manh*** |

*Lunch*

### ***Session 6*** *– Multi-scale modelling 2: Rate-equations and Reaction Diffusion models*

*Chair: Klaus Schmid*

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|---|---|
| 14:00 – 14:35 | Modeling isotope exchange in W using fill level dependent trapping (I17)<br>***Klaus Schmid*** |
| 14:35 – 15:10 | Macroscopic rate equation modeling of trapping/detrapping of hydrogen isotopes in tungsten materials (I18)<br>***Christian Grisolia*** |

*Coffee break*

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|---|---|
| 15:40 – 16:15 | Migration, trapping and release of deuterium from tungsten in the presence of high density of defects: theory and experiment (I19)<br>***Olga Ogorodnikova*** |
| 16:15-16:35 | Materials research in Jülich: hydrogen retention in beryllium (O5)<br>***Dmitry Matveev*** |

### ***Summary and discussion***

16:35- 17:15

Closing

# Poster session

P - 1 Thin tungsten oxide layers : structural properties and deuterium retention
*Younès Addab*

P - 2 The Xolotl Plasma-Surface Interactions Simulator
*Sophie Blondel*

P - 3 Path integral molecular dynamics for the nuclear quantum effects in the Frenkel defects in BCC Fe
*Bingqing Cheng*

P - 4 Experiment and modelling of hydrogen isotope exchange in beryllium layers as mean of T inventory control in ITER
*David Douai*

P - 5 DFT calculations of voids in α-Fe
*Dmytro Kandaskalov*

P - 6 Meta-stable state of 111-crowdion binding with $VH_6$ complex in tungsten
*Daiji Kato*

P - 7 Comparing He ion energy transfer to W and Fe surfaces through molecular dynamics simulations
*Peter Klaver*

P - 8 Joint experimental and theoretical efforts to bridge the gap between today's experiments and future fusion devices
*Timo Dittmar*

P - 9 Modelling and Experiments of Plasma-Material Interactions in Presence of fusion Neutrons
*Maya Padivattathumana*

P -10 Magnetic sheath effect on the gross and net erosion rates due to impurities
*Nicolas Mellet*

P -11 Aluminium studies for laboratory plasma: particle growth and hydrogen retention
*Jonathan Mougenot*

P - 12 $W_2$, $W_4$, WH, $WH_2$: Ab initio and DFT benchmarks
*Michal Novotny*

P - 13 Modelling of D atom absorption and diffusion dynamics in self-ion damaged tungsten exposed to deuterium atom beam
*Anze Zalzonik*

P - 14 Kinetic Monte Carlo simulation and rate theoretical approach for influence of vacancy on hydrogen diffusivity in tungsten
*Deqiong Zhu*

P - 15 Some aspects of determination of hydrogen binding energies with defects in metals
*Mikhail Zibrov*

P - 16 Raman spectroscopy investigation of beryllium based materials
*Cédric Pardanaud*

P – 17 Aspects of ion-metal and electron-metal interactions in fusion relevant energy regimes
*Svetlana Ratynskaia*

P – 18 The microphysics of ion-surface recombination and calculations of the heat sheath transmission factor
*Panagiotis Tolias*

P – 19 Hydrogen diffusion and vacancies formation in tungsten: DFT and statistical models
*Nicolas Fernandez*

# Abstracts

# Self trapping and trap mutation in bulk tungsten: a DFT and Molecular Dynamics investigation

J. Boisse[a,b], C. Domain[a,c], A. De-Backer[a,d]C.S. Becquart[a,*]

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[c] *EDF-R&D, Département MMC, Les renardières, F-77818 Moret sur Loing, France*
[d] *CCFE, Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK*

Being virtually insoluble in metals, but very mobile, He atoms can be trapped, associate with vacancies, forming platelets and bubbles. He atoms have been shown to contribute to swelling, cause intergranular embrittlement and produce roughening and blistering at metal surfaces. Being repelled by the metal atoms, they form stable clusters, which are also mobile. This tendency to form clusters is so strong that when too many He atoms are aggregated together it can be less costly to relieve the strain created by the interstitial elements by the ejection of one or more matrix atoms leading to the formation of one or more Frenkel Pairs (FP), i.e. vacancies and Self Interstitial Atoms (SIAs). When no vacancy is initially present, the He cluster will be trapped by the vacancy it created, in a self-trapping (ST) event; whereas when one or more vacancies are already associated with the He cluster, the same mechanism is referred to as trap mutation (TM) or loop punching, if more than one SIA is created.
We have investigated the thermodynamics and kinetics of ST and TM in tungsten using Density Functional Theory (DFT) calculations and Molecular Dynamics with a recently developed potential for W-He adjusted on DFT calculations.
The stability of helium-vacancy clusters ($He_nV_m$) as well as pure interstitial helium clusters in tungsten results from a competitive process between thermal emission of vacancies, self interstitial atoms and helium atoms, depending on the helium-to-vacancy ratio in mixed clusters or helium number in pure interstitial helium clusters and will be presented in this work. We investigated in particular the ground state configurations as well as the activation barriers of self trapping and trap mutation, i.e. the emission of one SIA along with the creation of one vacancy from a vacancy-helium or pure helium object.

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# New interatomic potentials for studying the behavior of noble gas atoms in tungsten

Fen Zhou [a], Jingzhong Fang [a], Huiqiu Deng[a,*], Jianglong Liu [a], Shifang Xiao [a], Xiaolin Shu [b], Fei Gao [c], Wangyu Hu [a]
[c]

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[c] *Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, Michigan 48109, USA*

The fiber-formed nanostructures ("fuzz") have been observed on the surface of tungsten as exposed to the low-energy and high-flux He plasma irradiation, however they were not formed on the W surface by exposure to Ar or Ne plasmas. To date the fuzz formation mechanism is still unclear. To study the different behavior of noble gas X (=He, Ne and Ar) atoms in the bulk and on the surface of tungsten, new *ab initio*-based potentials for W–He, W–Ne and W–Ar interactions were developed by fitting the results obtained from first-principles density functional theory calculations. The "s-band model" was used to describe the many-body interactions between each of the noble gas atoms and its neighboring W atoms. These potentials reproduced the formation energies of point defects and the migration barriers of single noble gas atoms. The simulations using these potentials successfully predicted that the tetrahedral interstitial site is more stable than the octahedral interstitial site for X (= He, Ne or Ar) interstitials. Based on the new potentials, the binding interactions of a single X atom with the Xn and Xn-Vacancy clusters and the diffusion properties of Xn clusters in bulk W were studied using molecular dynamics simulations. The simulation results indicate that the binding energies obtained using the new potentials are well in agreement with the results of the first-principles calculations. The migration energies of the clusters increase with both the increase in the atomic radius of noble gases and the increase in the size of the clusters. The diffusion, nucleation and clustering behavior of noble gas atoms in bulk W have been studied detailedly. The glide of dislocation loops induced by Xn clusters or bubbles has also been discussed.

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# Tungsten Fuzzy Nanostructure Growth by Molecular Dynamics and Monte-Carlo Hybrid Simulation

A. M.Ito[a,*], T. Murashima[b], T. Tamura[c], R. Kobayashi[c], A. Takayama[a], S. Kajita[d], S. Takamura[e], N. Ohno[d], M. Yajima[a], Y. Yoshimoto[f], S. Ogata[b], and H. Nakamura[a,c]

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[f]*The university of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan.*

Fuzzy nanostructure is induced by helium plasma irradiation onto a tungsten surfaces [1]. The fuzzy nanostructure which generated on the divertor walls in nuclear fusion reactors brings about the decrease of the thermal conductivity of the tungsten materials and the increase of the tritium retention. We have tried to clarify the formation mechanisms of the fuzzy structure by multi-scale simulation approach. The formation process of the fuzzy nanostructure can be classified into the irradiation process, the diffusion and agglomeration process, the bubble structure growth process, and the fuzzy nanostructure growth process, which we call the four-step process [2]. In the four-step process, the former three processes were clarifyed by using the binary collision approximation (BCA), the density functional theory (DFT), and the molecular dynamics (MD), respectively.

In the fourth processes, the fuzzy nanostructure growth had been successfully reproduced by the MD and Monte-Carlo (MD-MC) hybrid simulation [2,3]. In the MD-MC hybrid simulation, the long time diffusion of helium atoms was simulated by the random walk based on the MC, and the deformation of the tungsten material due to pressure from the helium bubbles was simulated by the MD. As a result, it was understood that the fuzzy nanostructure grew only when helium retention is under the steady state. In addition, the height of the fuzzy nanostructure increased proportionally to the square root of helium plasma irradiation time, which agrees with the experimental observations [4,5].

In this paper, we propose the mechanism of the enhancement of the convex-concave surface structure, and introduce the improvement of the MD-MC hybrid simulation to reproduce more long fuzzy nanostructure. If we achieve to create sub-micro-meter fiber, we can compare the surface fractal dimension which had been measured by the experiment [6].

[1] S. Takamura, N. Ohno, D. Nishijima, and S. Kajita, Plasma Fusion Res. 1 (2006) 051.
[2] A. M. Ito, et al, J. Nucl. Mater. (2015) in press, doi:10.1016/j.jnucmat.2015.01.018
[3] A. M. Ito, et al., in: IAEA Fusion Energy Conference, 2014, pp. MPT/1–MPT/3.
[4] M. Baldwin and R. Doerner, Nucl. Fusion 48 (2008) 035001.
[5] Y. Noiri, et al.,J. Nucl. Mater. (2015)*in press*, doi:10.1016/j.jnucmat.2015.01.036
[6] S. Kajita, et al.,Phys. Lett. A 387 (2014) 2533-2538.

