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Hydrogen Permeation in Fusion-relevant Materials

Summary Report of the First Research Coordination Meeting

Virtual Meeting

23 – 27 November 2020

Prepared by
K. Heinola
IAEA Nuclear Data Section

January 2022

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Abstract

The First Research Coordination Meeting of the Coordinated Research Project on *Hydrogen Permeation in Fusion-relevant Materials* was held on 23 – 27 November 2020 as a virtual meeting due to the global SARS-CoV2 pandemic. 22 Chief Scientific Investigators representing 16 Member States presented their Research Proposals and corresponding activities in the field of nuclear fusion fuel permeation through reactor materials and components. Meeting was attended in total by 51 participants, which comprised of project CSIs, meeting observers and IAEA staff. Open issues related to fusion fuel permeation, retention, solubility, trapping and diffusion were discussed and plans for coordinated research activities to be performed during the project were made. Proceedings of the meeting are summarized in this report.

January 2022

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Abbreviations

A+M	atomic and molecular
CRP	coordinated research project
DEMO	demonstration fusion reactor
DFT	electron density functional theory
EBSD	electron backscatter diffraction
FPP	fusion power plant
FW	first wall of a fusion device or reactor
GAP	Gaussian approximation potential
GDP	gas-driven permeation
H/D/T	hydrogen/deuterium/tritium
IBA	ion beam analysis
IDP	ion-driven permeation
ITER	international thermonuclear fusion device; next-step fusion device
MD	molecular dynamics
ML	machine learning
NEB; CI-NEB	Nudged Elastic Band method used with DFT; Climbing Image NEB
PDP	plasma-driven permeation
PMI	plasma-material interaction
PSI	plasma-surface interaction
PWI	plasma-wall interaction
RAFM steel	reduced activation ferritic/martensitic steel
RCM	research coordination meeting
RE	rate theory equation
$t_{1/2}$	half-life
TBB	T breeding blanket in DEMO and FPP
TBM	ITER test blanket module for T breeding experiment
TDDFT	time-dependent DFT
TDS	thermal desorption spectrometry
TST	transition state theory; hTST – harmonic TST
XRD	X-ray diffraction

1. Introduction

It is important to know as much as possible about the behaviour of the reactor wall materials and components of a nuclear fusion reactor with respect to permeation of hydrogen isotopes from the plasma. This is to assess the wall materials suitability for containing the deuterium-tritium (D-T) plasma fuel and isolating the T fuel particles from the surrounding fusion reactor components. Of particular concern is the trapping and retention of radioactive T inside the wall ($t_{1/2}\sim$ 12.3 years), and the possibility of T diffusing through the material and finding its way into the coolant liquid (typically H_2O) of the reactor components, where it would pose a potentially serious environmental hazard. The T inventory plays a crucial role in fusion systems since the dynamical behaviour of T, such as solubility, diffusion, trapping, de-trapping, re-trapping, permeation, etc, in these so-called *plasma-facing materials* (PFM) determines the in-vessel fuel inventory source term (i.e., T retention) and the ex-vessel fuel release term (i.e. T permeation). These in-vessel and ex-vessel T inventories are critical for assessing the retention and permeation of T in the next-step fusion device ITER due to the radiological hazard and therefore for licensing purposes. Further, this in-vessel and ex-vessel T containment information will be used in the fusion reactor safety assessments for licensing of future fusion facilities, such as the fusion demonstration reactor DEMO and the future fusion power plants (FPP). Minimizing the uncertainty associated with T permeation enhances the reliability of safety assessment and supports licensing of DEMO reactors and FPPs in participating countries.

For investigation and modelling the hydrogen permeation through plasma-facing components, validated hydrogen-material interaction parameters are required. Previous works[1] on these parameters must be revisited and missing data must be addressed in the corresponding interaction categories. Only a full set of qualified parameters allow for fundamental permeation data, which is currently missing for the present plasma-facing components in the first wall (FW) of main chamber and divertor planned for next-step fusion device ITER and for DEMO. These components comprise of various materials, such as tungsten (W), different steels and also beryllium (Be) in the case of ITER, but also of equal importance are elements used as joining materials and cooling pipes. As a crucial example is the divertor design of ITER, which comprises of W mono-blocks having internal copper-chrome-zirconium (CuCrZr) cooling pipe and an interlayer made of Cu between the W material and the CuCrZr pipe. Further, the ITER port plugs in the main chamber FW recessed areas comprise of stainless steel (SS316L). These ports have been assessed to be the main permeation source in ITER. Moreover, port plugs will be used for testing at least four reference T breeding blanket concepts for DEMO reactor specifications. These so-called test blanket modules (TBM) use reduced activation ferritic/martensitic (RAFM) steels, such as EUROFER97, F82H and CLAM as structural material. In DEMO reactor and beyond, T is bred in T breeding blanket (TBB), which surrounds the reactor main chamber and is positioned under the armour materials of the PFCs. Fundamental knowledge of T permeation in TBBs is mandatory for the design of economical and radiologically safe operation of DEMO and FPPs.

