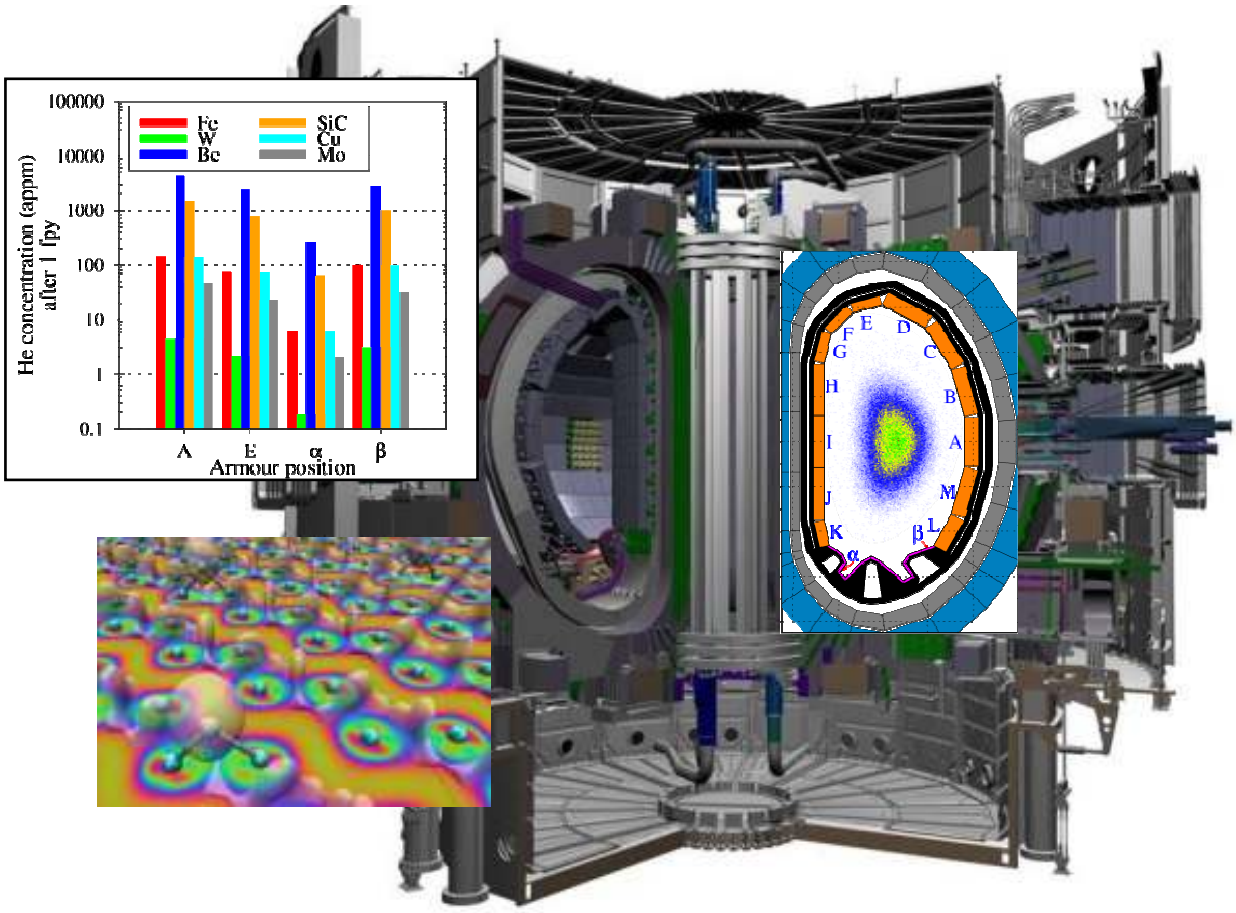
Second International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices

MoD-PMI 2016



BOOK OF PROGRAM AND ABSTRACTS

June 22-24 2016, Loughborough University, Loughborough, Leicestershire, United Kingdom

IAEA International Atomic Energy Agency

IOP Institute of Physics Computational Physics Group

CCFE Culham Centre for Fusion Energy

Oxford Materials

Invited Speakers

Andree de BACKER, Culham Centre for Fusion Energy, UK
Takumi CHIKADA, Shizuoka University, Japan
Dorothy DUFFY, University College London, UK
Chu-Chun FU, CEA Saclay, France
Tilmann HICKEL, Max-Plank-Institut für Eisenforschung GmbH, Düsseldorf, Germany
Karl HAMMOND, University of Missouri, USA
Felix HOFMANN, University of Oxford, UK
Andreas KIRSCHNER, Forschungszentrum Jülich, Germany
Xiao-Chun LI, CAS Institute of Plasma Physics, Hefei, PR China
Jaime MARIAN, University of California, Los Angeles, USA
Mihail-Cosmin MARINICA, CEA Saclay, France
Thomas MORGAN, Dutch Institute for Fundamental Energy Research, The Netherlands
Kazunori MORISHITA, University of Kyoto, Japan
Kai NORDLUND, University of Helsinki, Finland
Cedric PARDANAUD, Aix-Marseille Université, France
Thomas SCHWARZ-SELINGER, Max-Planck-Institut für Plasmaphysik, Garching, Germany
Hyung Jin SHIM, Seoul National University, Korea
Udo von TOUSSAINT, Max-Planck-Institut für Plasmaphysik, Garching, Germany
Blas UBERUAGA, Los Alamos National Laboratory, USA
Anna WIDDOWSON, Culham Centre for Fusion Energy, UK
Yi-Chun XU, CAS Institute of Solid State Physics, PR China

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Takuji ODA, Seoul National University, Korea
Klaus SCHMID, Max-Planck-Institut für Plasmaphysik Garching, Germany
Manoj WARRIER, BARC Visakhapatnam, India
Brian WIRTH, University of Tennessee at Knoxville, USA
Hong-Bo ZHOU, Beihang University, PR China

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Steve FITZGERALD, University of Leeds (Co-Chair)
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Kalle HEINOLA, JET, University of Helsinki
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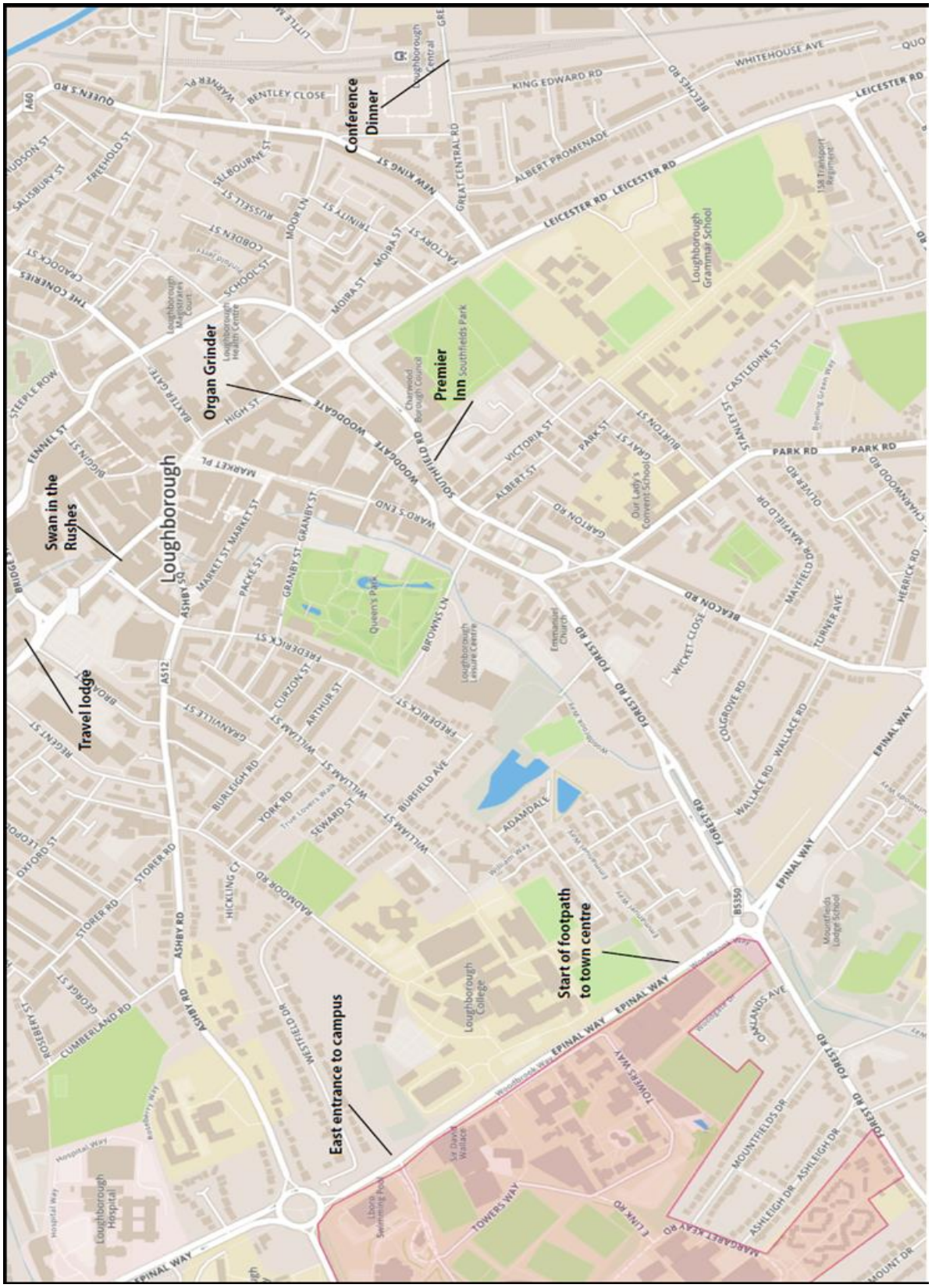
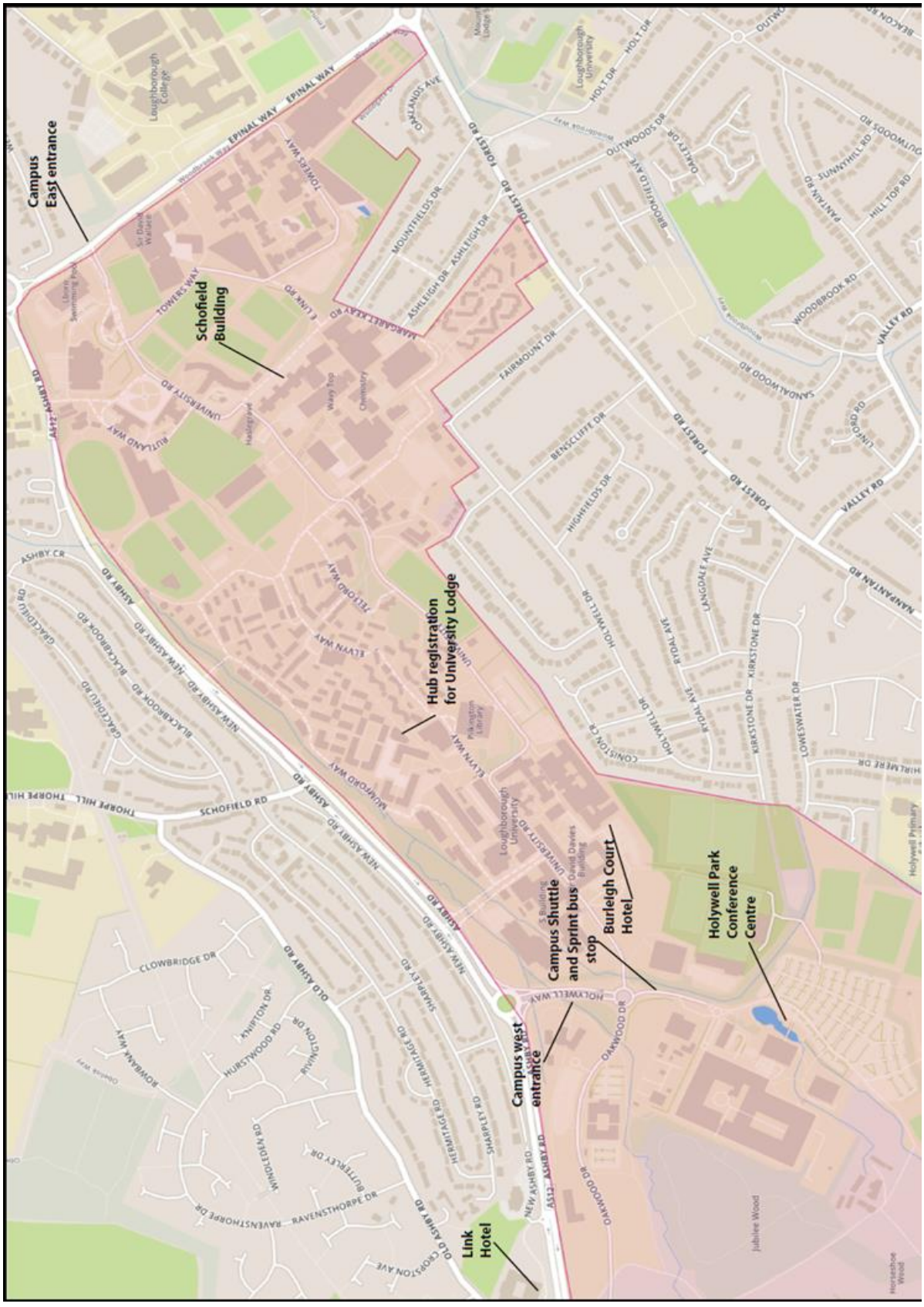