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# Modelling of Hydrogen Interactions with Beryllium Surfaces in Fusion Reactor

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Beryllium is a candidate material for the first wall of future fusion reactor. It is also considered as a neutron multiplier in the tritium breeding blanket. In both cases, hydrogen isotopes are generated inside beryllium bulk via transmutations induced by fusion neutrons and will interact with beryllium external and internal (gas bubble) surfaces. Therefore, theoretical investigation of such effects is of high importance for the understanding of beryllium behaviour in fusion environment.
This contribution reviews the results of the first principles modelling of hydrogen isotope interaction with beryllium surfaces. Using ab initio molecular dynamics, we simulated the hydrogen molecule dissociative adsorption on Be (0001) surface for various hydrogen surface coverages. Our simulations show that the H2adsorption energy depends on hydrogen coverage, being 0.75 eV for the clean surface and about 1.2 eV for 1ML coverage. Moreover, if the kinetic energy of impinging molecule is significantly higher than the barrier, but not sufficient for implantation under the surface, the molecule will be reflected with a high probability. This sheds light on the physical meaning of the sticking coefficient. Preferable hydrogen adsorption sites for different coverage were found. Adsorbed hydrogen atoms repel each other up to the third nearest neighbour distance, thus preventing H2associativedesorption at low H-coverage. The repulsion of hydrogen atoms at high coverage results in a notable surface stress and leads to surface reconstruction, which can be viewed as formation of chemical bonds characteristic for BeH2polymer chains. This tendency is further enhanced if subsurface hydrogen is present in addition to hydrogen at the surface. In this case, amorphous chemical compound containing structural units similar to those of BeH2is formed at the surface. These chains are elevated above the surface in the middle, but still attached to it by their ends. We suggest, therefore, that decomposition of BeH2formed at the external surface could be one of the possible hydrogen desorption mechanisms, as supported by experiments [1].
In addition, we have shown that adsorbed hydrogen notably changes the surface energy of the major crystallographic surfaces. The general tendency consists in the surface energy decrease with increasing hydrogen coverage, but then, at higher concentrations, hydrogen atoms begin to repel each other, and the surface energy increases again. The variations in the surface energies are, however, quite different for the diverse surfaces tested, leading to the change of the most energetically favourable surface from the basal (0001) plane for low H-coverage to the pyramidal type II ($11\bar{2}2$) for high coverage. Moreover, equilibrium H-coverage is different for different surfaces within one facetted gas bubble. This leads to the complex modification of the gas bubble form according to the H-surface coverage and its bulk concentration. Drastic changes in the bubble form were also observed in the high-dose hydrogen implantation experiments[2].

[1]R.P. Doerner, et al., J.Nucl.Mater. **390-391**(2009) 681-684
[2] S.P. Vagin, et al., J.Nucl.Mater. **258–263**(1998) 719-723

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# Modelling and Data Needs for Plasma-Material Interaction in Fusion Devices: Perspective from the IAEA Atomic and Molecular Data Unit

B. J. Braams* and H.-K. Chung

*Nuclear Data Section, Division of Physical and Chemical Sciences (NAPC), International Atomic Energy Agency (IAEA), Vienna, Austria*

The mission of the Atomic and Molecular Data Unit (AMDU) at IAEA is to support development of fusion as an energy source by the provision of internationally recommended data for atomic, molecular and plasma-material interaction (PMI) processes and related material microstructure properties. In the area of PMI the twin main concerns are erosion and tritium retention. Microstructure properties are important to us as they provide the link between radiation damage and tritium retention. The Unit has active Coordinated Research Projects (CRP) on PMI with beryllium [1], irradiated tungsten [2] and steel [3], and we are mindful of the importance of liquid metals as well. PMI is an important topic in our other meetings as well, for example [4] and [5]. We are keenly interested in uncertainty assessment and data evaluation, e.g. [6] and [7].

We will use the opportunity of speaking at MoD-PMI to highlight key issues in modelling and data development for problems of PMI for fusion. One key issue is the effective treatment of electronic excitation in the context of molecular dynamics (MD) simulations of radiation damage or other fast particle collision processes. This involves fundamental questions of the derivation of an effective model (perhaps Langevin dynamics for the nuclei coupled to a heat equation for the electron temperature) starting from quantum or Ehrenfest dynamics. It also involves assessment of suitable electronic structure methods and of the fitting of the resulting internuclear potential or the force. A second key issue is that of development and validation of accurate MD potentials just for the ground electronic state, but for relevant non-crystalline mixed materials at relevant high energies as after impact by a fast particle. A third key issue is systematic uncertainty quantification from the electronic structure calculations through the development of MD potentials (or of rates for other simulations) to the calculation of microstructure properties after exposure to plasma and/or radiation.

[1] CRP PMI with Beryllium: https://www-amdis.iaea.org/CRP/Beryllium/
[2] CRP Irradiated Tungsten: https://www-amdis.iaea.org/CRP/IrradiatedTungsten/
[3] CRP Steel Surfaces: https://www-amdis.iaea.org/CRP/SteelSurfaces/
[4] ICTP-IAEA Joint Conference on Models and Data for Plasma-Material Interaction in Fusion Devices: https://www-amdis.iaea.org/Workshops/ICTP2014/
[5] Decennial IAEA Technical Meeting on A+M+PMI Data for Fusion Science and Technology: https://www-amdis.iaea.org/meetings/AMPMI14/
[6] Joint IAEA-ITAMP Technical Meeting on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data: https://int-amdis.iaea.org/meetings/ITAMP/
[7] 4th Biennial Technical Meeting of the International Atomic and Molecular Code Centre Network: https://int-amdis.iaea.org/CCN/Meetings4/

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## Time-dependent simulation of electronic stopping from first-principles

J. Kohanoff[a,*], E. Artacho[b], and A. A. Correa[c]

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Materials in fusion reactors, especially those in the first wall, are subject to intense irradiation with 14.1 MeV neutrons. While most neutrons will go through the wall without interacting, a fraction of them will hit atoms in the material and transfer part of their kinetic energy to these, so-called, primary knock-on atoms (PKA). The PKA become them themselves projectiles that self-irradiate the material, damaging it. According to the velocity of the PKA, there are two asymptotic regimes: nuclear stopping at low velocities, and electronic stopping at high velocities. In the intermediate velocity region both mechanisms coexist. Most of the modelling work done so far has focused on the nuclear stopping regime, which can be addressed via molecular dynamics simulations based on empirical force fields. Although the fundamentals of electronic stopping have a long research history, from the first-principles simulation point of view, the electronic stopping regime has only been studied in the past few years [1].

Here I will present the approach we have been using to describe irradiation, and in particular self-irradiation, of materials in the electronic stopping regime. The methodology is based on time-dependent density-functional theory (TDDFT) and the Ehrenfest approximation, and is suitable for ion (or atom) irradiation. The simulation is started by assigning an initial velocity to the projectile and proceeds by integrating numerically the time-dependent Kohn-Sham equations of motion for electronstogether with Newtonian equations of motion for the nuclei. The forces on the nuclei arise from the time-dependent electronic density. This results in a continuous increase of electronic energy due to non-adiabatic energy transfer from the projectile to the electrons. The rate of energy transfer is directly related to the electronic stopping. In addition, it is possible to compute non-adiabatic forces on the nuclei and other quantities. We have used this approach to study proton and $\alpha$-particle irradiation of a number of materials such as LiF [1,2], Al [2,3,4], Au [5], Ge [6], and $SiO_2$, and the self-irradiation of Fe. The latter are directly relevant to fusion reactors.

[1] M. Pruneda, D. Sánchez-Portal, A. Arnau, J. I. Juaristi and E. Artacho, Physical Review Letters**99**, 235501 (2007).
[2] M. A. Zeb, J. Kohanoff, D. Sánchez-Portal and E. Artacho, NIMB **303**, 59 (2013).
[3] A. A. Correa, J. Kohanoff, E. Artacho, D. Sánchez-Portal and A. Caro, Physical Review Letters, **108**, 213201 (2012).
[4] A. Schleife, Y. Kanai and A. A. Correa, Physical Review B **91**, 014306 (2015)
[6] M. A. Zeb, J. Kohanoff, D. Sánchez-Portal, A. Arnau, J. I. Juaristi and E. Artacho, Physical Review Letters, **108**, 225504 (2012).
[6] R. Ullah, F. Corsetti, D. Sánchez-Portal and E. Artacho, Physical Review B **91**, 12503 (2015).

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# Quantum nuclei in materials: (when) do we need to worry?

M. Ceriotti*
*Laboratory of Computational Science and Modelling (COSMO), MXG 338 (Bâtiment MXG), Station 12, CH-1015 Lausanne*

I will present an introduction to the modeling of the quantization of ionic degrees of freedom in materials, that is necessary to describe zero-point energy or tunneling effects. I will discuss path integral molecular dynamics and colored-noise acceleration, the most relevant experimental observables related to nuclear quantum effects, and the situations in which they can be expected to be important - including water, hydrogen-containing materials and point defects in metals.

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# Quantum theory of transport and trapping of hydrogen in iron

Anthony T. Paxton* and Ivaylo H. Katzarov

*Department of Physics, King's College London, Strand, London WC2R 2LS*

I will describe recent progress in the calculation of diffusivity of hydrogen in body centred cubic iron. Electronic structure is described within the tight binding approximation and the dynamics of hydrogen is rendered using quantum statistical mechanical methods based within the Feynman path integral formulation. I focus in particular upon two aspects of the problem. One is the capture and escape from traps arising at crystal lattice defects, in particular the vacancy. The other is the isotope effect, which highlights the non classical dependence upon the mass of the diffusing particle.

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# Nuclear quantum effects in tritium diffusion in α-iron

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Molecular dynamics simulation is a very useful tool and has been extensively used in various fields including physics, chemistry, biology and material sciences. The working equations mostly used in the standard molecular dynamics simulation are Newton equations based on classical mechanics, where nuclear quantum effects, such as zero-point energy and tunneling, are completely ignored. The validity of classical dynamics has not yet been fully established in many cases since we do not have an exact quantum method that can be applied to dynamical processes with many degrees of freedom. Recently, ring-polymer molecular dynamics (RPMD) simulation have been becoming a practical and useful computational tool that can describe quantum nuclear effects in various dynamical processes at a relatively accurate level [1]. The RPMD method is an approximate quantum mechanical simulation technique based on path-integral formalism that enables inclusion of nuclear quantization effects. The RPMD model allows for the simulation of real-time dynamical trajectories and provides a consistent framework for simulating both quantum mechanical and classical mechanical degrees of freedom. This method has been recently applied to obtain various dynamical quantities including chemical reaction rate coefficients as well as diffusion coefficients [2-4]. However, it is also known that RPMD fails to describe high-frequency vibrational motions [5].

In this work, we apply the RPMD method as well as CMD (centroid molecular dynamics [6], also including nuclear quantum effects with a slightly different theoretical treatment) method to hydrogen diffusion in α-iron [7]. We have employed the embedded atom model potential energy interaction partly constructed with DFT calculations. It was found that the H and T diffusion has the crossover temperature of 500 and 300 K, respectively, derived from the temperature dependence of the calculated diffusion coefficients. This indicates that nuclear quantum effects are not negligible below these temperatures. In addition, we found that vibrational quantization is also playing an essential role in diffusion mechanisms because of the existence of second-order saddle point with imaginary frequencies.