Study of hydrogen permeation in the FW plasma-facing materials is further complicated by the elevated temperatures present under normal operation of a reactor and the anticipated damage they will suffer due to irradiation by the flux of energetic 14 MeV neutrons produced in the D-T fusion reactions. Also of relevance is the nature and evolution of the FW material surface, which is altered by interaction with the plasma through erosion and preferential sputtering of certain component atoms. The effect of annealing out of defects during recrystallization of W components under high heat loads may enhance the permeation process at the divertor. The effect of fast ions and charge exchange (CX) neutral atoms escaped from the plasma may have a strong impact to the surface and sub-surface modification of the FW components and their effect to hydrogen permeation needs to be scrutinized. The intense neutron flux from the D-T fusion reactions penetrate the FW surface and interact with the atomic elements of the wall creating neutron-induced large-scale lattice damage and transmuting the wall elements. These

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[1] F. Reiter, K. S. Forcey, G. Gervasini, A Compilation of Tritium-Material Interaction Parameters in Fusion Reactor Materials, Joint Research Centre EUR 15217 EN, Commission of the European Communities, Luxembourg1993

effects transform the wall component properties and will have a significant effect to the hydrogen retention and mobility in the wall.

Although the precise mechanism is not understood, it is well-known that trapped hydrogen reduces the ductility of many materials, including steels, a phenomenon known as hydrogen embrittlement or hydrogen-induced cracking. For safety and operational reasons, it is also important to understand and mitigate the potential damage that could be caused to key components in a fusion reactor, including the above-mentioned large number of diagnostic ports needed in ITER. Purpose of this Coordinated Research Project (CRP) on Hydrogen Permeation is to collect, assess and validate fundamental computational and experimental data that are needed to simulate hydrogen permeation and to extrapolate the results to ITER and DEMO plasma conditions. The present report is the output of a five-day Research Coordination Meeting (RCM) on data requirements for hydrogen permeation in the FW plasma-facing materials and components. Meeting was held fully virtual via Cisco Webex platform due to the global SARS-CoV2 pandemic.

Section 2 summarizes the presentations at the meeting. Section 3 summarizes the discussions and conclusions. Appendix I provides the list of participants and Appendix II the meeting agenda. Appendix III provides speaker summaries of the presentations.

2. Proceedings

The Head of the Nuclear Data Section, A. Koning welcomed participants and emphasized increasing interest and need for atomic and molecular data. Participants introduced themselves and the agenda in Appendix 2 was adopted without change. K. Heinola reviewed meeting objectives.

The meeting proceeded with presentations of 30 minutes each organized in five sessions throughout the week. Each 3-hour day comprised of oral presentations followed by a discussion session. Presentations were given by the corresponding Chief Scientific Investigators of each CRP participating Research Group who presented their Group's recent hydrogen permeation-related activities as well as their research plans for this CRP. In total there were 30 presentations given at this RCM.

Speaker summaries are provided in Appendix III and presentation material are available on the A+M Data Unit web page at https://amdis.iaea.org/meetings/hydrogen-permeation-rcm1/ and on the event's Indico conference web page https://conferences.iaea.org/e/hydrogen-permeation (access key required. For enquiries please contact *fusion-data@iaea.org*).

There were four presentations in the first session chaired by **K. Heinola** on the topic of **Session I: Atomistic Modelling** by **Yves FERRO** (University of Marseille, France) on "*Hydrogen diffusion at surfaces, defects and interfaces*", **Brian WIRTH** (University of Tennessee, USA) on "*Modeling and experimental investigation of hydrogen permeation in fusion materials*", **Musharaf ALI** (Bhabha Atomic Research Centre, India) on "*DFT studies on diffusion and permeation of hydrogen isotopes in iron (Fe) and tungsten (W)*" and by **Byeongchan LEE** (Kyung Hee University, Korea) on "*Interatomic potential development for H permeation in critical components*".