LOUGHBOROUGH TOWN CENTRE MAP



HOLYWELL PARK CONFERENCE CENTRE

PULLMAN DINING TRAIN

MoD-PMI 2016 PROGRAM

Wednesday 22nd June

8:15-8:45 Registration

8:45-9:00 Opening

Duc Nguyen-Manh, *Culham Centre for Fusion Energy*

Session 1 – **Tungsten Fuzzy Nanostructure**

Chair: ***Charlotte Becquart***

9:00-9:30 I1. Atom-level mechanisms behind time and temperature dependence of W fuzz formation

Kai Nordlund, *University of Helsinki*

9:30-10:00 I2. Accelerated Molecular Dynamics Studies of He Bubble Dynamics in Tungsten

Blas Uberuaga, *Los Alamos National Laboratory*

10:00-10:20 O1. Ballistic He penetration into W fuzz

Peter Klaver, *Dutch Institute for Fundamental Energy Research*

10:20-10:40 O2. The BCA-KMC Hybrid Simulation for Hydrogen Retention in Tungsten Materials

Atsushi Ito, *National Institute for Fusion Science, Gifu*

10:40-11:10 Coffee break

Session 2 - **Experimental Data for Modelling**

Chair: ***Felix Hofmann***

11:10-11:40 I3. Deuterium uptake, release and isotope exchange in self-damaged tungsten

Thomas Schwarz-Selinger*, Max-Planck-Institut für Plasmaphysik, Garching*

11:40-12:10 I4. Liquid metals as plasma facing materials for future fusion reactors

Thomas Morgan*, Dutch Institute for Fundamental Energy Research*

12:10-12:30 O3. Preparation and Characterization of Mixed Layers containing Beryllium and Deuterium

Cristian Lungu*, Plasma and Radiation Physics, Romania*

12:30-12:50 O4. Studies on plasma / Aluminium (as Beryllium surrogate) interactions: particle nucleation and hydrogen inventory in material defects

Jonathan Mougenot*, Université Paris 13*

12:50-13:40 Lunch

Session 3 - **H Isotopes and He Synergy**

Chair: ***Daiji Kato***

13:40-14:10 I5. Properties of helium and hydrogen in iron systems from atomistic simulations

Chu-Chun Fu, *CEA, Saclay*

14:10-14:30 O5. The behaviours of helium atoms and clusters in vanadium studied with atomistic simulations
Huiqui Deng, Hunan University

14:30-14:50 O6. Multiscale study of plasma induced trapping of hydrogen isotopes in tungsten
***Petr Grigorev**, SCK-CEN, Mol*

14:50-15:10 O7. Influence of He on hydrogen isotope transport and retention in tungsten – First observation of D accumulation around He implantation zone
***Sabina Markelj**, Jozef Stephan Institute, Ljubljana*

15:10-15:40 Coffee break

Session 4 - **Uncertainty Quantification**
Chair: ***Takuji Oda***

15:40-16:10 I6. Bayesian Experimental Design for Plasma-Wall-Interaction Simulations: Efficient estimation of Uncertainties based on parallel Gaussian Processes
***Udo von Toussaint**, Max-Planck-Institut für Plasmaphysik, Garching*

16:10-16:40 I7. Development of Sensitivity Analysis Techniques for Kinetic Monte Carlo Simulations
***Hyung-Jin Shim**, Seoul National University*

16:40-17:10 I8. KMC simulation of nucleation and growth of defect clusters in metals during irradiation: damage rate dependence
***Kazunori Morishita,** University of Kyoto*

17:10-17:30 O8. Interatomic potentials for modelling radiation damage in tungsten: A comparison with DFT calculations
***Charlotte Becquart**, Université Lille*

17:30-18:00 **General Discussion: Synergy of Experimental and Modelling Data**
Chair: ***Udo von Toussaint***

Thursday, 23rd June

Session 5 – **Multi-scale Modelling of PMI**
Chair: ***Kai Nordlund***

8:45-9:15 I9. Multiscale Plasma–Material Interactions Simulation: Continuum-Scale Models Informed by "Computer Experiments" Using Large-Scale Molecular Dynamics
***Karl Hammond**, University of Missouri*

9:15-9:45 I10. Modelling of plasma-wall interaction and impurity transport in fusion devices with the 3D ERO code
***Andreas Kirschner,** Forschungszentrum Jülich*

9:45-10:05 O9. Multi-scale simulations of fuel retention in JET-ILW
***Kalle Heinola**, University of Helsinki*

10:05-10:25 O10. Near Surface Helium Segregation in Tungsten with the Xolotl Plasma-Surface Interactions Simulator
***Sophie Blondel**, University of Tennessee, Knoxville*

10:25-11:00 Coffee break

Session 6 - **Experimental Methods for PMI**
Chair: ***Thomas Schwarz-Selinger***

11:00-11:30 I11. Material migration and fuel inventory in JET ITER-like wall from surface analysis techniques
***Anna Widdowson**, Culham Centre for Fusion Energy*

11:30-12:00 I12. Raman microscopy: a suitable tool for characterizing surfaces in interaction with plasmas in the field of nuclear fusion.
***Cedric Pardanaud**, Université Aix-Marseille*

12:00-12:30 II3. Helium Implantation Effect on Microstructure and Physical Properties of Tungsten for Plasma-Facing Fusion Reactor Components
***Felix Hofmann**, University of Oxford*

12:30-12:50 O11. Recent Activity in Russian Federation on Simulation of PMI in Fusion Devices
***Valeriy Kurnaev**, National Research Nuclear University, MEPhI*

12:50-14:00 Lunch

Session 7- **Cascades and Defect Clusters**
Chair: ***Yves Ferro***

14:00-14:30 I14. Energy landscape of nanosized interstitial clusters in Fe, W and V using ab-intio methods
***Cosmin Marinica**, CEA, Saclay*

14:30-15:00 I15 Scaling laws of cascade and sub-cascade formation in high energy ion and neutron impacts
***Andree de Backer**, Culham Centre for Fusion Energy*

15:00-15:20 O.12 Hydrogen effects on radiation damages in tungsten
***Daiji Kato**, National Institute for Fusion Science, Gifu*

15:20-15:40 O13. Modeling of effects of vacancy, vacancy clusters and grain boundaries on hydrogen behaviors in tungsten
***Takuji Oda**, Seoul National University*

15:40-16:15 **General Discussion: Multi-scale Modelling Tools for PMI**
Chair: ***Karl Hammond***

16:15-16:45 Coffee break

Session 8 – **Poster**
Chair: ***Andree de Backer***

16:45-17:45 See List of Poster

18:30-22:00 **Joint MoD-PMI2016 and COSIRES2016 Dinner**

Friday, 24th June

Session 9 – **Transmutation and Segregation**
Chair: ***Duc Nguyen-Manh***

8:45-9:15 I16. Modelling the kinetics of rhenium precipitation in neutron-irradiated tungsten
Jaime Marian, *University of California, Los Angeles*

9:15-9:45 I17. Radiation resistance of nano-crystalline iron: Coupling of the fundamental segregation process and the annihilation of interstitials and vacancies near the grain boundaries
Yichun Xu, *Institute of Solid State Physics, CAS*

9:45-10:05 O14. Effect of Re and Os in W under irradiation: comparison between numerical and experimental results
Tomoaki Suzudo, *Japanese Atomic Energy Agency*

10:05-10:25 O15. A Density Functional Theory investigation of H saturated W surfaces
Yves Ferro, *Université Aix-Marseille*

10:25-11:00 Coffee break

Session 10. **Quantum Excitations and Oxides**
Chair: ***Cedric Weber***

11:00-11:30 I18. Modelling electronic excitation induced effects in tungsten
Dorothy Duffy, *University College London*

11:30-12:00 I19. Ab initio thermodynamics of point defects in metals: Hydrogen, vacancies and their interaction
Tilmann Hickel, *Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf*

12:00-12:30 I20. Experimental and computational approaches to the elucidation of hydrogen isotope permeation in erbium oxide coatings for tritium permeation barrier
Takumi Chikada, *Shizuoka University*

12:30-12:50 O16. Electrodynamics of correlated materials: the optical conductivity as a probe for Mott and charge-transfer physics for copper oxides
Cedric Weber, *King College London*

12:50-13:00 **MoD-PMI2016 Summary**
Bas Braams, *IAEA Vienna*

13:00 Lunch

List of Posters (MD-PMI2016)

P1. Shape of hydrogen-covered bubbles in beryllium: ab initio study
Dmitry Bachurin, *Karlsruhe Institute of Technology*

P2. Modelling of Neutron Damage and PKA Spectrum for Synergistic Plasma Effects
Addab Hussain, *University of Manchester*

P3. Interstitial-mediated diffusion and clustering for transmutation elements Re and Os precipitation in W
Yu-Hao Li, *Beihang University, Beijing*

P4. Tungsten oxide thin films: D^+ and He^+ bombardment
Celine Martin, *Aix-Marseille Université, Marseille*

P5. Modelling the Timescales in Which Helium Embrittlement Occurs within Breeder Blanket Materials
Luke Menzies, *University of Manchester*

P6. Paschen curve approach to investigate electron density and deposition rate of Cu in magnetron sputtering system
Anand Pathak, *University of Hyderabad, India*

P7. Recent Progress in Modelling of Hydrogen Interactions with Beryllium (0001) Surface
Christopher Stihl, *Karlsruhe Institute of Technology*

P8. A new EAM interatomic potential for tungsten-hydrogen system
Li-Fang Wang, *Beihang University, Beijing*

P9. Tritium behaviour in beryllium investigated by DFT in the ITER context
Yves Ferro, *Aix-Marseille Université, Marseille*

ABSTRACTS
INVITED TALKS

I1. Atom-level mechanisms behind time and temperature dependence of W fuzz formation

K. Nordlund,[1,*] G. Valles,[2] I. Martin-Bragado,[2] A. Lasa,[1,4]
C. Björkas,[1] E. Safi,[1] J.M. Perlado,[2] and A. Rivera[2]

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[4]*Oak Ridge National Laboratory, Oak Ridge, TN37831-6169, USA*
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Recently, tungsten (W) has been found to form a highly underdense, nanostructured morphology ("W fuzz") when bombarded by an intense flux of He ions from a plasma, but only in the temperature window 900–2000 K. We have examined the formation of this fuzz using , Molecular Dynamics (MD) and Kinetic Monte Carlo (KMC) computer simulations. The DFT and MD showed that He bubbles can start forming by self-trapping in pristine W [1] and grow by dislocation loop punching [2,3]. The bubble growth and coalescence leads to surface roughening, which in turn slows down the fuzz growth rate due to the possibility of bubble rupture sidewards in a growing fuzz tendril [4]. Finally, using further KMC simulations that consider the He trapping and detrapping rate in specific He-defect complexes, we now show that the temperature dependence of fuzz formation can be understood based on He and point defect clustering, cluster growth, and detrapping reactions. At low temperatures (<900 K), fuzz does not grow because almost all He is trapped in very small He-vacancy clusters. At high temperatures (>2000 K), all He is detrapped from clusters, preventing the formation of the large clusters that lead to fuzz growth in the intermediate temperature range.

[1] K. O. E. Henriksson, K. Nordlund, A. Krasheninnikov, and J. Keinonen, , Appl. Phys. Lett. **87**, 163113 (2005)
[2] K. O. E. Henriksson, K. Nordlund, J. Keinonen, D. Sundholm, and M. Patzschke, Physica Scripta **T108**, 95 (2004)
[3] A. Lasa, K. O. E. Henriksson, and K. Nordlund, Nucl. Instrum. Methods Phys. Res. B **303**, 156 (2013).
[4] A. Lasa, S. K. Tähtinen, and K. Nordlund, EPL **105**, 25002 (2014).

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I2. Accelerated Molecular Dynamics Studies of He Bubble Dynamics in Tungsten

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[b] *Analytical Mechanics Associates, Inc., at NASA Ames Research Center, Moffett Field, CA, USA*
[c] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, USA*
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Tungsten has been proposed as a candidate material for the divertor in fusion devices, particularly ITER. However, upon exposure to high fluxes of He from the plasma, tungsten begins to degrade. The implanted He diffuses in the subsurface of the material, ultimately nucleating bubbles that can cause numerous detrimental phenomena, including blistering and the formation of so-called fuzz, a nanoscale foamy structure. There is thus great need to understand the origins of these effects so that they can be designed against.