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# The need for a better understanding of plasma-material interactions in ITER and the role of modelling

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ITER, currently being built in Southern France, aims at producing 500MW of output power for durations of 400s, thereby demonstrating the scientific and technological feasibility of fusion power for peaceful purposes. In a fusion device, power from the core plasma has to be exhausted by the plasma-facing components, mainly in the divertor area, a special area of the plasma chamber where the open magnetic field lines intersect the primary plasma facing components and where the plasma is neutralized and pumped away. The plasma-facing surfaces in the divertor are thus exposed to extreme heat (>10MW.m-2) and particle fluxes (up to 1024m-2s-1 or 1.6x105A.m-2) for extended durations and accordingly to unprecedented ion fluences. In addition, the very high localized heat fluxes caused by unmitigated edge-localized modes (ELMs) (several GW.m−2 for 0.5–1ms) are high enough to lead to material erosion, melting, and vaporization for most materials and represent a serious concern for the lifetime of the plasma-facing components. ELM mitigation is required in ITER to keep the energy density below the melting threshold of tungsten. A large number (>107) of mitigated ELMs (with E<0.5MJ.m-2) is however expected over the divertor lifetime.

Bombardment of tungsten surfaces by low-energy ions (D/He) is known to lead to strong morphology changes which are well-documented and subject to intensive investigations. The impact of those morphology changes on the long-term evolution of the material thermo-mechanical properties is however not known. Similarly, while significant surface damage can occur for surfaces exposed to large number of ELM-like transients even at the moderate energy densities expected during mitigated ELMs, the impact of the strong material cracking/roughening on the power handling capability of the material is not yet clear.

It is probably not possible to address all those issues experimentally before ITER starts operating, but the preparation for ITER operations implies building the strongest possible physics basis. Modelling has therefore a key role to play in the plasma-material interaction area. Ultimately, the goal of numerical simulations should be to build a model that is global enough to capture the behaviour of a material under fusion conditions and can ‘predict’ changes of the material thermo-mechanical properties under prolonged operation.

This talk will introduce the various challenges related to power exhaust and plasma-wall interactions in ITER with an emphasis on the open questions where further research is needed and modelling can help.

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# Vacancy defects studied in tungsten by using Positron annihilation spectroscopy

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Tungsten has been chosen to recover parts of the divertor and is a candidate material for first wall armor of future thermonuclear fusion reactors (ITER and DEMO) where it will be subjected to extreme conditions: neutron irradiation, He and H fluxes and high temperatures. The introduction of He, point defects and H in metals lead to the evolution of the microstructure and macroscopic properties such as mechanical properties (embrittlement, swelling..) that have to be understood to foresee the lifetime of the component in such extreme conditions.

Positron annihilation spectroscopy (PAS) is a well-known and established technique, able to characterize vacancy defects and free volumes in materials. It is sensitive to the size of the defects from the single vacancy and to their clustering or their decoration with impurities (such as He…) with a great advantage of probing thin damage region by using slow positron beams. In this presentation the principles of the technique will be reminded and some examples of the results obtained in W will be developed. We show how carefully designed experimental investigations using PAS and other techniques such as TEM, NRA (nuclear reaction analysis), and modeling can complement each other and provide a route to the understanding of the microstructure evolution of materials in these conditions.

On one hand, in the objective of determining the properties of vacancy defect and their interaction with He, the distribution and the nature of $^3$He implantation-induced defects in tungsten samples have been studied by PAS as a function of implantation fluence. The results show that monovacancies are generated along the ion path and that their concentration varies directly with the implantation fluence. The annealing induces agglomeration to form large vacancy clusters. These results are in good agreement with object kinetic Monte-Carlo (LAKIMOCA) simulations.

On the other hand, in the aim of studying and understanding the evolution of the microstructure of tungsten under irradiation in an environment close to the one of future fusion reactors such as ITER and DEMO, irradiation of W samples with W ions were carried out as a function of dose and temperature. PAS revealed small vacancy clusters. Their size and concentration increase with irradiation dose up to 1 dpa and annealing of irradiated samples a change in their size and concentration. TEM observations show that the formation of vacancy defects, namely voids or vacancy loops, depends on the irradiation dose and temperature.

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# Experimental studies of hydrogen transport parameters in tungsten

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Tritium inventory and permeation will certainly grow more in importance with ITER and next step devices employing metal plasma facing materials or components, as a consequence of the expanded use of tritium coupled with longer pulse or steady state operation. Specifically, tungsten is presently planned for use in the ITER divertor and possibly as an armor material for the first wall in next-step devices.

To improve our modeling and predictive capabilities of tritium inventory and permeation in fusion devices employing tungsten, we must solve the hydrogen transport equation, which requires solution to the diffusion equation with appropriate boundary conditions and trapping parameters. In general, the boundary conditions and trap parameters are time dependent due to the physico-chemical changes occurring at the tungsten surface from material mixing / erosion processes or changes in bulk material properties from neutron or heat loads. Presently, large uncertainties exist in accurately determining the nature of such boundary conditions and trap parameters, which hinders a robust and accurate estimate of tritium inventory and permeation in fusion devices.

In this presentation, we present our on-going efforts to establish the foundation necessary to quantitatively predict hydrogen transport (release, trapping, permeation) in tungsten. We address the following three phenomena that are important for quantifying tritium transport. First, the changes in boundary condition and its impact on the inward diffusive flux as function of temperature due to impurity induced near surface changes (C, N, He, Ar, Ne) or by surface melting are discussed. Second, we present our effort on determining the fundamental parameter of hydrogen diffusion coefficient in the temperature range of interest in fusion ($300 < T < 1000$ K). Third, we present novel ion/electron beam and tritium tracer experiments that appear promising in determining some of the fundamental parameters, which may allow testing and bridging of first principle simulations with laboratory experiments.

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# Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach

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The mechanical integrity of many materials is impacted by the presence of hydrogen and even minute amounts of a few *ppm* may give rise to fracture and embrittlement. This is particularly true for metallic alloys designed to withstand high mechanical loads. From a modeling point of view, the description of the impact of H on mechanical properties is challenging since it is well known to interact with almost all microstructural and point defects. Thus, a quantitative description of how H impacts and interacts with the various defects requires to model large length- and timescales while also having to take into account atomistic effects. In the talk it will be shown how combining *ab initio* calculation with thermodynamic concepts allows to determine free energies at finite temperatures with a hitherto unprecedented accuracy. These concepts have been successfully used to (i) identify the relevant mechanisms at atomic scale and (ii) to construct atomistically informed mesoscale/macroscale concepts that allow to model H embrittlement on the length and time scales relevant for experiment.

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# Setting up plasma pulse-scale simulations with electronic structure calculations

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In a fusion device, the interactions between the plasma and the surrounding armour material take place in time-scales ranging from microseconds to hours, and in length-scales from nanometres to centimetres. The experimental observations typically cover these time-scales, whereas the spatial resolution is usually observed as an integral over vessel surface areas. For understanding the underlying microscopic phenomena leading to observed larger scale events, dedicated laboratory experiments and computational studies need to be carried out focusing on the microscopic effects on the surface and in the bulk of the fusion relevant materials, such as tungsten (W) and beryllium (Be).

Use of electronic structure calculations is an essential tool in studying the microscopic effects theoretically. Obtained results are used as building blocks when increasing the knowledge on effects taking place in larger length and time scales, and studied with applicable computational tools such as Molecular Dynamics, kinetic Monte Carlo calculations, and further with the Rate Theory calculations. Computational studies extended into multiple length and time-scales allow understanding and extrapolating the experimentally observed materials effects under plasma conditions. Starting from electronic structure calculations we study the effects of hydrogen (H) trapping and diffusion in W, point defects, and defect clustering. The theoretical results will be used in multi-scale Rate Theory calculations, and compared with implantation experiments, and thermally activated desorption results. Recent W-Be-H results obtained with Molecular Dynamics calculations will be discussed and compared against the experimental erosion and deposition data obtained from JET's ITER-Like Wall campaign.

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# Hydrogen recycling in tungsten during plasma pulse simulations with rate equations

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Hydrogen recycling between fusion plasma and plasma facing materials is one of the most important issues to achieve stable steady state fusion operation. It affects also the hydrogen isotope retention (i.e. tritium inventory). Most of the particles in the plasma have entered the plasma through recycling from the plasma facing components.

Using rate theory equations we simulate hydrogen recycling and retention in tungsten during plasma pulses. Results show that there are short periods of times during which H particle flux back towards the plasma is larger than the flux into the tungsten material. Moreover, the vacancy formation in tungsten is simulated for both high energy deuterium irradiation experiments and below threshold displacement energies. The vacancy formation is seen to be flux dependent especially for low energy irradiations.

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# Multiscale modelling of radiation effects in materials: ion implantation versus neutron irradiation

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Modelling radiation effects requires bridging a wide range of time and length scales. For example, defects are produced in a picosecond timescale while diffusion of these defects can expand seconds or hours. A multiscale approach, using different simulation methods, have proven to be a very successful way to model damage production and damage evolution. However, care must be taken in the transfer of information from one simulation level to the next, to make sure all the relevant processes are included in the model.

In this presentation we will provide a description of the most commonly used multiscale modelling approach: combining density functional theory calculations, molecular dynamics simulations and object kinetic Monte Carlo, to provide information that can be directly compared to experimental measurements of damage in irradiated materials. We will focus on one example: damage produced in Fe and FeCr alloys. And we will discuss one particular issue: the differences between ion implantation and neutron irradiation. Currently, ion implantation is commonly used to obtain information about defect production and defect evolution, in an attempt to build models for neutron damage. We will point out the differences and commonalities between the two types of irradiation, and those aspects that should be taken into consideration when building models for neutron irradiation from information obtained from ion implantation.

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# Modeling isotope exchange in W using fill level dependent trapping

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Common diffusion trapping models for modeling hydrogen transport in metals are limited to traps with single de-trapping energies and a saturation occupancy of one. While they are successful in predicting typical mono isotopic ion implantation and thermal degassing experiments, they fail at describing recent experiments on isotope exchange at low temperatures. Following the predictions of DFT calculations we have developed a new diffusion trapping model [1] that is based on fill-level-dependent de-trapping, where each trap site can contain an integer number of hydrogen atoms and the de-trapping energy depends on the current fill level. This model allowed us to describe the isotope exchange experiments conducted close to room temperature where common diffusion trapping codes predict no-isotope exchange since all traps are filled and inactive.