The second day proceeded with **Session II: Gas-driven Permeation** chaired by **A. Houben**. Presentations were given by **Floriane LEBLOND** (CEA, France) on "*Permeation and trapping in EUROFER97: a wide-angle approach*", **Anne HOUBEN** (Forschungszentrum Jülich, Germany) on "*Hydrogen permeation studies on fusion materials and the influence of interfaces on the permeation: Gas-driven permeation measurements on bulk and layered substrates and hydrogen retention studies*", **Pablo BRUZZONI** (National Atomic Energy Commission, Argentina) on "*Study of hydrogen isotopes permeation and diffusion in F82H ferritic-martensitic steel for fusion applications*" and by **Anne GOLUBEVA** (Kurchatov Institute, Russia) on "*Gas-driven permeation of D through bronzes and other structural materials for fusion*". The second session of the day was **Session III: Plasma-driven permeation** and chaired by **H. Zhou**. Talks were given by **Anže ZALOŽNIK** (UCSD, USA) on "*Experimental validation of H permeability models for Be, W and RAFM steels*", **OYA Yasuhisa** (Shiziuoka

University, Japan) on “*Plasma-driven permeation of hydrogen isotope for W*”, **Li QIAO** (Lanzhou Institute of Chemical Physics, China) on “*Influence of the permeation barrier oxide layers on hydrogen permeation of W and RAFM steel*” and by **Haishan ZHOU** (ASIPP, China) on “*Plasma-driven permeation of hydrogen through materials and components*”. **Session IV: Ion-driven Permeation** was chaired by **K. Heinola** and had a presentation by **Wolfgang JACOB** (IPP Garching, Germany) on “*Ion-driven permeation experiments and modelling*”.

Third day of the meeting continued with **Session V: Hydrogen Isotope Retention** chaired by **S. Markelj**. Session had talks by **Sabina MARKELJ** (Jožef Stefan Institute, Slovenia) on “*Experiments and modelling of in-situ uptake, transport and release studies of hydrogen isotopes in irradiated tungsten*”, **Sergei DANILCHENKO** (Institute of Applied Physics, Ukraine) on “*Development of the X-ray diffraction and thermal desorption spectroscopy techniques for investigation of proton (deuterium/helium) induced near-surface effects in fusion-relevant materials*”, **Long CHENG** (Beihang University, China) on “*Deuterium retention in tungsten under fluences up to 10^{29} m^{-2}*” and by **Daniel PRIMETZHOFER** (Uppsala University, Sweden) on “*Analysis of materials exposed to hydrogen isotopes (H, D, T) in permeation experiments: surface pre-characterisation and post-exposure depth profiling of steel, tungsten and Cu-Cr-Zr*”.

The meeting’s fourth day comprised of the final scientific session **Session VI: Neutron-irradiated Materials** and was chaired by **D. Terentyev**. Presentations were given by **Dmitry TERENTYEV** (SCK-CEN, Belgium) on “*Recent irradiation experiments involving baseline and advanced tungsten materials performed at SCK-CEN*”, **Masashi SHIMADA** (INL, USA) on ”*Plasma- and gas-driven tritium permeation in fusion materials*”, **Olga OGORODNIKOVA** (MEPhI, Russia) on “*Deuterium and helium retention and corresponding modifications of W-based materials under transients*”, **Tommy AHLGREN** (University of Helsinki, Finland) on “*Hydrogen diffusion, retention and irradiation-induced damage in fusion-relevant materials*” and by **Mikhail Yu. LAVRENTIEV** (UKAEA, United Kingdom) on “*Combined experimental and theoretical studies of the retention and permeation of hydrogen isotopes in fusion-relevant materials*”.

The fifth and final day comprised of last technical discussion session and of summaries for sessions **I** – **VI** given by their corresponding chairpersons.

3. Technical discussion

3.1 Atomistic modelling and experiments

Session I: Atomistic Modelling comprised of presentations on computational studies utilizing electron Density Functional Theories (DFT) and classical Molecular Dynamics (MD). Topics covered varied from i) W and Fe surfaces, ii) hydrogen penetration through W and Fe surfaces, iii) effect of W surface oxidation to hydrogen and hydrogen penetration, iv) hydrogen diffusion in the bulk lattice of W and Fe, v) effect of defects to hydrogen lattice diffusion as assessed by the harmonic Transition State Theory (hTST) as well as vi) MD interatomic potential development and exploitation in permeability studies in fusion materials with and without defects.