Using accelerated molecular dynamics (AMD) methods, we examine the various kinetic processes related to He evolution in tungsten, including the migration of He through the matrix, the nucleation of He bubbles, and the subsequent growth of those bubbles. We focus on how mobile He clusters interact with existing bubbles to understand in detail the growth process of the bubbles. By using AMD methods, we can reach time scales – and thus bubble growth rates – that are much closer to experimentally relevant rates than possible with conventional molecular dynamics. As a consequence of the slower rates, we see that there is a cross-over in behaviour. When the growth rates are high, the system is over-driven and cannot respond to the high He flux. However, as the rates are reduced, thermally-activated events become possible, allowing the system to find alternative pathways to accommodate the He. In particular, bubbles interact more strongly with microstructural features such as the free surface in this regime. This leads to qualitatively different behaviour at slower growth rates.

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I3. Deuterium uptake, release and isotope exchange in self-damaged tungsten

T. Schwarz-Selinger[a,*], A. Manhard[a], K. Schmid[a], J. Bauer[a], L. Gao[a],
U. von Toussaint[a], W. Jacob[a], A. Založnik[b] and S. Markelj[b]
[a] *Max-Planck-Institut für Plasmaphysik, Boltzmannstr. 2, 85748 Garching, Germany*
[b] *Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia*

Hydrogen isotope retention in present day fusion experiments is of minor concern. Due to the limited particle fluences and target temperatures retention is restricted to the near surface. In a future nuclear device neutron bombardment will create additional traps for hydrogen isotopes throughout the material that will slow down transport but will increase fuel retention. Dedicated lab experiments are necessary to derive a physical understanding of the processes involved to allow for modelling and hence extrapolation.
Nuclear Reaction Analysis (NRA) and Thermal Desorption Spectroscopy (TDS) are the workhorses in the community to measure deuterium (D) retention and derive input parameters for modelling. In the first part of this presentation the basic principles for D detection with NRA are first briefly described in order to discuss the deconvolution challenge and the limitations of the technique in terms of detection limit, information depth and achievable depth resolution. The major aspects of TDS are shortly introduced with a few examples to highlight the main obstacles in interpreting TDS spectra such as the influence of the ramp rate as well as the trap and hence deuterium profile on the peak position. This is to motivate the need of having both at the same time to derive valuable input data for e.g. the de-trapping energies and the attempt frequencies.
The experimental challenge for tungsten is that the intrinsic defect density is low and defects are created only during the plasma or ion beam exposure. As long as the temporal and spatial evolution of these defects are not known extraction of model input parameters from lab experiments are hampered. In the second part I will present our approach to overcome these obstacles by separating D transport from defect creation. Defects are created in recrystallized tungsten by tungsten self-implantation with 20 MeV. Decoration of defects is done by exposing to a low-energy deuterium plasma (< 5 eV/D or 38 eV/D, < 10^{20}D $m^{-2}s^{-1}$) or D atoms (0.2 eV/D, <10^{19}D $m^{-2}s^{-1}$) to avoid creation of additional defects in the bulk as well as inhibit surface blistering. Decoration is either performed at low temperature to avoid any defect annealing as well as at elevated temperature to provoke defect migration and evolution. NRA is used to follow the migration of D into depth as function of D fluence. The dominant de-trapping energies with the pre-exponential factors are derived by measuring the shift of the desorption peak when varying the TDS heating rate of a set of identical samples. The initial implantation profile as well as the D reflection coefficient are calculated with SDTrimSP. While these mono-isotopic loading experiments can be described quantitatively with a diffusion trapping model without any free parameter it fails to describe isotope exchange experiments. Recent benchmark experiments conducted between 130 K and 600 K will be presented that show in how far the assumption of fill-level dependent de-trapping energies can describe the observed exchange.

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I4. Liquid metals as plasma facing materials for future fusion reactors

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The reliable long term performance of the divertor in DEMO and reactors beyond is of paramount importance in developing fusion energy as an economic and viable power source. Damage to the plasma facing material (PFM) region of a solid divertor surface over time due to the extremely high heat, ion and neutron loads expected may limit this lifetime significantly, demanding frequent and undesirable replacement to avoid component breakdown. The use of a liquid metal surface therefore offers advantages in this context, due to the liquid's nature permitting a continuous renewal of the surface. Further liquids are inherently disordered, thus avoiding many of the issues of neutron irradiation which affect atomic lattices and which are expected to play a strong role in degrading the structural and mechanical performance of solid PFMs [1].
Despite these benefits, use of liquid metals has several inherent difficulties. Firstly, implementation is more technologically complex than a solid PFM. Strong jxB forces in a tokamak may destabilise liquid surfaces, leading to the development of Capillary Porous Structures (CPS) [2] or thin trenches [3] which restrain motion via surface tension forces. Secondly, core plasma compatibility may be a significant challenge for high-Z candidates such as Sn, while fuel retention is of significant concern for Li due to its strong affinity for hydrogen isotopes [4]. Despite these difficulties however several LM concepts have been developed and are investigated at many research labs around the world, in both toroidal and linear devices as well as test stands. This talk will give an overview of the current status of liquid metal research and its prospects as the PFM for future fusion reactors.

[1] M.R. Gilbert et al. Nucl. Fusion 52 (2012) 083019

[2] V.A. Evtikhin et al. J. Nucl. Mater. 307–311 (2002) 1664–1669

[3] D.N. Ruzic et al. Nucl. Fusion 51 (2011) 102002

[3] M.J. Baldwin et al. Nucl. Fusion 42 (2002) 1318–1323

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I5. Properties of helium and hydrogen in iron systems from atomistic simulations

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In future fusion reactors, high energy neutron irradiation is expected to generate large concentrations of hydrogen and helium via transmutation reactions, in addition to the self-defects. It is now well known that these gas elements cause damage to structural materials through bubble formation, embrittlement, swelling, and hardening. Taking α-iron as the basis material, we perform atomistic studies employing a combination of first principles, classical molecular dynamics, and Monte Carlo methods.

In this talk, we present results on the dissolution, diffusion and clustering of helium and hydrogen in α-Fe systems[1-3], with particular focus on the dependence on local chemical and structural environments. In particular, the impact of impurities (carbon)[4] and alloying elements (chromium)[5] and of grain boundaries[6,7] will be discussed. Finally, we provide some hints to explain the synergistic effects of helium and hydrogen as suggested by some experiments.

[1] C.C. Fu, and F. Willaime, Phys. Rev. B 72 (2005) 064117
[2] E. Hayward, and C.C. Fu, Phys. Rev. B 87 (2013) 174103
[3] E. Hayward, R. Hayward, and C.C. Fu, J. Nucl. Mater 476 (2016) 36
[4] C. Ortiz, M.J. Caturla, C.C. Fu and F. Willaime, Phys. Rev. B 80 (2009) 134109
[5] E. Martinez, and C.C. Fu, Phys. Rev. B 84 (2011) 014203
[6] L. Zhang, C.C. Fu, and G.H. Lu, Phys. Rev. B 87 (2013) 134107
[7] L. Zhang, C.C. Fu, E. Hayward and G.H. Lu, J. Nucl. Mater 459 (2015) 247

I6. Bayesian Experimental Design for Plasma-Wall-Interaction Simulations: Efficient estimation of Uncertainties based on parallel Gaussian Processes

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Since PWI.simulations are expensive it is indicated to exploit the computational budget in the best possible manner. However, many of the input parameters are uncertain and a proper comparison of the simulation results with experimental data requires the quantification of the uncertainty of the code results as well. Unfortunately the curse of dimension often prohibits a straightforward Monte Carlo sampling of the uncertain parameters. Bayesian Experimental Design together with the use of surrogate models (Gaussian processes) suggests a more efficient approach. Employing the Kullback-Leibler-divergence as utility function we propose an optimized and automated sequentiell parameter selection procedure for the simulations. The proposed method is applied to PWI-simulations with several uncertain and Gaussian distributed input parameters. New approaches to reduce the wall-clock-time for the optimization as well as the performance of other utility functions are also discussed.

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I7. Development of Sensitivity Analysis Techniques for Kinetic Monte Carlo Simulations

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The kinetic Monte Carlo (KMC) method can provide the dynamical evolution of a rare-event system over a large timescale by simulating individual transition events with appropriate incremental time intervals.[1,2] Since Beeler's simulation of radiation damage annealing, KMC has been widely applied for analyses of material irradiation, gas surface interactions, statistical physics, etc. However the accuracy of numerical results estimated from KMC simulations is governed by the reliability of the transition rates used in the simulations. Sensitivity analyses may be useful to order the transition data by importance and quantify the uncertainty of the numerical results.

Monte Carlo (MC) perturbation methods such as the correlated sampling (CS) and the differential operator sampling (DOS) methods [3,4] have been successfully applied for reactivity coefficient estimations and nuclear data sensitivity and uncertainty calculations [5,6] in the MC particle transport analysis.

In the workshop presentation, a mathematical foundation of the KMC simulations will be expressed as the Neumann series solution with the time-flight and event kernels to a master equation in the form of the first-order partial differential equation. From the Neumann series formulation, perturbation formulations for the CS and DOS methods for the KMC perturbation analysis will be derived to efficiently and accurately estimate the changes of design parameters due to the transition data changes. The effectiveness of the developed formulations will be investigated for a simplified xenon decay chain problem and one-dimensional neutron irradiation simulations in pure BCC Fe by an in-house object KMC code, PAVIO [7].

[1] M. H. Kalos and P. A. Whitlock, Monte Carlo Methods, John Wiley & Sons (2008)
[2] K. A. Fichthorn and W.H Weinberg, J. Chem. Phys. 95 2 (1991) 1090
[3] H. Takahashi, Nucl. Sci. Eng. 41 (1970) 259
[4] H. Rief, Ann. Nucl. Energy 11 (1984) 455
[5] Y. Nagaya and T. Mori, J. Nucl. Sci. Technol. 42[5] (2005) 428
[6] H. J. Shim and C. H. Kim, J. Nucl. Sci. Technol., 48[12] (2011) 1453
[7] Y. H. Choi and H. G. Joo, Fusion Eng. Design 88[9-10] (2013) 2471

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I8. KMC simulation of nucleation and growth of defect clusters in metals during irradiation: damage rate dependence

Kazunori Morishita [a,*], Toshiki Nakasuji [a], and Yoshiyuki Watanabe [b]

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Fusion materials data are generally obtained using alternative irradiation facilities that provide different irradiation conditions from actual fusion environment, which reflects the fact that there are no actual fusion devices at present. This may result in a practical difficulty caused when fusion reactor design is made. To overcome this difficulty, some efforts of materials modelling have been made to bridge the gap, where multiscale phenomena occurred in materials during irradiation are clarified using various computer simulation techniques that are individually applied to appropriate time and length scales. In the present study, computer simulations are performed to investigate the formation of defect clusters in metals under various irradiation conditions.

Nucleation behaviour of defect clusters in Fe is widely and systematically investigated by Monte-Carlo technique, along with defect energies obtained in advance by molecular dynamics (MD) technique using the Finnis-Sinclair interatomic potential function and so on. Super-saturation of defect concentrations in Fe matrix is provided by the rate equation theory analysis. Nucleation rates of helium-bubbles, voids, self-interstitial atom (SIA) clusters, and solute-atom clusters (copper-vacancy clusters) in Fe are individually obtained as a function of damage rate and temperature.

Our results clearly shows that the nucleation rates of He-bubbles, voids and SIA clusters indicate an increasing function of dpa/s, while that of copper-vacancy clusters exhibit a decreasing function. Chemical compositions of clusters are also obtained as a function of time and other irradiation conditions. Furthermore, the effect of cascade clusters on nucleation rates is investigated. All of these findings could be useful to interpret the existing irradiation data for fusion reactor design.

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I9. Multiscale Plasma–Material Interactions Simulation: Continuum-Scale Models Informed by "Computer Experiments" Using Large-Scale Molecular Dynamics

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Helium interaction with metals such as tungsten in fusion reactors is a potentially enormous materials challenge, bringing with it the possibility of increased erosion rates, increased tritium retention, changes in conductivity, plasma disruptions, and material embrittlement. Considerable efforts have been put forth through the U.S. Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program on plasma–surface Interactions in the last several years to develop an understanding of helium accumulation and helium-induced surface damage in tungsten. Significant components of this effort are molecular dynamics simulations of helium plasma exposure with larger simulation sizes than are typically examined. In particular, we discuss simulations on the order of 50 nm × 50 nm × 30 nm, as well as a smaller subset of calculations for comparison purposes at 25 nm × 25 nm × 25 nm and 100 nm × 100 nm × 35 nm. These simulations use fluxes on the order 10^{25} m^{-2} s^{-1}, which is within a factor of ten of anticipated helium flux to the divertor in ITER. The results from these simulations, which extend to time scales of 1 μs and longer, show pronounced differences in surface evolution between different initial surface orientations and show significant trapping and segregation of helium near defects such as surfaces, grain boundaries, and dislocations. The primary purpose of the overall program is the development of Xolotl-PSI, a finite-difference simulation program intended to track helium and helium–vacancy cluster sizes for realistic times and experimentally-relevant length scales. The incorporation of the effects of other bubbles, surfaces, and grain boundaries into Xolotl, effects which have been largely discovered or at least informed by the molecular dynamics simulations as well as more targeted simulations, is an ongoing project. While the models embedded in Xolotl are incomplete, we are beginning to understand the important pieces of materials physics that are most important to the prediction of helium behavior in tungsten.