The main input data into the new fill-level-dependent de-trapping code is the fill level dependence of hydrogen binding energy in a particular trap site. These numbers are only available from DFT calculations at the moment and are thus limited to small defects like mono-vacancies. However from previous experiments it seems that in W trapping is probably dominated by dislocations [2]. Therefore the initial comparison with experiments using the data for mono-vacancies only qualitatively reproduced the data but a quantitative match required an ad-hock fit of the activation energies.

In this presentation we will discuss the implication of fill-level-dependent de-trapping both for mono-isotopic and for isotope exchange experiments. We will show that for mono-isotopic experiments the new model is indiscernible within experimental uncertainties from common diffusion trapping models. For isotope exchange experiments we will show that common diffusion trapping models not just underestimate the isotope exchange at low temperatures but that they also fail at correctly describing propagation of the diffusion front during isotope exchange experiments.

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# Macroscopic rate equation modeling of trapping/detrapping of hydrogen isotopes in tungsten materials

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Macroscopic rate equations (MRE) are used to investigate migration and trapping of hydrogen isotopes (HIs) in metallic materials at scales relevant to realistic experiments such as thermal desorption spectrometry (TDS) measurements realized after plasma or ions exposure of a tungsten (W) sample. In usual MRE models as TMAP7, HIIPC or our own code MHIMS (Migration of Hydrogen Isotope in MaterialS), each trapping site can only trap a single HI and each type of trapping site has a unique and constant detrapping energy. In the first part of this presentation, the free parameters of the MHIMS code are adjusted thanks to well defined TDS experimental data. Then, MHIMS is frozen and used to extrapolate to different experiences as retention versus ions fluence or evolution of retention of HIs in function of the sample temperature: the predicted results are in good agreement with the experimental data. However, DFT calculations have shown that in a single crystal of W at room temperature up to 6 HIs can be trapped in a single type of trap such as a mono-vacancy. In such a vacancy, the detrapping energy increases as the number of HIs decreases. These results are not the one used in MHIMS. Thus, a new version of the code called "MHIMS-reservoir" has been developed based on these DFT outcomes. This approach has been recently used by K. Schmid and co-workers to model the isotopic exchange observations which are difficult to reproduce with a usual MRE model. In the following part of the presentation, the newly implemented MHIMS-reservoir equations are first described and then, their outcomes confronted to experimental TDS measurements after ions implantation in a tungsten single crystal (SCW). In the simulation with no time lag between implantation and TDS, the TDS spectrum is composed of 3 peaks. The first TDS peak observed at low temperature corresponds to vacancies filled with 6 HIs; the second peak at medium temperature to vacancies filled with 5-3 HIs; and the third one at high temperature, which is the dominant one, to vacancies filled with 2-1 HIs. Experimentally, one or two peaks are observed. Complete simulation with all the step followed in the experiment shows that the number of peaks observed experimentally is highly dependent on the time lag between implantation and TDS measurements.
Using DFT values for detrapping energies, the MHIMS reservoir model is able to fit the experimental TDS measurements presented by Poon and co-workers taking into account the TDS chamber baking at 400 K during 1.5 h which precedes the TDS measurement. In the case of TDS measurement from Quastel and co-workers, we have to decrease the detrapping energies by 10 % in order to fit the experimental spectrum. This could be explained by the high impinging deuterium flux (1020 D/m²/s) used in those experiments which induces traps creation.

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# Migration, trapping and release of deuterium from tungsten in the presence of high density of defects: theory and experiment

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Due to practical importance of using of tungsten (W) as a plasma-facing material for fusion application and wide accumulated database, the deuterium (D) accumulation and release in W are analyzed in the present contribution. Those plasma-facing components of fusion reactors will be exposed to 14 MeV neutrons. Ion irradiation with energetic heavy ions is currently recognized as the only non-activating method to simulate the fast neutron damage produced in fusion reactors. Therefore, in this work, 20 MeV W ions were used to simulate n-induced damage in W samples. Following to the damage production by the irradiation at different dpa levels, samples were loaded by $D_2$ gas, D thermal atoms or low-energy D plasma. Each sample was exposed once to the certain experimental condition. Post-mortem measurements were nuclear reaction method (NRA) and thermal desorption spectroscopy (TDS). The D retention in damaged W was compared to that in undamaged W. The formation of blisters observed in the case of undamaged W was suppressed after pre-irradiation of W with self-ions because of creation of a high density of defects in damaged W which prevent any local super-saturation and, therefore, quenching blister formation.

Rate equations have been used to model experimental data. The diffusivity, solubility, reflection coefficient, surface barrier, binding energies of D with different types of defects and density of defects are input parameters for rate equation model. These parameters can be derived from the first-principle (DFT) calculations, effective-medium theory (EMT), molecular dynamics (MD) and TRIM calculations. Incorporation of binding energies of D with a vacancy and a dislocation recently calculated by DFT [1,2] and penetration probability and ion range calculated by MD and TRIM [3] in the rate equation model allows us to validate different predictions against experimental data. A comparison of calculations using different theoretical models with experimental values can clarify the physics underling the hydrogen-metal interaction and can provide an answer on several important questions, namely, (i) which type of trap corresponds to certain D binding energy, (ii) which is a range of validity of MD and TRIM models as well as limitation of DFT calculations and (iii) which process is rate-limited in respect to the D uptake and release in W. Modelling of experimental data of the D depth profile in pre-damaged W after exposure to thermal atoms, D2 gas or low-energy plasma did not show any local super-saturation that is in an agreement with experiments and explains the mechanism of the blister formation. It was shown analytically and confirmed experimentally that the D migration and trapping in a presence of high density of defects in W depends on the penetrated ion flux, incident D energy, defect density and sample temperature.

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# Influence of aluminum oxide coating oxygen presence in plasma on deuterium retention in tungsten

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The report presents the results of the experiments made in MIKMA device [1] with the samples of PLANSEE tungsten. The samples were irradiated by the ions of deuterium (or deuterium with oxygen addition) plasma.The irradiating ion current density was (3.9-7.9)×$10^{19}$ at/$m^2$sec, the sample temperature – 500 K. The amount of gases retained in the samples after each experiment were determined by Thermal Desorption Spectrometry (TDS). The samples were not annealed after each TDS.

Experimental results (fig. 1.) show that fluence dependence of deuterium trapping in tungsten is determined by ion energy. Aluminum oxide coating increases retention of the implanted deuterium atoms preventing their diffusion to the surface. Irradiation of the tungsten with ions of the oxygen added plasma leads to the decrease of deuterium trapping. Oxygen seems to initiate surface reactions activating deuterium atom recombination and release from the surface. The same processes courses the release of pre-implanted deuterium atoms from the aluminum oxide coated tungsten, when the last one is irradiated by the ions of the oxygen added hydrogen plasma. The irradiation activated processes leading to observed phenomena are discussed.

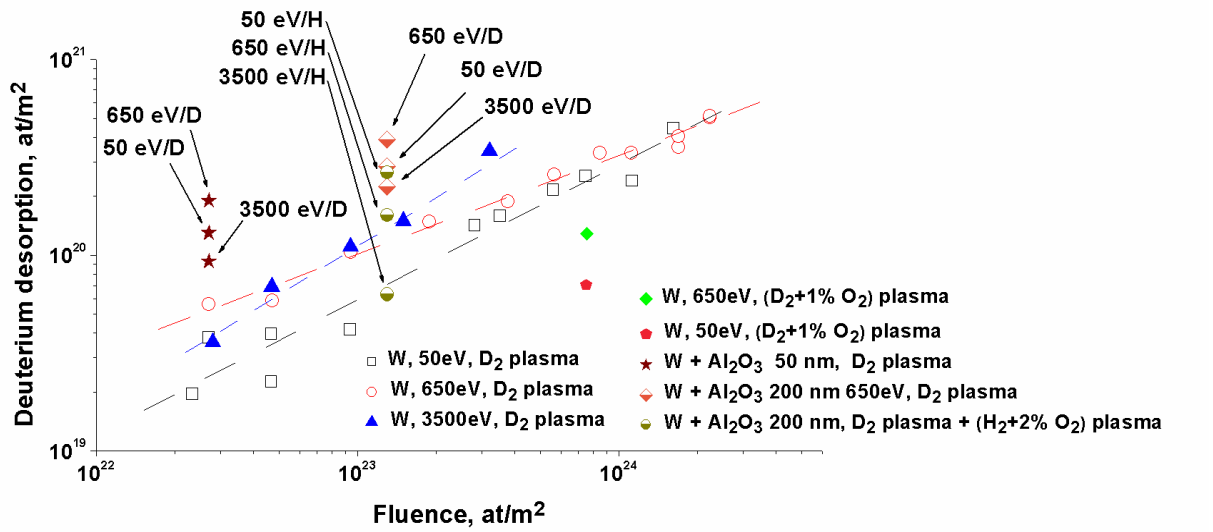


Fig.1. Deuterium retention in both tungsten and tungsten with aluminum oxide coating after irradiation under various conditions.

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# Deuterium retention in polycrystalline tungsten at low fluences

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Fuel retention is one of the critical issues for plasma facing materials in fusion devices because of nuclear safety regulation related to the tritium inventory. In this contribution, we will present our progress in building a consistent database on deuterium retention in tungsten, which is being used in an integrated experiment-multi-scale modeling approach dedicated to reveal fundamental mechanisms behind deuterium and tritium retention in tungsten materials (WHISCI A*MIDEX project). This is a mandatory step for any reliable and predictive ITER wall model to be developed.

In an introducing part, we will present our experimental setup which has been designed to avoid any spurious effects related to contamination and air exposure. In our apparatus, tungsten samples are prepared, implanted with deuterium ions and characterized all *in-situ* in ultrahigh vacuum. For precise quantification of deuterium retention, a high-sensitivity Temperature Programmed Desorption (TPD) is used allowing exploring fluences as low as a few $10^{17}$ D/m$^2$. This sensitivity eases the comparison with theoretical methods and allows detecting any surface effects in retention/release processes. We underline the fact that a great number of parameters are controlled independently in this apparatus, such as the ion kinetic energy, the ion flux, the sample temperature during ion implantation, the time between ion implantation and retention measurement… as well as the quality of the sample since we obtained implanted polycrystalline samples exhibiting a single deuterium desorption peak.