Discussions continued on the input requirements of research groups performing multi-scale simulations.

- Calculations based on quantum mechanical DFT can be done generally on systems comprising of thousands of atoms. Results are accurate but limited with system sizes studied. Upscaling of computational results from DFT requires potential landscapes describing the various atomistic environments of the material. Landscapes for perfect lattices including point defects or 1-2 single defects located close to each other can be obtained with DFT fairly straightforward. However, large-scale defects such as large clusters of defects, voids and grain boundaries in their full scale are currently out of reach or very challenging for DFT calculations. Other parameters related to particle or defect transition pathways, such as potential energy barriers needed for trapping or dissociation, can be only obtained with Nudged Elastic Band (NEB) method or with Climbing Image NEB (CI-NEB) method.

- Classical MD is an efficient tool for simulating features and properties of atomistic systems including several millions of atoms making it an attractive method for studying material defect properties at length and time scales currently unreachable with DFT. The reliability of the interatomic potential used for MD simulations plays a crucial role in validating predictions done with MD. Moreover, different MD interatomic potentials have been developed using different known materials properties as input hence projections describing features outside this input data need to be validated. As a proposal, sets of recommended interatomic potentials known to be reliable for certain features would be desirable, but regretfully, that recommendation activity lies outside the scope and available resources of this CRP. However, this CRP has a research proposal which includes development of a machine learned (ML) MD potential for W using the Gaussian Approximation Potential (GAP; ML-GAP) formalism, which potentially can overcome the problems with conventional interatomic MD potentials.

In the discussions it was highlighted the importance of surface in assessing hydrogen permeation and the related dynamics. DFT can provide energy landscape data from mono-vacancy systems up to surfaces, however, the large-scale defect properties need to go through interpolation. Activation barriers from surface to bulk can be calculated reliably with DFT, e. g. for hydrogen penetration from an oxygenated W surface to the bulk. In this connection it was noted that it would be very helpful to have any kind of experimental data or observations of oxygen monolayers on W in order to validate the predictions done with DFT. This request was further discussed among the meeting participants. In general, one of the outcomes of this CRP is to collect a database of experimental diffusivity, surface properties (incl. oxidation) data and to recommend a validated data or fit. Importance of understanding the effect of surface oxidation to hydrogen permeation was considered as high importance. In addition, real systems will always have fractions of carbon present which should be included to the list of studied elements affecting hydrogen dynamics on fusion materials surfaces. In this context both DFT and MD computations are complementary: with DFT one has calculated local effects and energies whereas MD simulations are suitable for examinations of effects and dynamics on larger scales, but both methodologies require experimental validation. A proposal was raised for the DFT groups to prepare a review of computational results, which would highlight data already available and more importantly the focus areas where experimental data is needed. Due to current lack of resources, this proposal was left for discussion in the future meetings.

Irradiation-induced damage due to neutrons and high energy fusion plasma ions will have an effect to hydrogen retention, diffusion and permeation. The damage predictions can be done computationally with MD simulations (e. g. LAMMPS, MDRANGE) or with codes based on binary-collision approximation (BCA), such as SDTrimSP, Marlowe, or the widely used SRIM code. In-depth discussion on the validity of the current version of SRIM took place and the code's reliability in predicting primary knock-on energies, angular distribution of damage and quantity of predicted damage was assessed. This topic was agreed to be discussed more in detail in a special session at Technical Meeting on Hydrogen Permeation planned to take place from 4 – 6 October 2021.

Many research groups performing multi-scale computations of hydrogen retention and permeation utilize the concept of Rate Theory Equations (RE). REs are deployed in a variety of existing codes, such as TMAP7, FESTIM, TESSIM-X, MHIMS, advanced RE (aRE) and CRDS. Discussions took place about a potential RE code comparison activity. It was noted, that EUROfusion has had already such comparison activity, but those results should be checked and codes participating that activity could be invited to participate to an extended comparison activity. In addition to the previously studied evolution of hydrogen concentration in the bulk this new activity should include dynamics of hydrogen at surfaces and at materials interfaces. However, it remained open who would lead this extended RE code comparison activity, but IAEA will check for available resources.