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I10. Modelling of plasma-wall interaction and impurity transport in fusion devices with the 3D ERO code

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The erosion of wall material and resulting impurity transport and deposition are critical issues in fusion research. Besides the limitation of the life time of wall components also long-term tritium retention by co-deposition has to be addressed. Experiments at existing devices in combination with modelling are necessary to understand the involved physics and eventually being able to make predictions for future devices like ITER or DEMO.
The present contribution provides a description of the 3D Monte-Carlo code ERO [1], which is used to model plasma-wall interaction and impurity transport in fusion devices. ERO considers physical and chemical erosion processes and simulates the transport of impurities in the test particle approximation in a given background plasma. The spatially resolved erosion/deposition at wall components is given as output together with the impurity distributions and their 3D light emission in the plasma around the wall component of interest. So far, ERO is designed to be used for rather local applications, normally wall components of sizes in the range of ~100 cm^2 surrounded by a simulation box. However, currently a major upgrade is envisaged including in particular massive parallelisation to allow for global transport applications covering much larger parts of the first wall of fusion experiments. The current status of the ERO upgrade activities will be summarised.
Some ongoing applications of the ERO code will be presented to demonstrate its application and comparison with experimental results. As an example, modelling of WF_6 and MoF_6 experiments at TEXTOR indicate that the local deposition of W and Mo suffers from an in-situ enhanced re-erosion if large deposition fluxes occur. Such enhanced re-erosion has also been observed earlier for carbon. As another application the erosion of beryllium (Be) wall tiles at JET has been studied in detail by comparison of modelled and observed Be light emission. The main aim is to qualify the sputter yield of Be as experimental data from laboratory experiments show very large scattering. It has been concluded from this modelling that Be erosion at plasma-wetted areas at JET rather follows the lower limit of the above-mentioned scattering than the upper one.

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I11. Material migration and fuel inventory in JET ITER-like wall from surface analysis techniques

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Two experimental campaigns have now been completed with the JET ITER-like wall configuration (JET-ILW); 2011-2012 (ILW-1) and 2013-2014 (ILW-2). Following each JET campaign a set of components have been removed for analysis. Results from the analysis of these components provide direct measurement of material erosion, re-deposition, fuel retention, surface and particulate morphology. In conjunction with campaign statistics, such as the distribution of strike points in the divertor, and additional real time diagnostics, an insight into the key plasma parameters driving material migration and fuel retention can be obtained.

This presentation provides an overview of fuel retention and material migration drawing on a range of analysis techniques. The results show that co-deposits still dominate fuel retention particularly on plasma shadowed surfaces and regions in the SOL where surface temperatures are lower. Deposits > 15 µm per campaign and with a rough topology have formed at the upper inner divertor in the scrape off layer (SOL) accounting for the majority of fuel retained in the divertor. In the main chamber deuterium retention is highest on the ends of beryllium limiter tiles where deposition occurs in the SOL compared with the centre of the tile where strong erosion occurs due to plasma interaction in limiter plasmas. Fuel retention in bulk tungsten also varies according to plasma exposure. In shadowed regions fuel inventory is up to 10^{17} D at./cm^2, where as in regions exposed to plasma the inventory is an order of magnitude lower. The influence of strike point on material migration to the remote divertor corners is clearly shown. Deposits in the outer corner are ~5 times higher for ILW-2 than ILW-1. This correlates with differences in the outer strike point distributions for the two campaigns. Micrographs of deposits in the outer corner show a layered structure which likely due to variations in plasma parameters and strike point location. In addition material migration by line of sight transport of sputtered neutrals to deposition monitors in the remote corners show a clear dependence on strike point position.

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[†] See the Appendix of F. Romanelli et al., Proceedings of the 25th IAEA Fusion Energy Conference 2014, Saint Petersburg, Russia

I12. Raman microscopy: a suitable tool for characterizing surfaces in interaction with plasmas in the field of nuclear fusion

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Raman microscopy, which is sensitive to chemical bonds, defects, structure,... is a suitable tool that can give information on how a material can be modified by interacting with ions. We are developing the Raman microscopy analysis of Be and W materials as a suitable tool to understand processes at work on the walls of tokamaks by comparing samples extracted after interaction in the tokamak plasmas and samples devoted to mimic tokamak samples synthesized in laboratory controlled conditions[**].

We will first give concrete examples on how this technique can be used to characterize, with a micrometric resolution, and on meter scale, samples extracted from old carbon tokamaks, and from one JET ITER like wall mirror [1]. We will then give concrete examples on what information can be obtained from the spectra by doing a study on laboratory materials such as Be (implanted by D ions [2]), Be_xW_y [1], BeC and WO_3 (implanted by D [3]), benchmarking Raman microscopy with other techniques (such as atomic force microscopy, electron microscopy, ion beam analysis,...) and/or DFT calculations.

We will conclude that depending on the processes at play, bands related to Raman active vibrational transitions are modified (band intensity variation, broadening, shifting) and new defect-induced bands can appear, related to structural and/or chemical modifications by plasma/wall interactions. Some of our findings are:

- when diminishing the size of Be crystallites to some nanometers, the phonon density of states appear in the spectrum
- when implanting Be with 2 keV D^+, high hydrogen retention is observed in the form of nanometric dendrites composed of BeD_2 hydrides
- when co-depositing Be and C, new Raman bands appear, these new bands being attributed to BeC_2, with the help of DFT calculations [4].

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** *<u>Origin of the samples studied/collaboration:</u> Be, Be_xW_y and BeC samples were deposited by the group of C. Lungu, in Romania [1]. Be implanted by D have been synthesized by the group of Ch. Linsmeieir, in Germany (IPP+FZJ) [2].*

I13. Helium Implantation Effect on Microstructure and Physical Properties of Tungsten for Plasma-Facing Fusion Reactor Components

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Tungsten is likely to be used for divertor armour components in future fusion reactors. During service it will be exposed to high temperatures, intense neutron flux and ion bombardment. Here we concentrate on the effect of injected helium on the mechanical and physical properties of tungsten.

Using X-ray micro-diffraction and laser-induced transient grating measurements, we observe lattice swelling and modulus change due to helium-implantation in tungsten. Surprisingly, a fraction of a percent lattice expansion, driven by the accumulation of helium and implantation defects, causes an order of magnitude larger reduction of the elastic modulus. These observations are interpreted using a combined elasticity and density functional theory based model. We find that our experimental observations are consistent with a damage microstructure dominated by Frenkel defects with helium-filled vacancies [1]. Measurements on helium-implanted single crystals confirm the slight increase in elastic anisotropy predicted by our calculations.

Transient grating measurements can also determine the thermal transport properties of the implanted layer. We show that even a modest concentration of injected helium leads to a substantial decrease in thermal diffusivity. Using a kinetic theory model this effect can be explained in terms of the implantation-induced damage microstructure [2]. Importantly the changes in thermal transport properties are not a trivial function of the implanted ion dose.

X-ray micro-diffraction measurements of lattice strains in samples heat-treated after ion-implantation show significant evolution of the damage microstructure. Indeed they suggest that at elevated temperatures defects migrate deeper into the material bulk [3]. Thus we can start to form a joined-up picture of helium-implantation-induced damage in tungsten and its diverse effects on microstructure and physical properties.

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I14. Energy landscape of nanosized interstitial clusters in Fe, W and V using ab-intio methods

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The size limitation of ab initio calculations impedes first principles simulations of crystal defects at nanometer sizes. Considering clusters of self-interstitial atoms as a paradigm for such crystal defects [1-4], we have developed an ab initio-accuracy model to predict formation energies of defect clusters with various geometries and sizes. Our discrete-continuum model combines the discrete nature of energetics of interstitial clusters and continuum elasticity for crystalline solid matrix. Moreover, the present energetic model can be adapted in order to address the free energy landscape of defects in body-centered-cubic metals up to the melting temperature. This energetic model is matched against atomistic free energy methods in which the phase space is sampled using adaptive molecular dynamics methods [5-7]. The discrete-continuum model is then applied to interstitial dislocation loops with <100> and 1/2<111> Burgers vectors, and to C15 [8] clusters in body-centered cubic crystals Fe, W and V, to determine their relative stabilities as a function of size. We find that in Fe the C15 clusters were more stable than dislocation loops if the number of self-interstitial atoms involved was fewer than 51, which corresponds to a C15 cluster with a diameter of 1.5 nm. In V and W, the 1/2<111> loops represent the most stable configurations for all defect sizes, which is at odds with predictions derived from simulations performed using some empirical inter-atomic potentials. Further, the formation energies predicted by the discrete-continuum model are reparameterized by a simple analytical expression giving the formation energy of self-interstitial clusters as a function of their size. The analytical scaling laws are valid over a very broad range of defect sizes and can be used in multi-scale techniques including kinetic Monte Carlo simulations and cluster dynamics or dislocation dynamics studies.

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I15. Scaling laws of cascade and sub-cascade formation in high energy ion and neutron impacts

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A critical constraint associated with the application of defect production cluster size scaling laws established in recent studies [1,2], to radiation phenomena occurring over a broad range of irradiation conditions, is the limitation on the energy of the incident particles at which the scaling laws still apply. Incident neutrons or ions, with energies exceeding a certain energy threshold, produce a complex hierarchy of collision sub-cascade events, which impedes the use of the defect cluster size scaling law derived for an individual low-energy cascade. By analysing the statistics of sub-cascade sizes and energies, we show that defect clustering at super-threshold energies can be described by a convolution of two scaling laws, one for the energies of sub-cascades and the other for the sizes of defect clusters formed in sub-cascades. The statistics of sub-cascade sizes exhibits a transition at the threshold energy, where the sub-cascade morphology changes from a single molten domain below the threshold, to several or many molten sub-domains above the threshold. The number of sub-domains then increases in proportion to the energy of the primary knock-on atom. The model has been validated against direct molecular dynamics simulations and applied to W, Fe, Be, Zr and sixteen other metals, enabling the prediction of full statistics of defect cluster sizes with no limitation on the energy of a cascade event. We found that populations of defect clusters produced by the fragmented high-energy cascades are dominated by individual Frenkel pairs and small defect clusters, whereas the lower-energy non-fragmented cascades produce a greater proportion of large defect clusters.

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I16. Modeling the kinetics of rhenium precipitation in neutron-irradiated tungsten

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High-dose, high-temperature neutron irradiation of W-based alloys results in the appearance of transmutation elements Re, and Os, among others. Both of these elements are soluble in W up to 30% atomic concentration at high temperatures under equilibrium conditions. However, above 1 dpa fast neutron irradiation dose, these transmutants are seen to form small intermetallic precipitates at concentrations of less than 2% atomic. Moreover, these result in substantial hardening of the W matrix. In this work, we present a kinetic model based on Monte Carlo simulations of W-Re precipitation parameterized entirely using DFT calculations, and including both vacancy and interstitial-defect mediated solute transport. The model is used to study radiation enhanced diffusion and radiation induced precipitation as a function of temperature and irradiation dose, as well as assess the conditions under which the formation of solute clusters is favored. Results from Monte Carlo calculations are then used to parameterize more efficient continuum-level kinetic models to predict the long term kinetics of fusion tungsten materials.

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I17. Radiation resistance of nano-crystalline iron: Coupling of the fundamental segregation process and the annihilation of interstitials and vacancies near the grain boundaries

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Finding novel nuclear materials with high radiation resistance is very important for the nuclear industry and requires the understanding of the self-healing of radiation damage in such novel materials as nano-crystalline iron. Combining molecular dynamics simulations, molecular statics calculations and the object kinetic Monte Carlo method, we found that the self-healing capability of nano-crystalline iron is closely related to the coupling of the individual fundamental segregation and annihilation processes of vacancies and interstitials near the grain boundary (GB). Statically, both near the GB and at the GB, a low-energy-barrier/barrier-free region forms around the interstitial which promotes the annihilation of vacancies. The annihilation process was found to always involve the collective motion of multiple atoms due to the recovery of the strained atoms around the interstitial. Dynamically, the annihilation involves two coupled processes. Before segregating into the GB, the interstitial annihilates lots of vacancies near the GB as it diffuses near the GB together with the low-barrier region. In addition, although the interstitial is tightly bound to the GB after segregation, it efficiently removes the vacancies near the GB while moving along the GB, with the low-barrier region extending into the neighborhood of the GB and even into the grain interior. These two mechanisms were found to work at low temperatures, even temperatures where the vacancy was immobile. This study revealed the interaction of the major radiation defects at different scales and thereby uncovered the origin of the high radiation resistance of nano-crystalline iron.