Then, we will present systematic studies on how deuterium retention depends on some of these parameters. First, we will confirm a “universal” retention *vs.* fluence relationship for polycrystalline tungsten by extending *in-situ* results of Ogorodnikova *et al.* [1] to low fluences, from $10^{21}$ D$^+$/m$^2$ down to $10^{17}$ D$^+$/m$^2$. Second, we will evidence a release of implanted deuterium from tungsten at room temperature, a behavior that can be rationalized with recent DFT results [2]. Third, the deuterium retention dependency with the implantation temperature will be presented for low fluences. These new results will be compared with high fluences results from Roszell *et al.* [3] as well as post-implantation annealing experiments performed in our laboratory.

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# Hydrogen trapping at vacancies and hydrogen impact on vacancy diffusion and self-diffusion in Ni

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We study possible implications of vacancy-hydrogen clusters in environmental damage of "structural" metallic alloys (oxidation, hydrogen (H) embrittlement, eventually irradiation). In Ni (and Pd), Fukai has shown that gigantic concentrations (up to 25 at. %) of vacancies can be stabilized by H [1,2,3] and that it could increase by several orders of magnitude the diffusion coefficients of the host metal. The conditions, however, are extreme: originally, the project concerned hydrides at high temperature (600-900C, pH2=3GPa). One can wonder if these effects exist in the service conditions of Ni based alloys: room temperature and CH=2000ppm for H embrittlement and 600K, CH= 2500ppm to 1at.% for stress corrosion cracking in pressurized water reactors. We have performed EAM and DFT calculations of H segregation energies at vacancies in Ni. The maximum binding is 0.27eV and 0.4eV in the single and divacancy respectively, in good agreement with Fukai's Thermal Desorption Spectroscopy results. By a comprehensive calculation of the formation energy of VHn clusters (n=1 to 14), it was shown that segregation occurs mostly on the octahedral site (off-centered) in the vacancy (O1) with almost no O1-O1 interactions, strong O1-T1 (tetrahedral) repulsion and weak attractive O1-O2 interaction. Approximately constant effective pair interactions can be extracted from these formation energies. Together with the segregation energies in the dilute limit, they constitute a simple energetic model from which we can derive the equilibrium distributions and concentrations of VHn (analytical formulas are validated against Monte Carlo simulations). The knowledge of the statistical weight of the various clusters enables to select a limited number of configurations to evaluate migration barriers, and from this, the diffusion coefficient of the clusters. H drastically slows down the vacancies, but this effect is overcompensated by the increase in equilibrium vacancies and finally Ni self-diffusion is markedly increased.
We have also studied the trapping of H at vacancies. We show that we can use a random walk model to derive the effective diffusion coefficient, as a function of the vacancy concentration. The use of First Passage Time Analysis [4] enables to consider the inner sites connectivity in the model and go beyond Oriani's formulation. Finally, a simple model is proposed which is valid at high vacancy concentrations (KMC simulations are used as a check) and for defects larger than vacancies, like small precipitates. We believe such modeling can be useful to design microstructures optimized to slow down H penetration.

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# Vacancy nanoclusters in irradiated W and W alloys: First-principles assessments and multi-scale modelling

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Understanding of irradiation-induced vacancy behaviour in tungsten is one of outstanding and debate issues since the 1960s although numerous studies have been taken with regard to the generation and formation of defect structures formed under irradiation. On one hand, a nucleation and growth of vacancies into voids and dislocation loops can be observed in damage microstructures in W and W alloys using neutron and ion irradiation. On the other hand, the vacancy population produced by irradiation was unaccounted for in form of vacancy defects which could not be reliably sized within nano scale using TEM but small vacancy clusters can be detected by Positron Annihilation Spectroscopy (PAS).

By employing multi-scale approach based on first-principles assessment for which the inhomogeneous and low electron density in vacancy-cluster regions has been taken into account, we have performed a systematic study of energetic and kinetic properties of nano-vacancy in bcc TMs with a particular focus on tungsten and origin of the observed anomalous effects of solute segregation in W alloys. The formation and migration energies of vacancy clusters in nanometer-size scale as well as different dissociation pathway of vacancy clusters have been investigated in order to assess the stability and transformation of different defect configurations by using density functional theory (DFT) calculations in combination with molecular relaxation and kinetic Monte-Carlo simulations at various ranges of temperature and time. Importantly, our ab-initio data base for vacancy cluster calculations have been used to designing a new EAM-type interatomic potentials for which the surface corrections to the embedding functional have been implemented. By cross-checking both formation and migration energies for nanoclusters of vacancies, the agreement between new corrected EAM potentials with DFT calculations is very satisfactory. The predicted temperature of vacancy-cluster dissociation is consistent not only with observation of the voids ibut also with the variation of dislocation length in high-temperature annealing of self-ion irradiated tungsten [1]. Finally, we describe briefly the extension of a combined DFT-MC formalism by considering vacancy as a new element in a multi-component alloys in order to study the origin of coherent precipitates in W-2%Re alloys under irradiation [2].

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## Materials research in Jülich: hydrogen retention in beryllium

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Interactions of the beryllium first wall with hydrogenic plasma species and intrinsic and seeded plasma impurities represent a particular interest for ITER. The main issues are the wall lifetime, formation of mixed layers (e.g. Be-W-N) in the divertor, and tritium retention. Forschungszentrum Jülich focuses its activities on these aspects of plasma-wall interactions, as well as on the development of advanced materials for first wall components. This contribution will give a short overview of experimental setups in Jülich, namely the linear plasma device PSI-2 and two multi-purpose experiments combining surface preparation, treatment and analysis (Artoss and the new XPS facility). Furthermore, the synergy of modelling and experiments will be illustrated on the example of hydrogen retention in Be addressed by means of diffusion-trapping modelling.
The diffusion-trapping model for Be is based on a system of coupled reaction-diffusion equations incorporated in the CRDS code [1] and supplied with an input from DFT simulation results [2]. The code is used to interpret experimental results on hydrogen retention in Be [3, 4]. The model allows introducing multiple diffusing species including mobile traps, multiple trapping in mono-vacancies, and surface-limited desorption processes. CRDS was successfully applied earlier to explain temperature-programmed desorption (TPD) experiments with monocrystalline and polycrystalline Be irradiated to low D fluences (~ $3\times10^{19}$ D/m$^2$) in the Artoss facility [1]. In this contribution, we revise hydrogen retention and transport mechanisms addressed in earlier works and investigate how different model assumptions with respect to involved processes and their parameters influence the simulated TPD spectra. The particular interest represent low-temperature desorption peaks (below 500 K) observed for fluences above $2\times10^{21}$ D/m$^2$.

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# Thin tungsten oxide layers : structural properties and deuterium retention.

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Because of its favorable physical properties such as a low erosion yield, a high melting temperature, a high thermal conductivity and a low hydrogen isotope permeation, tungsten is the material used for plasma facing components (PFCs) receiving highest fluxes in operating tokamaks (ASDEX-upgrade, JET-ILW) and will compose the ITER divertor. However, tungsten has a strong chemical affinity with oxygen and native oxide is naturally present on tungsten surfaces. On PFCs, oxide layers ($WO_{3-x}$) can be formed due to the presence of $O_2$ as a contamination, PFCs high temperature (few hundred degrees) and in case of accidental scenarii. Oxidation will induce a modification of tungsten wall properties especially regarding the erosion yield [1,2], the reflectivity and the deuterium retention [3,4,5] which will depend on the structure, the stoechiometry and the thickness of the oxide layers formed.
In order to study the effect of oxidation on tungsten PFCs properties, the behavior of oxide layers under deuterium bombardment and thermal cycling in divertor-like conditions, we have produced thin $WO_{3-x}$ layers which mimic the possible oxidation of tungsten PFCs. Tungsten samples were thermally oxidized, controlling temperature and oxygen partial pressure. We used recrystallized and non recrystallized polycrystalline tungsten samples.
Once characterized, W samples were put into vacuum (~$10^{-7}$mbar) and thermally oxidized at 400°C and at different oxygen partial pressures. The tungsten oxide layers formed were 80nm - 250nm thick. Different growth rates of oxide layers depending on $P(O_2)$ at 400°C have been measured. X-rays diffraction shows the existence of monoclinic and orthorhombic structure. The local structure of the formed oxide layers is investigated at different scales by Raman spectroscopy, SEM, TEM, and AFM. Annealing of the tungsten oxides is being performed and shows an evolution of oxide layer. Deuterium bombardment and annealing under deuterium atmosphere of the samples are under investigation. Retention, chemical erosion, stoechiometry and structure modification of the tungsten oxides will be studied.

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# The Xolotl Plasma-Surface Interactions Simulator

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Plasma surface interactions in fusion tokamak reactors involve an inherently multiscale, highly non-equilibrium set of phenomena, for which current models are inadequate to predict the divertor response and feedback on the plasma. In this presentation, we describe the code development of Xolotl, a new continuum advection-reaction-diffusion cluster dynamics code which simulates the divertor surface response to fusion relevant plasma exposure. Our initial effort focused on the simulation of the behavior of tungsten material during the exposure of 100 eV helium plasma.

The rate-equation theory used by Xolotl to predict the time evolution of the divertor surface will be first described, including the different reactions taking place, the diffusion of mobile clusters, the drift of small helium clusters toward the surface, how they are modeled after what is seen in atomistic simulations, and how the physics parameters were obtained.

As well, an uncertainty quantification effort is being conducted as a part of the development of Xolotl. It aims at understanding the effect of the input parameters – physical quantities obtained from atomistic simulations for instance – on the final results of the simulation. The uncertainty quantification strategy and tools will be presented.

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# Path integral molecular dynamics for the nuclear quantum effects in the Frenkel defects in BCC Fe

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The Frenkel defects created from irradiation damage have significant influence on the mechanical properties of metals. Molecular dynamics (MD) simulations have been routinely used to probe the defect production rate and mechanism of the displacement cascades [1]. In the conventional MD simulations, nuclei are typically treated as classical point mass. On the other hand, the quantum nature of the nuclei, even for the heavy ones such as Fe, can affect the relative free energy between different configurations. Therefore, it is of interest to investigate how nuclear quantum effects (NQEs) alter the free energy associated with the Frenkel defects.

In the present study, path integral molecular dynamics simulations were employed to evaluate the quantum correction term in the free energy estimation for the Frenkel defect in BCC iron. Using the empirical EAM force field for bulk iron with a Frenkel pair embedded, we predicted that the quantum nuclear effects stablize the Frenkel defects by a small amount. The nuclear quantum contribution to the free energy associated with a Frenkel pair was estimated to be -14±1 meV. We also found that the NQEs promote both the interstitial and the vacancy formations. The quantum effects are quite localized near the defects, spreading only towards the nearest neighboring atoms.

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# Experiment and modelling of hydrogen isotope exchange in beryllium layers as mean of T inventory control in ITER

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In the nuclear phase of ITER, wall conditioning will certainly contribute to the control of the tritium inventory - a major safety issue since the agreed safety limit inside the vessel must be kept under 640g during D:T operation [1] - by depleting tritium from the walls and in particular from that co-deposited with beryllium. High isotopic exchange efficiency in Glow Discharge Conditioning (GDC) or Ion Cyclotron Wall Conditioning (ICWC) plasmas have been reported [2]. However, the mechanisms at play in the interaction between hydrogen and beryllium layers are still poorly understood at a microscopic level, and there is in particular no specific theory or model in the literature to describe isotopic exchange.

We present here a 1D Diffusion Trapping Model for Isotopic eXchange - DITMIX - developed in order to understand the interaction mechanisms between hydrogenic species and beryllium co-deposited layers. The model is based on existing approaches to simulate hydrogen transport in metals [3,4] and includes processes like hydrogen implantation, trapping in ion-induced trap sites, detrapping to a solute (mobile) state, diffusion in Be and recombination to molecular form at the surface. Simulated profiles of hydrogen atoms are in a good agreement with those measured by $^{15}$N-NRA on pre-characterized 600 nm thick Be:H layers, which were irradiated by $D^+$ ions with well-defined fluxes and energies, for different durations and surface temperatures. However, the model predicts larger amounts of D atoms in the bulk of Be:Hlayers than those experimentally obtained from $^4$He-ERD measurements, casting some doubt on the processes involved.

DITMIX yields important information on the efficiency of the foreseen conditioning techniques for T inventory control. Hence GDC applied in ITER during one day or more is just efficient enough to remove an amount of tritium comparable to the estimated retention in a nominal ITER D:T shot [2], even in combination with baking at 513 K. Pulsed ICWC at 343 K - the wall temperature during ITER operation – would be efficient for $D^+$ fluxes to the wall as high as $10^{20}$–$10^{21}$ $m^{-2}.s^{-1}$.

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# DFT calculations of voids in α-Fe

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The point defects such vacancies are known to play significant role on diffusion in crystals. Vacancies and cavities can still lead to changes in micro-structure with subsequent changes in materials properties. They induce damage on the mechanical properties for alloys and metals displacement, such fragility, tensile strength, crack resistance, ductility, creep behaviors, and lead to premature aging structures. The formation of vacancy clusters occurs via various types of reactions of vacancy's point defects.
We present a first principles study of multi-vacancies ($V_n$, n=1, until 15) in α-Fe bulk and monovacancy on (100) and (110) surfaces by means of the density functional theory [1-2]. For the monovacancy, the formation energy ($E_f$=2.16 eV), diffusion coefficient ($D_0$=0.16 $cm^2/s$) and migration activation energy ($E_m$=0.64 eV) are found in agreement with experimental and theoretical data of the literature [3-5]. The vacancy formation energy on Fe(100) surface is more than twice smaller than on Fe(110)surface.
The second and first nearest neighboring configuration (2NN & 1NN) for divacancies is found to be the most stable configurations. Other divacancies configurations (3-7NN) have binding energy close to 0.0 eV. We show that most stable divacancy (2NN) diffuses through the 1NN configuration with a barrier equivalent to the one of the monovacancy.
To complete the description of divacancies, the mechanisms of formation/dissociation from isolated monovacancies are discussed in detail. We finally present results on $V_n$ vacancies with n ={3, 15}. We show that most stable vacancy is more compact vacancy which contains biggest number of 1NN and 2NN fragments.
Our calculations are performed using the Vienna *ab initio* simulation package VASP using projected-augmented wave (PAW) method for the description of the pseudopotential. Exchange and correlation are described with the functional of Ceperley and Adler parameterized by Perdew and Zunger with the nonlocal generalized gradient approximation (GGA) of Perdew and Wang 91.

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# Meta-stable state of 111-crowdion binding with $VH_6$ complex in tungsten

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Since tungsten will be used for plasma facing component materials in ITER and is a candidate material also for DEMO reactors, tritium retention in neutron damaged tungsten is a key issue. Recently, experimental works with fission neutrons and high-energy heavy surrogate ions have been performed to evaluate the radiation effects [1, 2]. These works show significant enhancement of the retention in the damaged tungsten and primary roles of radiation induced vacancies and/or vacancy clusters (voids).

In divertor plasmas, the tungsten target would be exposed to low-energy and high-flux plasma particles as well as neutron. Strong enhancement of the hydrogen retention in single- and polycrystalline tungsten specimens has been observed at higher fluxes [3]. A distinct feature of plasma irradiation from gas permeation obeying the Sieverts' law is that incident hydrogen atoms/ions from the plasma can readily overcome permeation barriers of the surface without high pressures. One can, therefore, assume that under the continuous high-flux implantation local concentration of hydrogen atoms can exceed the solubility limit of the tungsten. In such cases, the tungsten matrix may contain super-saturated hydrogen atoms and sustain extremely high stresses. Therefore, the blistering of tungsten surfaces may be induced by the exceedingly high local concentration of hydrogen atoms beyond the solubility limit of the tungsten [3, 4].

For a better characterization of radiation damages in the tungsten under the divertor condition, we examined impact of hydrogen cluster formations on the radiation damages in the tungsten. The present density functional theories (DFT) calculations revealed that an octahedron hydrogen cluster prevents the vacancy from recombining with a self-interstitial-atom in a neighbouring 111-crowdion. The formation energy of the meta-stable state is smaller than sum of the individual formation energies for the $VH_6$ complex and the 111-crowdion indicating that the $VH_6$ complexes can trap the 111-crowdion. This implies that the radiation damage remaining after collision cascades by energetic primary knock-on atoms will be increased in the presence of the hydrogen clusters.

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# Comparing He ion energy transfer to W and Fe surfaces through molecular dynamics simulations

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Exposing W and Fe surfaces to similar He plasma leads to different surface evolution. We investigate, through molecular dynamics (MD) simulations, if a difference in energy transferred from He to the surfaces contributes to the different surface evolution. W and Fe surfaces with four different orientations were bombarded with 60 eV He ions, impacting 0-10 degrees from the surface normal. Comparable numbers of He atoms reflect back from the W and Fe surface monolayers or escape again after first penetrating a little below the surface. However, due to the less unequal mass ratio between He-Fe compared to He-W, He ions transfer energy to Fe more efficiently. As a result, He atoms that reflect from Fe surfaces carry away less kinetic energy than those reflecting from W. This rules out ion energy transfer as an explanation why similar plasma exposure on W leads to several times thicker fuzz layers than on Fe. Somewhat counter-intuitively perhaps, He ions that do not reflect or escape back to the vacuum thermalize at a greater depth below the surface in Fe than in W (25.4 vs. 11.8 Angstrom), despite the more efficient energy exchange between He and Fe. The thermalisation depth result also shows the limits of binary collision approximation (BCA) results, such as from the TRIM code. TRIM results for reflected He ion energies were quite close to MD results. However, the rather simple model of the BCA does not reproduce the unexpected deeper thermalisation depth of He ions in Fe, making it quite doubtful if what happens to He inside W and Fe is described properly.

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# Joint experimental and theoretical efforts to bridge the gap between today's experiments and future fusion devices

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Extrapolating from existing fusion experiments to next generation plasma devices like ITER, DEMO and beyond means bridging several orders of magnitude in almost every plasma and device parameter. To allow for reliable predictive scaling of available results to future devices, a good understanding of the involved processes and validated modelling is crucial. This presentation will illustrate how this can be achieved in a close interplay between dedicated experiments and modelling.
Three experimental setups are selected to demonstrate such a successful combination of experiments, density functional theory (DFT) calculations and modelling: the XPS setup, the ARTOSS experiment and the linear plasma device PSI-2.
The new XPS-setup experiment which is dedicated to investigate chemical reactions and ion-surface interactions was used to measure valence band spectra of Be and Be-N. These were then used to verify DFT results on phase formations expected at first wall. In addition, we compare measured core levels of different tungsten compounds to calculated core levels using the DFT code Fleur [1].
ARTOSS, combining classic surface science tools with accelerator based techniques, focuses on studies on hydrogen retention and release behaviour, especially in Be and Be-based materials. DFT-calculations [2] predict different kinetics for hydrogen and Be self-interstitial diffusion parallel and perpendicular to the basal plane of Be single crystals. Temperature-programmed desorption (TPD) experiments of monocrystalline and polycrystalline Be irradiated with low D fluences (~ $3\times10^{19}$ D/m$^2$) in ARTOSS are modeled using a diffusion-trapping model implemented within the CRDS code. This leads to a refined model of hydrogen retention and transport mechanisms in Be based on DFT calculation results.
Last but not least, the PSI-2 linear plasma device is dedicated to the understanding of plasma-material interactions at reactor-relevant wall loading conditions. Besides giving an overview of experimental capabilities of the device, we present the data and modelling results on the influence of the particle flux density, plasma impurity content and tungsten material microstructure on the D retention.

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# Modelling and Experiments of Plasma-Material Interactions in Presence of Fusion Neutrons

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The interaction of the hydrogen isotope plasma along with the energetic neutrons (14MeV) and alpha particles (3.5 MeV) can cause material erosion, structural damage, fuel retention and changes of thermo-mechanical properties of the material that lead to the eventual mechanical failure of the material depending on the choice of the wall material. In this work we report on neutron induced material damage and the subsequent plasma wall interactions in tungsten, which is the proposed divertor material for ITER. The modelling of neutron damage is currently a priority need due to the non-availability of a fusion relevant high fluence neutron source. ITER-like neutron fluxes can cause very high dpa (displacement per atom) which is a measure of the damage in the system. The interaction of the fusion plasma with the neutron damaged material can trigger hitherto unobserved phenomena which might lead to the failure of the materials much before the anticipated life-time. Hence it becomes extremely important to understand the damage created by the neutrons and the subsequent plasma-wall interactions due to the hydrogen isotopes and alpha particles.