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I18. Modelling electronic excitation induced effects in tungsten

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Structural modification of materials by radiation is caused by either by energy transfer directly to the atoms or by the relaxation of radiation induced electronic excitations. Low energy ion irradiation mostly transfers energy to the atoms, whereas photons and very energetic ions excite electrons. High energy knock-on atoms from fusion neutrons fall in the intermediate regime, where energy is transferred to both the atoms and the electrons. The effects of energy transfer to the atoms is modelled by large scale molecular dynamics (MD) but modelling the electronic effects is more challenging. We include the effects of electron-phonon coupling and elecrtonic stopping in MD simulations by coupling to a continuum model for the electronic energy (2T-MD) [1]. The method can be used to model radiation effects from moderate energy ions, swift heavy ions and lasers [2].

Highly excited electrons affect the interactions between the atoms and the resulting non-thermal forces can induce ultrafast melting or other phase transformations. We have investigated the interactions between excited atoms of tungsten using high temperature density functional theory (HTDFT). The calculated phonon spectra for high electronic temperatures revealed a soft mode, which was indicative of a structural phase transformation. It was found that, at an electronic temperature (T_e) of 10000 K the fcc crystal structure has lower free energy than the bcc structure and above 15000 K there is no energy barrier associated with the bcc to fcc transformation along the Bain path [3]. Furthermore, ab initio molecular dynamics simulations at a T_e of 20000 K revealed that the initial bcc crystal transformed to fcc within 2 ps, further confirming the existence of the electronic excitation induced bcc to fcc phase transformation [4].

We have used HTDFT to fit a set of interatomic potentials that depend on the electronic temperature [4]. These electronic temperature dependent interatomic potentials can be used, in conjunction with 2T-MD, to include the effects of both electron-phonon coupling and modified interactions in large scale radiation damage simulations of cascades, swift heavy ions and lasers [5].

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I19. Ab initio thermodynamics of point defects in metals: Hydrogen, vacancies and their interaction

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Point defects such as vacancies and hydrogen atoms are frequently observed in metals that are subject to irradiation damage. The thermodynamic stability and kinetics of these defects is decisive for the long-term performance of these materials. While many ab initio approaches are limited to ground state properties, the dependence of the free energy on temperature and chemical potentials is very important for the defect stability. Furthermore, the activation energies for jumps of vacancies and interstitial atoms are decisive for their kinetics. Both quantities can be significantly altered by the interaction with other defects.

In this contribution, we apply our highly accurate ab initio methods to determine the free energy of vacancies [1]. Among all considered entropy contributions, we will in particular stress the relevance of anharmonic lattice vibrations. We will demonstrate that such an ab initio approach yields a non-linear temperature dependence, resulting in substantial deviations between low and high temperature results [2]. Further, thermodynamics concepts including defect complexes are applied to explain the exceptionally high vacancy concentration in intermetallic alloys and the exciting effect of superabundant vacancies in metals [3]. In particular, the hydrogen-vacancy interaction is addressed. At the end, consequences for the coalescence of vacancies and the molecule formation of hydrogen atoms are evaluated.

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I20. Experimental and computational approaches to the elucidation of hydrogen isotope permeation in erbium oxide coatings for tritium permeation barrier

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Establishing an efficient fuel breeding/recovering system is one of the main issues of D-T fusion reactors. Structural materials for DEMO reactors, such as reduced activation ferritic/martensitic steels, have high permeability for hydrogen isotopes in the operational temperature range. Fabrication of a thin ceramic film as a tritium permeation barrier (TPB) has been studied over several decades to mitigate tritium permeation to an acceptable level [1]. In recent years, research efforts in the development of TPBs have been dedicated to erbium oxide (Er_2O_3) coatings due to its potential to apply in liquid blanket systems [2]. In this presentation, experimental and computational results related to hydrogen migration behaviours in Er_2O_3 coatings are reviewed to organize the current status and further challenges on the TPB development. Latest investigations on multi-layer structure and irradiation effects on the permeation are also introduced.

A series of studies provided precise hydrogen isotopes permeation behaviours, such as the effects of surface coverage, grain size, multilayer structure etc., as well as permeation reduction factors of up to 10^5 at 873 K by high-purity Er_2O_3 coatings deposited on reduced activation ferritic/martensitic steel substrates. The development of fabrication process toward plant-scale fabrication has also progressed using a liquid-phase method. Accumulation of the experimental data on the Er_2O_3 coating properties and its hydrogen permeation behaviours provided a simplified model, suggesting that the primary requirement is to secure surface coverage of the coating and secondarily to control the microstructure of the coating.

For a further understanding of microscopic migration behaviours of hydrogen isotopes in Er_2O_3, first-principle calculations using density functional theory (DFT) and molecular dynamics (MD) simulations have been performed. The DFT results indicated that deuterium diffusivity, solubility and permeability in a single crystal Er_2O_3 showed a clear discrepancy with those of experimental data, due to the existence of grain boundaries in the Er_2O_3 coatings. On the other hand, the hydrogen diffusivity along grain boundaries estimated by MD simulations corresponded well to the experimental data within one order of magnitude.

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I21. Molecular dynamics simulations of H/He/dust interaction with W

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Tungsten (W) and W alloys are regarded as the most promising candidates for plasma facing materials (PFMs), which will be widely used in the next generation of fusion reactors. However, blistering in W-PFM induced by extremely high fluxes of low-energy hydrogen (H) and helium (He) ions irradiation will seriously influence the plasma stability and limit the lifetime of PFM. Dust issue is also an important problem in fusion devices. On one hand, dust can penetrate into plasma and cause the increasing of impurity. On the other hand, PFMs can be damaged by the impacting dust particles. These dust can cause damage on material surface and produce impurities by sputtering.

Based on the W-H-He potential developed by ourselves, we systematically investigate the interaction between H/He and different kinds of defects in W using molecular dynamics (MD) calculations. We have demonstrated the physical origin of H-H repulsion and He-He attraction in W, and given the binding energy dependence of H/He, vacancy and self-interstitial atom to the H/He-vacancy cluster on H/He-vacancy ratio. The formation and growing process of H-vacancy clusters and He-vacancy clusters have been demonstrated, respectively. However, higher H concentration is needed to form the H-vacancy clusters, while the He-vacancy clusters tend to form spontaneously.

In addition, the diffusion behaviour of small He clusters was also investigated by means of mean squared displacements (MSDs). The diffusivities of He clusters generally decrease with the cluster size increasing, and generally rise with the temperature increasing. When the size of the clusters is greater than 5, the cluster hardly diffuse in W. However, it is possible for He atoms to separate from the clusters under high temperatures. He atoms can form several small clusters at low temperatures, but large clusters at higher temperatures. Thus, the He bubble formation will be greatly influenced by the temperature, which is due to the fact that the small clusters hardly diffuse at low temperatures, and become mobile at high temperatures.

We investigate the interactions between Be/W dust and Be/W PFMs with the aid of MD simulations. The results show that W dust can cause serious damage on both W and Be surface. On W surface, a semi-sphere crater is formed. On the other hand, a more significant damage forms on Be surface where a vase-shaped crater generated. Because of the great deviation of W and Be, W atoms can penetrate deeply in Be material. However, the damage caused by Be is less significant. For both Be and W material, the crater is shallower and smaller. This is because the mass of Be dust is much less than that of W.

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ABSTRACTS
ORAL TALKS

O1. Ballistic He penetration into W fuzz

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Under exposure to intense low energy He plasma, W surfaces may turn into fuzz, a very low density structure consisting of nanorods. The exact growth mechanism of fuzz is not yet fully known. We present results of large-scale Molecular Dynamics simulations of low energy He bombardment of W fuzz structures. The goal of these simulations is to see if ballistic He penetration through W fuzz offers a more realistic scenario for how He moves through fuzz layers than He diffusion through fuzz nanorods. Instead of trying to grow a fuzz layer starting from a flat piece of bulk W, we employ a new approach of creating fully formed fuzz structures 0.43 μm thick out of ellipsoidal pieces of W, consisting of up to 37 million atoms. Lack of detailed experimental knowledge of the three-dimensional structure of fuzz is dealt with by simulating He bombardment on five different structures of 15vol% W and seeing how much difference the details of how the structure was created makes for how deep He penetrates. Results show that the by far most important factor determining He penetration is the amount of open channels through which He ions can travel unimpeded. For a more or less even W density distribution He penetration into fuzz falls off exponentially with distance and can be described by a 'half depth'. In a 15vol% fuzz structure, the half depth can reach 0.18 □m. In far sparser fuzz structures that were recently reported, the half depth might be 1 μm or more. This means that ballistic He penetration offers a more likely scenario than He diffusion through nanorods for how He moves through fuzz. It may provide an adequate explanation for how He penetrates through the thickest fuzz layers reported so far.

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O2. The BCA-KMC Hybrid Simulation for Hydrogen Retention in Tungsten Material

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To achieve the fuel balance and the recycling in fusion reactors, it is necessary to understand hydrogen and helium behaviours in plasma facing materials. In experience, the plasma-material interaction (PMI) strongly depends on the particle balance between the flux of plasma particles and the diffusivity in materials. Therefore, the long time scale simulation to reproduce realistic flux and fluence corresponding to experiments is a key issue for the particle balance. In our previous work, the formation of the fuzzy nano-structure induced by helium plasma irradiation had been successfully represented by Molecular Dynamics and Monte-Carlo (MD- MC) hybrid simulation [1,2] which can treat the realistic flux, 10^{22} $m^{-2}s^{-1}$, and fluence, 0.5×10^{22} m^{-2}, corresponding to experimental conditions. However, the MD-MC hybrid had not treated the collision cascade process of the helium ions, and the diffusion of helium atoms in material is just simple random walk in uniform lattice.

In the present work, we further develop the Binary Collision Approximation and Kinetic Monte-Carlo (BCA-KMC) hybrid simulation. In the BCA-KMC hybrid simulation, the BCA part treats the collision cascade process of incident plasma particles and the KMC part treats the diffusion processes of hydrogen isotope atoms and vacancies in tungsten materials. A shot of the collision cascade process is regarded as an event in the KMC algorism. The reason why the BCA is used for the collision cascade process is that the calculation speed of the MD is insufficient to achieve realistic flux and fluence. Here, the elapsed time of the BCA-KMC hybrid simulation can reach the time scale of 10^{-2} s beyond 10^{10} times of the gap with the time scale of atomic migration. In addition, the modification of the BCA code to treat any structured target materials [3] based on the ACAT [4] code is important for the present hybridization. The BCA-KMC hybrid simulation is here applied into the problem of hydrogen retention. Hydrogen retention amount at laboratory experiment flux, 10^{20} $m^{-2}s^{-1}$, to ITER divertor environment flux, 10^{24} $m^{-2}s^{-1}$ have been estimated.

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O3. Preparation and Characterization of Mixed Layers containing Beryllium and Deuterium

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The characteristics of fuel retention and release have been extensively studied [1-2]. Hovewer studies concernig the behaviour of pure and mixed materials containg beryllium (Be) are not so numerous, due to the difficulties to handle beryllium material. At the National Intitute of Laser, Plasma and Radiation Physics, Romania, a beryllium handling facility is operational since 2005, dealing with Be coatings on inconel and marker tiles [3] and Be containing solid and gaseous co-depositions [4]. These kind of mixed materials are supposed to play an important role in the fuel retention mechanism during the operation of ITER. In order to obtain samples with deuterium (D) inclusions a RF deuterium plasma was ignited during the beryllium deposition process using a HiPIMS system, having argon/deuterium mixture as working gas. D ions were generated in the produced plasma and were co-deposited with pure Be, and Be/W targets on the substrates kept at room temperature.
SEM measurements have been performed on the prepared samples, in order to investigate the films morphologies. 12x14x1 mm^3 Be, W, C and Si were used as substrates for each deposition.
X-ray diffraction spectra taken by use of CuKα radiation reveled the presence of hexagonal beryllium polycrystalline phase characterized by sharp peaks for all preferential orientations especially for Be(100) Be(002) and Be(101)
Thermal desorption spectral (TDS) measurements were performed for all types of samples: Be+D, Be/W +D films of 1 µm. In order to assess the nuclear fuel retained, the release of of HD and D_2 molecules were measured. All of the known trapping states for Be-D are observed as peaks and shoulders according to [5] (D/Be up to 1; 450-500K; BeD_2; 550-600K; BeO; 700K; defects; 800-900K) during the TDS experiment but in different proportions depending on the deposition conditions. Substrate for instance changes the nucleation process and gives the layer different structure. This makes different trapping states predominant for each substrate. The D amount has comparative values for films coated on Be and W substrates and much lower values for the films coated on Si substrate. This is due to the absence of the diffusivity phenomena of D in Si. This is why we can assume that some D also diffused in the W and Be substrate during the deposition.