One of the standard approaches is to simulate the neutron damage by creating the equivalent damage by the use of energetic heavy ions. The surrogate ion irradiation is modelled as a series of elastic collisions with the lattice atoms and inelastic scattering by the electron cloud. The elastic collisions result in the formation of primary knock-on atoms (PKA) which results in the formation of ion-vacancy pairs (Frenkel pairs) and their dynamics leading to the formation of vacancy and interstitial clusters. The evolution of these clusters has two consequences: (1) trapping of D/T ions from the plasma at the defect sites leading to fuel retention and (2) microstructural changes leading to the thermo-mechanical failure of the material. The consistent modelling of such a system involves different time and space scales which makes it an inherent multi-scale problem. Here we outline our approach to this problem starting from ab-initio/density functional calculations of activation energies of specific defects to rate equation models of predicting the fuel retention and the material damage. The crucial part is understanding the dynamics on the individual scales and how to link the different scales. Specifically, we discuss the Frenkel pair generation due to energetic tungsten and gold ion irradiation using molecular dynamics simulations and binary collision models. The details of the collision dynamics and the short-time (~few ns) evolution of the Frenkel pairs will be presented which will be eventually used in a higher level Monte Carlo code for calculating the long-term evolution of point defects and their clustering.

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## Magnetic sheath effect on the gross and net erosion rates due to impurities

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In fusion reactors, erosion processes determine the lifetime of plasma-facing components and the contamination of the confined plasma by impurity production. In the vicinity of the surface, the magnetized sheath plays a primary role in gross erosion. Acceleration of impurity ions across the strong electric field layer defines their impact angle and energy, which both influence the sputtering yield and reflection coefficient. While the increase of impact energy is taken into account in most edge fluid codes, the angular deflection has been implemented only recently (for example in [1] for the main species). In [2] we have shown that the deflection is larger for the impurities than for the deuterium in the Tore Supra limiter conditions. The sheath also affects the net erosion rate through its influence on prompt or local redeposition. Two mechanisms contribute: (1) the redeposition of the atoms of tungsten ionized in a distance smaller than the gyro-radius of the singly charged ion, which are promptly redeposited in their first Larmor gyration, and (2) the redeposition of the ions, which do not have sufficient kinetic energy to escape the sheath potential [3].

The average impact angle of various impurities for the case where only the cyclotron motion is taken into account was compared with a self-consistent particle-in-cell (PIC) model of the sheath [4]. Two limits can be distinguished: (1) A low density limit that corresponds to far SOL regions, where the sheath decreases the impact angle and (2) a high density limit that is relevant for WEST or ITER divertors, where the sheath increases the impact angle. In the case of tungsten self-sputtering in WEST, the gross erosion obtained with the full sheath treatment can differ by a factor two with respect to the ballistic approximation where only the ion cyclotron motion is taken into account.

To calculate the local redeposition we use the data provided by the PIC simulations of the magnetic sheath: the electric field, the electron density, and its energy distribution function. We also concentrate on the effect of the ionization cross section. In the case of ITER detached scenario, the electrons are in most cases not energetic enough to ionize the eroded tungsten atoms. The mean free path could be thus be mostly determined by the auto-ionization of formerly excited tungsten atoms. Comparisons with existing models [3,5] and calculations of the net erosion velocity for a set of impurities assuming WEST and ITER conditions are performed.

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# Aluminium studies for laboratory plasma: particle growth and hydrogen retention

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Prediction of tritium retention by plasma-wall material and plasma dusts is a major question according to the well-functioning and safety of tokamaks. That is why erosion, particle growth and retention processes are studied for different plasma-facing components PFCs (as tungsten, beryllium or carbon). However experimental studies in laboratory on beryllium are limited by its toxicity. Aluminium is an alternative element (Be-like) which can replace him to characterize the formation of compounds, especially the oxides and possibly the hydrides [1]. Both experimental and numerical studies on aluminium are currently leading in our lab. We focused here on the numeric works partially supported by Eurofusion WP-PFC (SP3/4) project.

Our first objective is to describe dust formation (carbon, aluminium and tungsten) magnetized plasma. We consider a laboratory discharge system where plasma is ignited by ECR between 0.1 and 1 Pa. Observed particles may be formed from hydrocarbon precursors introduced in the feed gas but also through plasma-surface interaction in $H_2$/Al or $H_2$/W system. We develop a 1D model for hydrogen discharge obtained in this system. We solve for the transport equations of hydrogen ions ($H^+$, $H_2^+$, $H_3^+$, $H^-$), electron energy (that yield the electron temperature) and H-atom in the radial direction discharge on the dipolar magnet equatorial symmetry plane. We have obtained characteristics of the $H_2$ discharge. In this system we are now implementing aluminium particle formation by sputtering and aerosol growth and transport inside the discharge.

Our second objective is to describe surface finish and hydrogen retention in material using HIIPC (Hydrogen Isotope Inventory Processes Code) model. Resulting from several collaborations, this model simulates the hydrogen inventory in the PFCs (tungsten, beryllium or carbon) [3]. It describes the hydrogen retention in the tungsten during a real tokamak material thermal cycle [4] and will be extended to reproduce hydrogen desorption spectrum (in collaboration with A*MIDEX WHISCI project). The model is also currently used to describe hydrogen retained in aluminium.

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# $W_2$, $W_4$, WH, $WH_2$: Ab initio and DFT benchmarks

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Large-scale simulations investigating properties of tungsten in plasma facing materials and first wall plasma interaction in fusion devices are based largerly on DFT data. We report benchmark calculations on selected properties of model systems ($W_2$, $W_4$, WH, $WH_2$) to compare the density functional data with wave-function based data. Some of these systems were studied previously [1-4] but the systematic comparisons with DFT are scarce. For geometry optimization we used GAUSSIAN09 program [5] exploiting DFT with various popular functionals: BLYP, B3LYP, B3PW91, PW91PW91, mPW91PW91, PBEPBE, PBE1PBE, M062X, M06L, LC-BLYP, LC-ωPBE, LC-PW91PW91, B97X, B97XD; and two basis sets: cc-pVDZ-PP, cc-pVTZ-PP. For the wave-function based calculations we used the MOLCAS program package [6] in conjunction with ANO-RCC basis set. $X^1\Sigma^+_g$ state of $W_2$ calculated with just four functionals (ωB97XD, M06L, M062X, B97D) is compared with data in [4]. For quintet $W_4$ and $^6\Sigma^+$ WH/WD we used scalar relativistic coupled-cluster method - DK-CCSD(T). To obtain the spectroscopic constants for WH/WDwe performed the Dunham analysis. For $^5B_2$ $WH_2$ the geometries and harmonic frequencies were compared with data from [2,3]. We have also tested the effects of both semiempirical and ab initio dispersion corrections. The dispersion corrections were calculated either with standalone functionals already containing dispersion (B97D, ωB97XD, B97D3) or adding a semi-empirical dispersion potential to the conventional Kohn-Sham DFT energy. Several schemes were constructed for these purposes from which we chose the Grimme D3 method with a Becke-Johnson damping function [7]. Except for $W_4$ the benchmarks show that most of the functionals are quite reliable to describe such systems. We have also shown that for these cases dispersion has only a negligible effect.

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# Modelling of D atom absorption and diffusion dynamics in self-ion damaged tungsten exposed to deuterium atom beam

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The study of plasma-material interaction is important in order to successfully predict and understand the evolution of the first wall and its feedback on plasma operation. The majority of the experiments on plasma-material interaction are performed with energetic ion or plasma bombardment of the material. However, the edge plasma in fusion device consist not only of ions, but also of neutrals (molecules and atoms). Therefore, experiments studying interaction of neutral species with material are needed in order to fully understand the edge plasma-material interactions and retention mechanisms. Moreover, low energy (< eV) atom beam is also advantageous over the ion beam experiments whenever creating additional damage in the material is not desirable, since defects in the material act as strong binding sites for hydrogen.

*In* situ studies of D retention and diffusion dynamics in self-ion damaged tungsten were performed. Polycrystalline W samples were pre-irradiated by 20 MeV W ions, simulating the neutron damage that will be created in fusion reactors, and exposed to neutral D atom beam at different sample temperatures [1]. Deuterium concentration depth profiles were measured by Nuclear Reaction Analysis (NRA). The modelling of these experimental data will be performed using TESSim code [2,3]. We have implemented surface processes into the code, taking into account interactions of deuterium atoms with the surface and different desorption mechanisms (Langmuir-Hinshelwood and Eley-Rideal), coupled with the diffusion into the bulk of the material. It also allows using multiple adsorption sites with different binding energies. The damage profile will be included, taking into account various defects with different binding energies. The code will be used to determine some important parameters of deuterium-tungsten interaction potential (e.g. binding energies of different adsorption sites and energy barrier for diffusion into the bulk). Hot-atom desorption mechanism will be additionally implemented into the code in order to improve the accuracy of the current model.

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# Kinetic Monte Carlo simulation and rate theoretical approach for influence of vacancy on hydrogen diffusivity in tungsten

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Tritium retention in reactor materials needs to be minimized for establishing an efficient and sustainable tritium fuel cycle in fusion reactors. Large tritium retention also causes radiation-safety concerns. Therefore, understanding and controlling tritium behavior such as release and accumulation in fusion reactor materials is an important research subject. Since the retention in plasma-facing components (CFCs) may get large, the tritium behaviour in tungsten, a promising candidate for CFCs, have received increasing attention.

The diffusion coefficient is one of the fundamental physical quantities that govern the tritium behavior in tungsten. It is directly relevant with the rate of tritium release and permeation from/through tungsten. In addition, it is a vital input in analyzing experimental results of thermal desorption spectroscopy (TDS) and nuclear reaction analysis (NRA), which have been widely performed to acquire information on hydrogen-defect interactions.

Among several reported hydrogen diffusivities in tungsten, the one given by Frauenfelder [1] has been most utilized: $D = 4.1\times10^{-7}\exp(-0.39\ eV/kT)$. However, DFT calculation results showed disagreement with the experimental result: specifically, DFT calculation indicates around 0.20 eV as the diffusion barrier [2]. Heinola and Ahlgren [3] examined this disagreement by using transition-state theory (TST) coupled with DFT calculation. It was shown that the diffusion coefficients obtained with DFT+TST approach are comparable with those of Frauenfelder's experiment, if experimental data at low temperatures (<1500 K) are excluded. The exclusion was suggested considering that low-temperature data were significantly affected by defects that act as hydrogen trap [3].