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O4. Studies on plasma / Aluminium (as Beryllium surrogate) interactions: particle nucleation and hydrogen inventory in material defects

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Prediction of tritium retention by plasma-wall material and plasma dusts is a major issue related to the well-operating and safety of tokamaks. That is why erosion, particle growth and inventory processes are studied for different Plasma-Facing Components (PFCs) such as tungsten or beryllium. However experimental studies in laboratory on beryllium are limited by its toxicity. Aluminium is an alternative element (Be-like) which can replace it 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 aluminium nanoparticle formation in magnetized plasma. We consider a laboratory discharge system where plasma is ignited by microwave Electron Cyclotron Resonance (ECR) between 0.1 and 1 Pa [2]. Observed particles are formed through plasma-surface interaction in H_2/Al or Ar/Al systems. We develop a 1D model for hydrogen and Ar discharge obtained in this system in the radial direction discharge on the dipolar magnet equatorial symmetry plane. In the obtained discharge conditions we then solve for the Al cluster growth created by sputtering of neutral Al and follow all neutral, negative and positive cluster growth in order to understand the possible nucleation route.

Our second objective is to describe hydrogen retention and bubble growth in the aluminium bulk using HIIPC (Hydrogen Isotope Inventory Processes Code) model. Resulting from several collaborations, the model simulates the hydrogen inventory in the PFCs (tungsten, beryllium) [3] enabling simulating Temperature Program Desorption (TPD) experiment. This work is focused on the bubble growth model description, data and confrontation with experimental results obtained with our ECR device [4].

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O5. The behaviours of helium atoms and clusters in vanadium studied with atomistic simulations

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Vanadium (V) based alloys have been identified as one of leading candidate materials for fusion first-wall and blanket structure applications due to their favourable mechanical and physical properties [1, 2]. Understanding the interaction between helium (He) and the host structural materials is of fundamental importance within a fusion reactor environment. However, up to now, few works have been performed to study the He behaviours in vanadium with atomistic simulation approaches. In the present study, a new interatomic potential for V–He interactions is developed by fitting to the results obtained from first-principles density functional theory calculations. The nudged elastic band and mean square displacements methods are used to get the migration energy barriers and diffusion coefficients of He atoms and clusters. With molecular dynamics simulations, the diffusing, clustering, and trapping of interstitial He atoms in vanadium are studied in detailed. It has been found the He atom prefers to occupy the tetrahedral interstitial site (TIS) in vanadium, and it can migrate quickly with very low barrier (0.06 eV) along the TIS-TIS path. Compared with iron and tungsten, however, the He atoms aggregate into clusters with lower binding energies of an additional He atom to He_n and He_n-vacancy clusters, and the trapping of He atoms depends much strongly on the pre-existing traps in host vanadium. The weak hybridization between the d state of V atom and the p state of He atom is responsible for the low binding energy for He-He pairs in vanadium [3]. The production and clustering of cascade defects have been investigated in vanadium with interstitial and substitutional He atoms. The effect of He concentration, PKA energy and irradiation temperature are also discussed.

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O6. Multiscale study of plasma induced trapping of hydrogen isotopes in tungsten

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Tungsten is a primary candidate material for plasma facing components in future fusion reactors. One of the current issues in the design of plasma facing component is trapping and retention of tritium since it is toxic and radioactive. Last years an extensive number of experimental studies were aimed on systematic study of mechanisms of hydrogen isotope (HI) retention in tungsten under fusion relevant plasma exposure conditions. However, the experimental data, available in literature is very scattered and does not allow one to create a physical model. Simulations of HI retention and desorption from tungsten samples with classical diffusion trapping simulation codes does not give a convincing result due to a large number of ad-hoc parameters needed to reproduce the experiment. In this work we would like to present our understanding of mechanisms governing plasma induced HI retention and material modification. Based on atomistic simulation results we propose a model of non-equilibrium HI trapping and bubble formation operating at sub-surface region of the material during plasma exposure. We link this model to classical diffusion-trapping retention mechanisms relevant for retention in the bulk of the material. The proposed model allows one to relate HI trapping with the microstructure of the material together with plasma exposure conditions. We use the model for interpretation of recent experimental results.

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O7. Influence of He on hydrogen isotope transport and retention in tungsten - first observation of D accumulation around He implantation zone

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As one progresses towards burning fusion plasma the influence of the presence of He on hydrogen retention comes into focus. Recent experiments with He seeded D plasmas showed that helium forms nano bubbles in the near surface layer, blistering is reduced and most importantly D retention is decreased [eg. 1]. While there are several attempts to explain the observations, the actual cause remains unclear. One possibility for the reduced retention is that He might act as diffusion barrier. Likewise nano-sized bubbles might open up additional pathways of D back to the surface thereby decreasing its transport to the bulk. Contrary to these experimental findings density functional theory (DFT) calculations show strong attraction between He and hydrogen [2,3], indicating preferential trapping of deuterium around He clusters.

In order to unravel this mystery of He acting as possible diffusion barrier and preferential binding of H around He, we took a different approach. We tried to separate the surface effect from the He effect by moving the He interaction zone into depth. Moreover, the study was made on saturated self-damaged W to decouple the possible influence of displacement damage created by He irradiation from the He-H interaction. In the experiment a recrystallized tungsten sample was first implanted by 20 MeV W ions creating a damage dose of 0.25 dpa. The sample was then exposed to a well-characterized low-temperature plasma at 290 K in order to decorate the defects induced by the W ion implantation reaching a homogenous D depth profile within the first 2 μm with a D concentration of about 2 at. %. One half of the sample was then irradiated by 500 keV He ions, fluence of 7.0×10^{20} He/m^2, obtaining 4 % of He buried 1 μm deep, approximately in the middle of the W ion damage zone. In the first experimental series isochronal annealing (2 h) was performed and after each temperature step the D depth profile was measured by Nuclear Reaction Analysis (NRA) in-situ on the He irradiated and no-He irradiated half of the sample. At 450 K strong accumulation of D in the He implantation zone was observed, increasing from 2 at. % to 3.5 at. %., whereas in the no-He half 20% decrease of deuterium retention was observed over the whole damaged zone as expected from previous studies. Hence no indication was found that He acts as a diffusion barrier. With further temperature increase the total amount of D started to decrease also at the He half of the sample and complete D desorption on both halfs was observed at 800 K. Consecutively the empty sample was exposed to D atoms (0.2 eV, flux 3.7×10^{18}D m^{-2}s^{-1}) at 600 K to study D uptake. The speed of D loading of the He half matched theno-He half however we again observed strong accumulation of D around the He implantation zone, obtaining an almost 3 times higher concentration on He half as compared to the no-He half by the end of exposure (fluence 1.28×10^{24}D m^{-2}s^{-1}).

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O8. Interatomic potentials for modeling radiation damage in tungsten: a comparison with DFT calculations.

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We have compared, for tungsten, the behaviour of five empirical interatomic potentials from the literature and one very recently derived, in situations related to the creation of the primary damage and threshold displacements with density functional theory (DFT) results obtained using two kinds of potentials: the minimal set regular planar augmented wave (PAW) potential and one PAW potential taking into account semi-core electrons. Threshold displacement energies (TDE) have been calculated over all directions using the method proposed by Nordlund et al. [1]. The comparison with the DFT results is not straightforward as the distributions obtained can be very wide depending on the direction. The evolution of the total energy of the system when one moves one atom step by step along one symmetric direction is compared with DFT results and provide a good assessment on the potential behavior. These results are confirmed by studies of replacement collision sequences (RCS) in the same direction, which also indicate that for the RCS along the <100> and the <111> directions, the softer the potential, the longer the « decay », the less energy transmitted to the « head on » atom and the later. For the <101> direction, the softer the potential, the longer the « decay », the more energy transferred to the « head on » atoms. The analysis of the minimum distance between atoms during the RCS collisions, indicates that the smallest distances between atoms are found for the RCS along the <111> direction and vary from 0.38 to 0.76 lattice units according to DFT. These interatomic ranges are thus the ones that need to be carefully adjusted when one hardens equilibrium potentials. Regarding equilibrium properties related to point defect generation: point defect formation energies, vacancy migration energy and spatial extension of the crowdion, our results underline the importance of reproducing correctly the crowdion.

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O9. Multi-scale simulations of fuel retention in JET-ILW divertor

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Experimental analyses done on samples retrieved from JET plasma-facing compo- nents reveal the extent of plasma-material interactions taking place during the JET operation. Results from the present JET all-metallic ITER-Like Wall have shown a substantial fuel retention rate decrease by a factor of 20 when compared to the oper- ation with the all-carbon JET wall [1]. Moreover, the fuel retention correlated with the erosion/deposition pattern measured in JET plasma-facing components. Analyses were performed with Ion Beam methods (IBA) and with Thermal Desorption Spec- trometry (TDS). The IBA results show the elemental composition of the deposits. The release properties of the co-deposited fuel species in the deposits are determined with TDS.

In the present work, the fuel retention and release properties in JET divertor samples are studied using the concept of Multi-scale calculations. A set of Rate Theory Equa- tions [2] describing the fuel mobility, release and re-trapping events are parametrized with Density Functional Theory calculations. The thicknesses of the deposited layers and the elemental composition of the deposits (main impurity Be, minor impurities C and O) are obtained from the previous experimental IBA results [1] and used directly as an input in the setup of the Rate Equations. The Multi-scale calculations for the TDS spectra, i.e. the fuel release at elevated temperatures show the effect of the thickness of deposited layers and their impurity (Be, C, O) composition as well as the effect of the deposit morphology.

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O10. Near Surface Helium Segregation in Tungsten with 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 latest code development and benchmarking of Xolotl, a new spatially-dependent reaction diffusion cluster dynamics code to simulate the divertor surface response to fusion relevant plasma exposure. The initial focus of our effort has involved simulating the behavior of tungsten to 100 eV helium plasma exposure.

Atomistic simulations reveal that the helium behavior near surfaces and grain boundaries is modified from that in the bulk, as a result of elastic interaction forces [1]. We used a hierarchical approach to scale bridging incorporating atomistic studies based on a reliable interatomic potential to parameterize Xolotl [2]. We extended our continuum model to two spatial dimensions in order to take into account the biased drift of mobile helium clusters toward the grain boundaries observed in atomic-scale simulations.

Finally, we extensively compared the results from large-scale molecular dynamics simulations to those from Xolotl to verify our model as well as understand its limitations.

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O11. Recent Activity in Russian Federation on Simulation of PMI in Fusion Devices

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The19th Annual Conference on Plasma Surface Interactions was held at MEPhI this January. Many presentations were devoted to experimental and computer simulations of plasma and its components interactions with plasma faced materials (PFM) for fusion devices. The conference agenda covered a broad list of topics related to MOD PMI Workshop including:

- materials behaviour under high heat fluxes;
- hydrogen isotopes retention in PFM;
- influence of oxygen on hydrogen recycling at plasma exposure;
- lithium and liquid metals as PFM
- tungsten fuzz behaviour

The aim of this presentation is to make a brief review of new results and findings important for PMI modelling obtained in Russian laboratories during the last year. Some of these results are given below:

The movement of molten layer, distribution of plasma pressure near the target as well as influence of the magnetic field and auxiliary acceleration on molten layer were measured at pulsed plasma accelerator in TRINITI (Troitsk) [1].

Physical conditions of droplet emission from the molten tungsten exposed to the plasma flux parallel to surface as a result of the wave crests blowing out were found by Yu.Martynenko [2]. It was shown that generation of waves and droplet emission are also possible at normal incidence of the plasma flux.

Testing of ITER grade tungsten under 0.2 -1.5 MJ/m^2 pulsed plasma loads ($P\sqrt{t}$ = 9 – 67 MJ/m^{2}s$^{1/2}$) at QSPU-T facility [3] demonstrated the threshold ~0.7 MJ/m^2 of crack‘s formation. Three types of cracks and its networks on the surface identified. The largest cracks of type I (0.2-1mm deep with density of network knots 10-50 cm^{-2}) and type II (0.1mm deep and density of knots 1-5·10^3 cm^{-2}) are generated below or near threshold of melting, while the cracks of type III (0.01-0.07mm deep, density of knots 2-3·10^{4}cm^{-2}) are generated above melting threshold. W coverage with deposited metal layer increases the threshold of crack’s formation.

The He concentration in W fuzz was estimated by V.Efimov et al [4] on the base of comparative thermal desorption measurements to be (13 ±2)%.

The role of oxygen in hydrogen transport trough oxidized surfaces is emphasized in qualitative model proposed by L.Begrambekov [5].