In the present study, kinetic Mote Carlo (KMC) simulation is performed to quantitatively evaluate the influence of vacancy on hydrogen diffusivity in tungsten. For simplicity, three processes are only taken into account: (i) hydrogen migration, (ii) hydrogen trap by vacancy, and (iii) detrap from vacancy. Kinetic parameters of these processes such as migration energy and trapping energy are determined based on DFT calculation results. Consequently, the low-temperature data of Frauenfelder's experiment [2] are nicely reproduced by KMC simulation if a reasonable concentration of vacancy is assumed. In addition, an equation to evaluate the lower limit of hydrogen diffusivities in defective tungsten is derived by a rate-theoretical approach. The indicated lower limit fairly agrees with reported experimental data.

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# Some aspects of determination of hydrogen binding energies with defects in metals

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Hydrogen inventory in metals with a positive heat of solution strongly depends on the presence of defects; therefore precise determination of hydrogen-to-defect binding energies is essential. In most cases, these energies are obtained by fitting numerically simulated thermal desorption (TDS) spectra to experimental ones. However, determination of the binding energies is ambiguous in this approach, as the parameters describing the defects are free parameters in the model, and therefore one spectrum can be fitted by using several combinations of various parameters.

There also exists a method of a direct determination of H binding energies with defects from a series of TDS measurements of identical samples performed with different heating rates. Although this method is known since 80-s [1, 2], no strict justification of its applicability has been made so far. Based on diffusion-trapping equations, it was shown in this work that such approach is valid in the case of infinitely high recombination rate at the surface, independently of the trap profile and the initial distribution of trapped hydrogen.

In order to demonstrate the feasibility of this method and explore its possible limitations, numerical simulations of TDS spectra from tungsten with different heating rates by using the TMAP7 code were performed. Various binding energies, trap profiles, and initial trap populations were used. In order to model different surface conditions, various recombination rate coefficients were used. It was observed that the binding energies can be correctly determined only in the case of a high H-H recombination rate at the surface, whereas the reduced recombination rate leads to overestimated values of binding energies. Based on the results of the simulations, a new transport parameter characterising the regime of H release was proposed. This parameter involves the surface recombination rate, the H diffusivity in the material, and the parameters of the trapping sites. It was shown that H release from the material is not affected by surface processes only in the case when the parameter proposed is much larger than unity.

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## Raman spectroscopy investigation of beryllium based materials

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Hydrogen isotope retention in beryllium is an important issue as this element is the dominant plasma-facing component (PFC) in ITER [1-4]. The aim here is to study the ability of Raman spectroscopy, a non-contact technique based on inelastic scattering of photons, to give information on the structure and composition of Be samples containing D, N and W. Two types of materials are investigated. First a polycrystalline Be sample bombarded by D ions (a few keV/atom, a few $10^{17}$ $cm^{-2}$), provided by IPP in Garching. Atomic quantification was performed using ion beam analysis. Second, Be and $Be_{50}W_{50}$ deposits containing few percents of D or N, provided by IAP in Bucharest. They were synthesized using the thermionic vacuum arc method [5]. Atomic quantifications were performed using ion beam analysis at IST in Lisboa.

Vibrational changes induced by D irradiation were then identified in Raman spectra. We report the presence of 6-7 bands that we attribute to Be-D vibrations whereas the pristine sample contains only one band due to the Be-Be vibrational stretching mode. DFT (density functional theory) calculations of vibrational frequencies were done to interpret these results. Atomic force microscopy was used to characterize the surface roughness. We found that in the bombarded sample dendritic structures are present within the implantation spot. These structures are typically a few micrometers long and are composed of nanodomes, typically 100 nm high. The Be-D bands are located mainly on these dendritic structures. The Raman spectra analysis suggests that ion implantation induces stress in the material and that these dendrites are formed as a consequence of stress saturation. These observations show that the bombardment induces growth processes and surface modifications.

On the contrary, no such structures, nor such Raman bands, were found for arc-deposited materials and 3 different bands, not observed after ion implantation, were observed. One of these bands may be attributed to Be-O bonds. The two other bands, observed for D and N containing samples, are interpreted as defect induced bands. In addition, for the $Be_{50}W_{50}$ sample, the Be-Be vibrational stretching mode was not observed, showing that Be and W are not forming separated clusters in the sample but are forming an alloy.

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# Aspects of ion-metal and electron-metal interactions in fusion relevant energy regimes

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The microphysics of ion-metal and electron-metal interactions in the plasma boundary of fusion devices affect not only the wall material but also the surrounding plasma. These interactions involve processes such as secondary electron emission [1], electron-backscattering [2], low-energy electron-reflection [3], ion-backscattering [4], ion-surface recombination [5] and surface assisted molecule formation. Such processes have been studied experimentally and theoretically in regimes that correspond to impact energies much higher than the ones encountered in divertor plasmas. Extrapolations to fusion relevant regimes are not viable, since the microphysics change drastically in very low energy ranges.

Furthermore, thermionic emission [6] is a very important process for dust and droplet dynamics. Thermionic electrons control the onset of a thermal instability that occurs due to the strong coupling of charging and heating [7]. Through this instability, thermionic emission effectively controls dust melting and impurity generation in fusion plasmas. Consequently, dust dynamics can be expected to be very sensitive to the treatment of the thermionic current. However, experimental data are very sparse for the tungsten Richardson constant and the work function at very high surface temperatures, whereas they are no experimental data for liquid metals (where by electronic structure arguments deviations from the Richardson-Dushman expression can be expected).

In this presentation we shall discuss: (i) why low energy extrapolations are not valid for plasma-solid interactions, (ii) which experimental data are needed in order to enhance the predictive power of codes, (iii) the necessity for updated data compendia for plasma material interactions by providing instances of outdated datasets currently used in fusion.

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# The microphysics of ion-surface recombination and calculations of the heat sheath transmission factor

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Ion-surface recombination refers to the neutralization of ions in the vicinity of a metal surface induced by quantum tunneling of bound electrons [1]. It is accompanied with energy absorption by the metal, making it an important heating mechanism not only for plasma-facing-components but also for dust in case the plasma temperatures are low ( $T_e < 10$eV). Currently, in fusion plasmas the micro-physics of recombination are not properly taken into account and it is wrongly assumed that the energy released to the PFC for each event is equal to the ionization energy of the ion [2].

Low energy ions present at the Ångström vicinity of metal surfaces are 100% neutralized due to the relatively large interaction times and the metal electron availability for tunneling. Neutralization mainly occurs through resonant and Auger processes [3]. *Resonant neutralization* refers to the constant energy transition of an electron from the metal continuum of states to the discrete atomic states; hence it is not accompanied by energy transfer to the metal. *Auger neutralization* refers to the transition of metal electrons at a higher binding energy atomic state; hence it is accompanied by potential energy release absorbed by the valence electrons, which leads to either electron emission or heating of the metal. Neutralization can also occur by a combination of these processes. The contribution of each process to the neutralization rate strongly depends on the particular ion / metal combination.

A first-principles approach without adjustable parameters has not been developed yet [4]. However, for sub-keV ions theoretical approaches can be developed based on Hagstrum's elementary theory [3] by **(i)** assuming that the level shift stems from the image interaction, **(ii)** assuming that when both two-electrons and many-electron processes are permissible, the former dominate, **(iii)** utilizing the theoretical electronic density of states of the metal.

We developed such an approach for the tokamak relevant case of $\mathrm{H}^+$and $\mathrm{He}^+$ions incident on W surfaces [5]. In the /W case, resonant neutralization dominates and there is no PFC heating. In the $\mathrm{He}^+\mathrm{H}^+$/W case, resonant channels are forbidden and Auger neutralization dominates leading to 10.5 eV heating per incident ion. For comparison, neglecting the micro-physics leads to 13.6 eV and 24.6 eV per ion. With these revisions, we revisited Pilot-PSI results for the sheath heat transmission factor ( ) in the high recycling regime [6] and managed to explain the observed discrepancies with analytical sheath theory [2]. Finally, we shall discuss implications stemming from the aforementioned difference between H and He ions.

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# Hydrogen diffusion and vacancies formation in tungsten: DFT and statistical models

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The interaction of hydrogen with tungsten and vacancies is investigated by mean of Density Functional Theory (DFT). Because DFT is limited to small models of about one hundred atoms at zero temperature, this work is complemented by a statistical approach with the aim to yield temperature dependent data that can be directly compared with macro-scale thermodynamic and kinetic experimental data.

It follows that DFT data are included in a statistical model based on transition state theory and thermodynamic. Such model allows revising the solubility and diffusivity of hydrogen in tungsten. The discrepancy between the experimental diffusion coefficient from Frauenfelder *et al* [1] and other DFT results [2] is understood and two diffusion regimes are proposed depending on the temperature.

The trapping of multiple hydrogen atoms in tungsten vacancies is also investigated. The hydrogen population in vacancies and the vacancy concentration in tungsten are shown to depend on the temperature. TDS spectra are simulated using simple kinetic laws; despite the simplicity of the model, the agreement is good agreement with experimental results recorded on single crystalline samples [3,4].

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# DFT calculations and statistic models for the evaluation of accidental beryllium and tritium releases in ITER facility

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The safety analysis of the ITER experimental facility principally aims to evaluate the amount and chemical speciation of radionuclides that can be released to the environment in accident conditions (the so-called source term). Initially, only tritium, tungsten dusts and corrosion products present in the coolant system of the vacuum vessel were taken into account. However, in addition to these products, the beryllium dusts have an extreme chemical toxicity and must also be considered, which is the focus of the present work. To improve the source term evaluation, electronic properties, thermodynamic functions of gas and solid beryllium compounds and interaction between them are key issues.

As the first step, the thermodynamic properties of the gaseous Be-O-H-T system have been recently investigated on the basis of quantum chemistry calculations [1]. To achieve a reliable thermo-chemical database of beryllium compounds, the thermodynamic properties of Be(c), $BeH_2$(c) and $BeT_2$(c) have to be known. Also the kinetic of formation of these mixed Be/H and Be/T materials are of high interest and both their kinetics and thermodynamics will be investigated in this study. To this end, a theoretical approach associating solid state physics and quantum chemistry is developed: it is based on electronic structure calculations by mean of Density Functional Theory (DFT) methods as implanted in the *Quantum Espresso* package.

Beryllium and beryllium hydride models are established and constructed. The procedure incorporates the supercell size and simulations parameters optimization like the plane wave cutoff energy, the Brillouin zone k-points and the smearing width. The crystal structure, mechanical properties and electronic structure of Be and $BeH_2$ are calculated and compared with the available and experimental data [2-4].

The next step will be about hydrogen trapping in beryllium vacancies, hydrogen interaction on the beryllium and hydride beryllium surfaces and the phonon properties of these systems.

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