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O12. Hydrogen effects on radiation damages in tungsten

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Tungsten is a prime candidate as the divertor material of the ITER and DEMO reactors, which would be exposed to unprecedentedly high-flux plasmas as well as neutrons. For a better characterization of radiation damages in the tungsten under the divertor condition, we examine influences of super-saturated hydrogen on vacancies in the tungsten. The present calculations [1-3] based on density functional theory (DFT) reveal unusual phenomena predicted at a super-saturated hydrogen concentration: strongly enhanced vacancy and di-vacancy concentrations under the super-saturated hydrogen concentration are predicted by a thermodynamics model assuming multiple-hydrogen trapping, i.e. hydrogen clusters formation, in the vacancies; and DFT molecular dynamics revealed that hydrogen clusters can prevent a vacancy from recombining with the neighboring crowdion-type self-interstitial-atom. These suggest that neutron damage effects will be increased in the presence of the hydrogen clusters.

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O13. Modeling of effects of vacancy, vacancy clusters and grain boundaries on hydrogen behaviors in tungsten

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Tritium retention in and leakage through plasma facing components need to be suppressed for radiation safety and fuel cycle sustainability of fusion reactors. In order to accurately predict the tritium behaviors during reactor operation, deep understanding of the influence of lattice defects is vital. In this study, we investigate effects of vacancy, vacancy clusters and grain boundaries (GBs) on hydrogen solution, diffusion and permeation in tungsten using thermodynamic models.

First of all, molecular dynamics (MD) simulation was performed with LAMMPS code. The purpose of the MD simulation is to quantify the effect of each defect on hydrogen diffusivity and solubility and to clarify the mechanism of it. Since the quality of available potential models for W-H system is not satisfactory for this purpose, the MD simulation was performed with bcc-Fe, in which hydrogen-defect interactions are similar to those in bcc-W and a good potential model is available. Based on observations in the MD simulation, theoretical models to describe the effects of those defects were constructed by means of rate theory and equilibrium theory. The validity of the constructed models was confirmed in comparison with MD simulation results. Subsequently, model parameters for bcc-W were determined by first-principles calculation using VASP code. Finally, by combining models on vacancy, vacancy clusters and GBs, hydrogen behaviors in various conditions were evaluated.

The constructed model nicely reproduced available experimental data on hydrogen diffusivity and permeability. It was indicated that hydrogen in bcc-W diffuse dominantly along GBs at temperatures below around 1000 K. The contribution of diffusion in the crystal lattice (tetrahedral sites) is negligible. This is because the binding energy at GB is large (~1 eV) while the energy barrier for diffusion along GBs are comparable with that in the crystal lattice. It was also indicated that hydrogen solubility and permeability are larger in materials of smaller grains. This point should be taken into account when developing advanced materials having small grains.

MD simulation of vacancy clusters showed that vacancy clusters have smaller trapping capabilities than isolated mono-vacancies if the concentration of vacancies is fixed. This phenomenon can be explained by considering an effective number of hydrogen trap sites, which decreases as the cluster size increases because hydrogen atoms basically can stay only on the inner wall of vacancy cluster. In the present MD simulation, H_2 molecule formation in vacancy clusters could not be appropriately described. In order to correct it, the amounts of H_2 molecules in vacancy clusters were roughly estimated. The estimation indicated that the total amount of trapped hydrogen become comparable between isolated mono-vacancies and vacancy clusters if hydrogen gaseous pressure in clusters is ~GPa.

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O14. Effect of Re and Os in W under irradiation: comparison between numerical and experimental results

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Tungsten is expected to be a promising plasma-facing material for future fusion devices, but radiation-induced precipitation (RIP), which leads the material to hardening, is a concern at their practical use. One of the keys to accurate prediction of the emergence of RIP is stability and migration of solute atoms, rhenium (Re) and osmium (Os), that are produced by nuclear transmutation through irradiation. We conduct a series of numerical simulations using *ab initio* and an atomic kinetic Monte Carlo method to investigate the behaviour of these solute elements[1,2].

We find that tungsten interstitial atoms displaced by radiation favourably form mixed dumbbell with the solute atoms, and these mixed dumbbells have 3D motion instead of 1D motion of SIAs. We believe that the shift of migration dimension greatly influences the diffusivity of the solute elements and their aggregation as precursor of the RIP. Our computational results suggest that the aggregation would be caused by recombination of vacancy and interstitial both of which are associated with solute atoms, and this notion is supported by experimental evidences.

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O15. A Density Functional Theory investigation of H saturated W surfaces

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This work takes parts in an ongoing effort to better understand the interaction of hydrogen with tungsten at the atomic scale and to produce macroscopic data that can be compared with experimental results. Calculations are performed within the Density Functional Theory framework.

Understanding the amount of hydrogen that saturates tungsten surfaces and the atomic-scale recombination processes taking place on the saturated surface is of paramount importance to improve the accuracy of macroscopic models used in large scale fusion research.

The interaction of hydrogen with the three most stable surfaces of tungsten (001), (110), and (111) surfaces of tungsten was investigated. The comparative stabilities of the (001), (110), and (111) surfaces are first calculated and the binding energies of various stable configurations of hydrogen are determined depending on the surface coverage. These results are intended to complement and improve the statistic model previously built [1] and provide data necessary to refine the parameterization of potentials used by the molecular dynamics community.

We found both (110) and (001) surfaces capable of accommodating high surface concentration of hydrogen. The (110) surface can accommodate more than 2 H *per* W atom, while the (100) surface accommodates more than 4 H *per* W atom. We will present our latest results on W surface saturated by H atoms.

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O16. Electrodynamics of correlated materials: the optical conductivity as a probe for Mott and charge-transfer physics for copper oxides

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Phenomena that are connected to quantum mechanics, such as magnetism, transport, and the effect of impurity atoms and disorder, and their relation to material design and energy needs are important for almost every branch of the industry. Density functional theory (DFT) was successful at making accurate predictions for many materials, in particular compounds which have a metallic behaviour.

However, one bottleneck of DFT is that it fails at describing well some of the compounds where strong correlations are present, in particular because the theory has to capture both the band-like character of the uncorrelated part of the compound and the Mott-like features emerging from the local strongly correlated centres.

A recent progress has been made in this direction by the dynamical mean-field theory (DMFT), that allows describing the two limits (metal and insulator) in a remarkable precise way when combined with DFT.

We review here how DFT+DMFT can be used to investigate intermediate energy properties of the copper oxides, by comparing theoretical predictions of the optical spectra with experimental data.

In particular, we identify coherent and incoherent spectral features that result from doping a charge-transfer insulator, namely quasiparticles, Zhang-Rice singlet band, and the upper and lower Hubbard bands. We investigate the asymmetry between particle and hole doping. We discuss how the doping and temperature dependence of the optical spectral weight can be used to evaluate the strength of the correlations in hole and electron doped materials, and discriminate between Mott insulators and Slater insulators.

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ABSTRACTS
POSTERS

P1. Shape of hydrogen-covered bubbles in beryllium: ab initio study

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Beryllium is very promising material for fusion energy applications due to its ability to multiply neutrons efficiently. High-energy neutrons arising from thermonuclear reaction in the plasma lead to a production of helium and beta-radioactive tritium in beryllium pebbles and, as a consequence, to formation of helium bubbles and embrittlement. Assessment of radioactive inventory of tritium in beryllium pebbles is very important from the safety point of view as well as for handling of the radioactive beryllium wastes after the end-of-life of the tritium-breeding blanket. The present design concept of ITER considers beryllium also as a plasma facing material for the first wall. In both cases hydrogen isotopes will interact either with the outer surface of the first wall or with internal surfaces of helium bubbles.

In this study five principal low-indices close-packed beryllium surfaces were investigated: basal (0001), prismatic type I $(1\ 1\ \bar{2}\ 0)$ and type-II $(2\bar{1}\ 1\ 0)$, pyramidal type-I $(1\ 1\ \bar{2}\ 1)$ and type-II $(2\bar{1}\ \bar{1}\ 2)$. Relaxation of the outermost surface layers covered with hydrogen atoms was studied for all above listed planes. Drastically different relaxation patterns with respect to pure beryllium were found. Similar behavior of the surface energy calculated with consequent addition of hydrogen atoms was revealed for most of the surfaces: the energy first reduces, reaches a minimum and thereafter rises with the increase of hydrogen coverage. A knowledge of the surface energy as a function of hydrogen surface coverage allowed us determination of the equilibrium shape of a bubble via Gibbs-Wulff construction. The hydrogen concentrations at different surfaces were calculated by minimizing the free energy of the perfect single crystal with a void. Here we consider the case with different hydrogen coverage on various surfaces and compare the results with the case of equal hydrogen coverages reported previously [1]. For 0% coverage Wulff polyhedron is composed mainly of basal, prismatic type-I and pyramidal type-I faces, while at critical coverage of 1 ML only pyramidal type-II facets are present. As a result, we obtained an expression for chemical potential as a function of hydrogen concentration. Assuming that chemical potential at equilibrium must be constant for all surfaces, the new hydrogen concentrations were estimated and Wulff polyhedra were constructed. Although the topology of the Wulff polyhedra slightly differs from that found in the case of equal coverages, the obtained equilibrium shapes still do not describe all the features observed experimentally. The discrepancies between the predicted equilibrium shapes of gas bubbles with the experimental results are discussed.

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P2. Modelling of Neutron Damage and PKA Spectrum for Synergistic Plasma Effects

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A fundamental concern for a hypothetical DEMO reactor is that of synergistic effects between plasma and neutron damage. This is detailed in the work [1] where phenomenon such as tritium retention and changing material properties are mentioned. One fundamental concern is that the various scales (both time and length) over which the effects occur at. As a direct corollary of this, the fundamental nature of damage through plasma and neutrons was investigated. A primary concern became that of the length scales on which these occur.

In the current landscape, experiments for neutron damage are done using ions as a proxy [2,3]. However, ion damage (like plasma) occurs fundamentally in the surface (order of 10 micro meters) considering fusion energy levels. The mean free path for a 14 MeV neutron itself would be in the centimetre scale which is further testified by sputtering theory combined with neutron sputtering experiments [4-6].

We have carried out work using a coupled MCNP4C and SRIM analysis with tungsten as the material. This has shown that, in terms of a standard Displacement per Atom (DPA) measure, damage is indeed lower in the first twenty microns; with the bulk of collisions occurring sub surface at the centimetre (meso) scale. Furthermore, we have also managed to construct a spectrum of Primary Knock-on Atoms (PKA) as a function of space and energy which shows that thermal events may occur subsurface. This leads us to hypothesise that plasma and neutrons are unlikely to interact due to the vastly different length scales over which the damage occurs.

The work done, however, provides a static picture in terms of DPA. In order to fully understand the nature of neutron damage, further work must be undertaken. Therefore, we will detail our current investigation in cascade evolution using MD simulations in order to contribute to the current work already being done. We hope that this will allow us to conclude that plasma neutron synergies will be less likely than previously expected as well as question the appropriate the use of ions as a proxy for neutron damage.

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P3. Interstitial-mediated diffusion and clustering for transmutation elements Re and Os precipitation in W

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Tungsten (W) and W alloys are considered as the most promising candidates for plasma facing materials (PFMs) in future fusion reactor. However, as a PFM, W will be exposed to 14 MeV high energy neutrons under a fusion environment, leading to the burn-up reaction and producing the transmutation elements. Rhenium (Re) and Osmium (Os) are the major transmutation production in W. Re and Os will precipitate under irradiation, and form new Re/Os-rich precipitate, which has significant effect on the microstructure and mechanical properties of materials. However, the formation mechanism of Re and Os precipitates has not been well understood.

Here, we have investigated the mechanism for the irradiation-induced Re/Os clustering in W using the first-principles method. It is found that the interaction between substitutional Re/Os atom (SS-Re/Os) is very weak. Taking into account the configurational entropy, the substitutional Re/Os clusters are thermodynamic instability. The diffusion energy barrier of Re/Os via the vacancy-mediated path is very high, which suggests that the formation of Re/Os clustering in W by the vacancy-mediated way is difficult. Further, we found that there is strong attraction between Re/Os and self-interstitial atom (SIA) in W. The SIA can be easily trapped by Re/Os once overcoming a low energy barrier (0.25 eV for Re and 0.09 eV for Os), and form W-Re/Os complex dumbbell. The diffusion energy barrier of W-Re/Os dumbbell (0.12 eV for Re and 0.40 eV for Os) is much lower than that of Re/Os diffusing via mono-vacancy (1.63 eV for Re and 1.36 eV for Os) or even vacancy clusters (0.99 eV for Re and 0.95 eV for Os). Most importantly, the W-Re/Os dumbbell can be easily trapped by the SS-Re/Os, and form high stable Re-Re/Os-Os dumbbell structure. The Re-Re/Os-Os dumbbell can serve as trapping centre for subsequent interstitial-Re/Os, leading to the growth of Re/Os-rich clusters in W. Our finding suggests an interstitial-mediated mechanism dominating the irradiation-induced Re/Os clustering in W, which will facilitates our understanding the microstructure evolution of W-PFM under long-time irradiation.

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P4. Tungsten oxide thin films: D^+ and He^+ bombardment

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Because of its favorable physical properties such high melting temperature, high thermal conductivity and low erosion yield, tungsten will compose the ITER divertor. As a drawback, tungsten has a strong chemical affinity with oxygen and native oxide is naturally present on tungsten surfaces. In this work, thin WO_3 thin films which mimic the possible oxidation of W Plasma Facing Components (PFCs) are produced to study their behaviour under low energy D^+ and He^+ bombardment. The aim is to improve our understanding on elementary mechanisms involved in erosion and retention processes and to study the effects on the structural properties of tungsten oxides.

The formed oxide tungsten layers have been characterized using scanning electron microscopy (SEM), atomic force microscopy (AFM), Raman spectroscopy, X-ray diffraction (XRD) and transmission electron microscopy (TEM) techniques. The thickness of the oxide tungsten layers were, controlled using the above approaches and, found to be in the range of 20 nm - 250 nm. A set of virgin tungsten and tungsten oxide samples will be exposed to D and He plasma and/or ion beams with E=0.01 - 1.0 keV and high fluxes (10^{20}-10^{24} m^{-2} s^{-1}). Preliminary low energy D plasma exposure (11 eV/D^+) of tungsten oxide has been performed at PIIM laboratory (Marseille-France). Following to D^+ implantation, the formation of tungsten bronze (D_xWO_3), a change in the oxide structure, a change in the layer colour due to an electrochromic effect and a deep diffusion of D^+ have been observed [1]. Therefore, a comparative study of D versus He (high affinity to induce the creation of bubbles, holes and nanostructure morphology [2]) exposures is mandatory in order to determine the elementary processes of implantation and to dissociate chemical and physical effects

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P5. Modelling the Timescales in Which Helium Embrittlement Occurs within Breeder Blanket Materials

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Within a DEMO like reactor, material will be exposed to high energy neutron fluxes. This will result in a in an accumulation of helium through transmutation. This causes most concern within the breeder blanket region, since steels (an iron based alloy) in this region will experience the highest rate of helium transmutation within the reactor. Helium being highly mobile and insoluble, leads to gas bubbles forming at the grain boundary of the metal, causing dilatation of the grain interfaces. This mechanism is known as helium embrittlement and renders the metal unusable [1].

Research has been done to predict the timescales in which this would occur under DEMO conditions. In current models, this can be as low as 2 years, which falls 3 years short of the minimum life time for breeder blanket components to enable fusion to be economically viable [2]. The previous model, developed by Mark Gilbert *et al.* is considered to be an extreme worst case scenario where all the helium migrates to the grain boundary (GB). In reality intergranular activity will act to pin the helium, affecting the rate at which helium migrates to the GB. A more elaborate model is being developed, accounting for pinning mechanisms that will reduce the rate of migration.

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P6. Paschen curve approach to investigate electron density and deposition rate of Cu in magnetron sputtering system

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In this work, Paschen curve for Ar gas was obtained during Cu deposition using DC magnetron sputtering system. Five process parameters of Paschen curve were used to obtain the electron density and deposition rate of the deposited nano structured thin films. Plasma parameter such as electron density was correlated with the deposition rate. It is proposed that maximum deposition rate of finest grain size may be obtained at plasma process parameter corresponding to Paschen minimum. Furthermore, low electron density and high hardness were obtained at paschen minima. This investigation helps to understand and optimize the quality of nano structured thin film dependence on process parameter.

Key words: Paschen curve, Electron Density, Deposition Rate, Grain size and Hardness

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P7. Recent Progress in Modelling of Hydrogen Interactions with Beryllium (0001) Surface

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Beryllium is a candidate material for the first wall of future fusion reactor and is also foreseen as a neutron multiplier in the tritium breeding blanket. Hydrogen isotopes are either generated inside beryllium bulk via nuclear transmutations or come from fusion plasma. In either case they interact with external surface of the Be first-wall tile or internal surfaces of helium gas bubbles. Therefore, theoretical investigation of such interactions is of crucial importance for the understanding of beryllium behaviour in fusion environment.

This contribution presents recent progress of the first principles modelling of hydrogen isotope interaction with beryllium (0001) surface. It was found that at coverages less than one hydrogen per surface Be (< 1H/Be), the interlayer relaxation pattern changes significantly, but the arrangement of the surface Be atoms remains stable. At local coverage of 1 H/Be, the H no longer adsorbs in the hcp and fcc hollow sites, but adsorbs at the bridge sites tending to form two bonds with surface beryllium. The surface exhibits significant in-plane relaxations when a critical coverage of 1 H/Be is accumulated locally. The energy barrier for dissociative adsorption of H2 increases with H-coverage until it stops completely at 1 H/Be, while atomic hydrogen is still attracted to the hydrogen covered surface. However, atomic hydrogen impinging on a surface preadsorbed with 1 H/Be ultimately results in desorption of a hydrogen molecule.

Further increase of the near-surface H-concentration is possible if subsurface positions are occupied by transmutation induced tritium diffusing from the bulk. Hydrogenation of the surface changes hydrogen diffusion barrier profile towards the surface drastically. Instead of a fast drop in barriers from bulk-like 0.56 eV to just 0.02 eV at the surface in the case of the clean surface, the barriers now practically does not change (0.6-0.62 eV). It was found that hydrogen residing in the first subsurface layer tends to close the half rings (Be-H-Be) previously formed at the external surface side. Thus formation of a BeH2-like compound at the surface was revealed in our energy minimization runs. The barriers for subsurface hydrogen to reach the outer Be-H layer and to build up the correct H/Be ratio of two were found to be between
0.14 eV and 0.35 eV.

These findings reveal that atomistic kinetic Monte Carlo technique based on the simple concept of ridged lattice should be extended to simulate hydrogen interaction with beryllium surface.

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P8. A new EAM interatomic potential for tungsten-hydrogen system

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The choices of interatomic potential used in W-H system are very limited. Only three interatomic potentials are available for W-H system, which are W-C-H potential by Juslin et al. (P_Juslin)[1], W-H-He potential by Li et al. (P_Li)[2], and W-H-He potential by Bonny et al. (P_Bonny)[3]. Both P_Juslin and P_Li are bond order potentials, which are not efficient enough to simulating large W-H system. P_Bonny is an embedded-atom method (EAM) potential, but it seems not accurate enough to simulating some properties of W-H system. We have developed an efficient and more accurate EAM potential for a binary W-H system, which reproduce better properties of W-H system.

In the new EAM potential, an existing EAM potential [4] is adopted with parameters unchanged for W-W interaction. For W-H and H-H interaction, the analytical form of the potential is the same as the model successfully applied in Ni-H system [5], and the fitting parameters are adjusted to give desired properties of the W-H system, based on the database of first-principles calculations. The new W-H potential has been thoroughly assessed, compared with other interatomic potentials of W-H system. It predicts correctly the formation energy of H atoms in tetrahedral and octahedral interstitial sites, substituted sites, and the migration energy of H atom in bcc W. The interaction between H atoms in bcc W is also reproduced based on the new potential, which has a great consistence with the results from first-principles calculations. As for interaction between H atoms and self-interstitial atoms in W, the new potential gives consistent binding energies with first-principles calculations and reasonable configurations of H atoms and self-interstitial atoms. On the simulation of properties of H-vacancy clusters in bcc W, the new potential gives the right binding energy of H atom to H-vacancy clusters, and predict the same configuration of H atoms in vacancies as the first-principles do. The potential could also reproduce the formation of H molecule in vacuum, which enables the simulation of H molecule around the W surface. In conclusion, the new W-H potential has a great performance on simulating the W-H system, and has an efficient computational ability.

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P9. Tritium behaviour in beryllium investigated by DFT in the ITER context

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Beryllium is one of the plasma-facing materials foreseen for ITER. It will have to sustain high fluxes of hydrogen isotopes, as a consequence of what a significant amounts of tritium could be retained in the wall. This amounts being dependent on temperature, the temperature dependency of the trapping and release processes is an important issue that needs to be understood, such as to limit tritium inventory below 700g in nominal operation. From the safety point of view, it is also of primarily importance to predict the amount of tritium released in case of accidental loss of confinement.

These are the motivations that led us to calculate by Density Functional Theory some of the elementary atomic processes for hydrogen in beryllium. Indeed, as mentioned by Oberkofler *et al.* [1], although much experimental data have been acquired in the past, the details of these elementary processes remain unclear.

Firstly, we determined the most stable interstitial sites and the most favorable diffusion pathway. The migration barrier we found is in excellent agreement with the one of Ganchenkova *et al.* [2]. Then we calculated the formation energy of a single-vacancy (V), in which up to five atoms could be trap (VH_n, n=0-5). The formation of hydrogen molecules inside the vacancy is not observed for all occupancy number. The many different pathways for H leading to the formation of a VH_n vacancy were also calculated, and the corresponding trapping and detrapping energies were determined. These data were finally incorporated in an MRE code developed at Jülich; a very good qualitative agreement was found between both the simulated and experimental TDS spectra.

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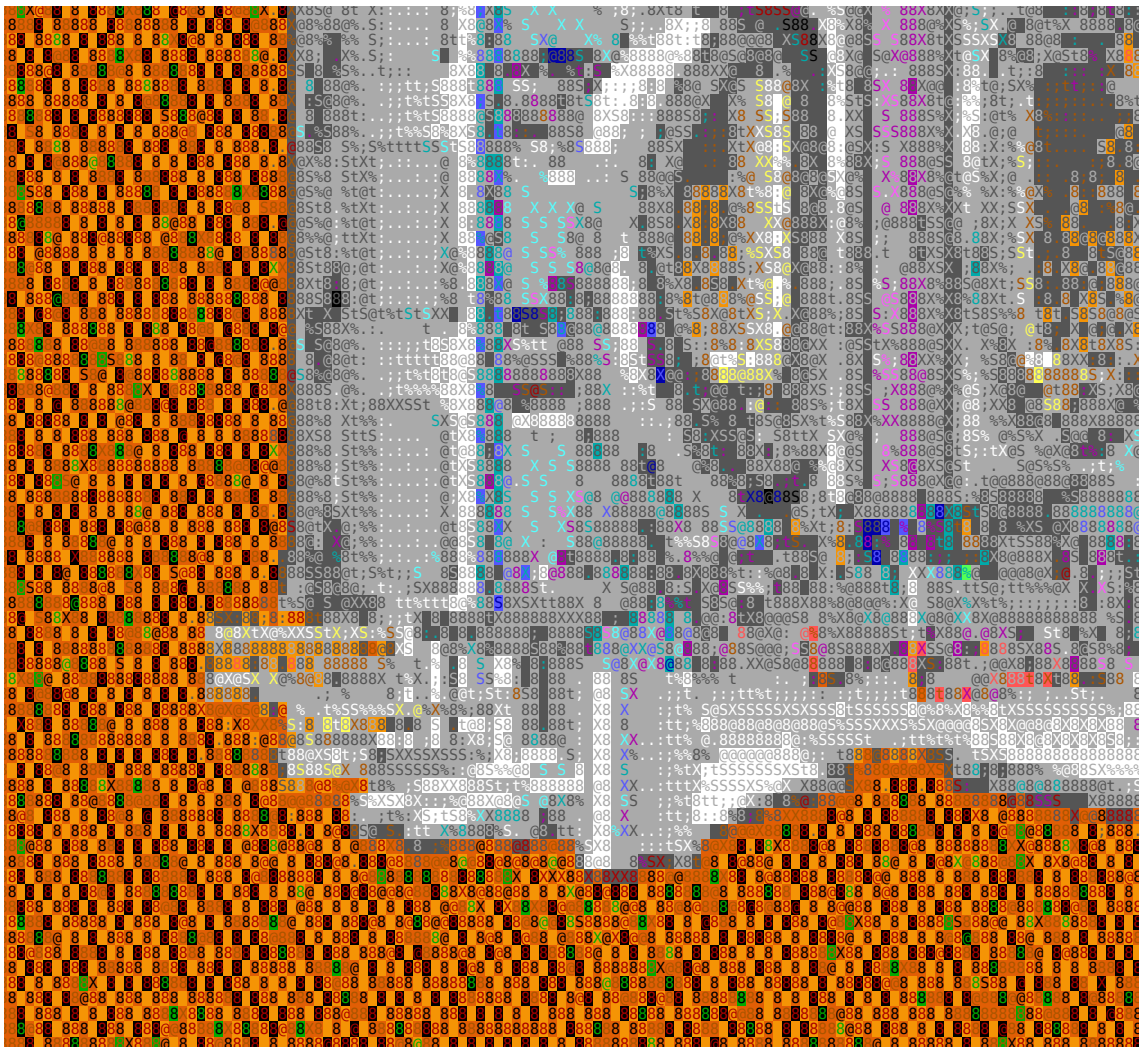

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