New IAEA-hosted databases were presented at the discussion session

- DefectDB (https://db-amdis.org/defectdb), a database for atomic structures and energy landscapes for bulk systems with and without impurities, surfaces and small-scale defects as calculated with DFT

- CascadesDB (https://cascadesdb.org/), database for MD simulations of neutron-induced collisional cascades in nuclear materials (fusion and fission)

3.2 Gas-driven permeation

Discussion on **Session II: Gas-driven Permeation** summarized talks on gas-driven permeation (GDP) research of hydrogen permeation and trapping in EUROFER97; GDP and retention measurements on bulk and layered structures of steels and W; effect of interlayers on permeation in F82H and W, and GDP permeation in bronzes (CuCrZr) and structural materials for fusion.

Materials under study with GDP are steels (RAFM, SS316L), W, CuCrZr and samples with different coatings. GDP is mainly performed using D_2 gas, but one group in this CRP is able to utilize T_2 as well. Presented experimental studies comprise of combination of GDP and TDS included with relevant modelling utilizing RE codes, such as TMAP. Specific research areas are

i) low temperature effects to diffusion and permeation
ii) effect of various surface properties to permeation, effect of polished, oxidized and damaged surface
iii) effect of interfaces existing in the material or created by layered structures
iv) effect of materials intrinsic microstructure and its temperature-dependent evolution.

Discussions raised the important question of using and preparing standards for permeation studies with GDP. As a primary example was presented the use of Ni-based foils as a permeation standard. However, the availability and production of standard Ni-foils was addressed as a concern. It was concluded, that having a joint GDP standard sample would be an ideal situation, but preparing such sheets meeting the criteria of each GDP laboratory's needs would probably not be realistic due to the variations in required standard sample thicknesses, size, microstructure in different directions, etc. As an alternative approach, it was concluded to recommend each GDP laboratory to take care of the preparation of a Ni-foil standard according to their needs and to report their progress on this issue at the follow-up meetings.

A cross-comparison activity of different GDP devices using the same or similar samples was proposed. Purpose of this round-robin activity is to coordinate GDP facilities to study a system as identical as possible allowing detailed comparisons of the participating facilities. For this, organizing material distribution by one source or sample provider is the key for valid comparisons. To secure the material identicality, pre-characterization of the materials must take place. This pre-characterization comprises of analyzing sample thickness, surface features (oxidation, etc), microstructure and so on. In summary, procedure for this GDP facility cross-comparison activity is to use one material from one source and batch, use same characterization for each sample and finally perform GDP measurements with identical parameters (gas loading, temperature, etc). The activity coordinator would be Forschungszentrum Jülich (Germany) and the material studied was chosen to be EUROFER97 provided by IPP Garching (Germany). It was agreed the Forschungszentrum Jülich would prepare a Pd-coating to the samples and the sample sizes were agreed between each participating GDP facility. Participating institutes so far are Forschungszentrum Jülich, CEA (France), National Atomic Energy Commission (Argentina) and Kurchatov Institute (Russia) and the call is open for participation. It was also proposed to arrange a combination of sputtering and GDP experiments. As a reference is the IAEA's ongoing round-robin activity on steel surfaces sputtering in connection of Steel Surfaces CRP (F43022). Idea was found interesting and useful and the decision to carry out a combination activity with sputtering and GDP was left for future discussions. Finally, outcome of any GDP research was recommended to be compared with any available similar Ion-driven and Plasma-driven permeation experiments.

A proposal for a database of the GDP sample microstructures was presented. This database would be in addition to GDP data made available through this CRP. It was concluded that any sample information could be included in the IAEA's recent database for fusion energy research HCDB (https://db-amdis.org/hcdb) and be connected with the corresponding GDP results.

3.3 Plasma-driven permeation

Session III: Plasma-driven Permeation discussions summarized talks on validation of hydrogen permeability models for Be, W and RAFM steel using plasma-driven permeation (PDP), PDP of hydrogen in W, effect of oxide layers as permeation barrier in W and in RAFM, PDP experiments using fusion reactor components and PDP experiments performed using T_2 gas with a linear machine.

Discussion on PDP highlighted various features needed to take into account as follows

i) characterization of plasma: determining the plasma elemental composition may be challenging but needs to be approximated in detail due to the plasma impurities affecting the conclusions of the plasma exposure. Impurities may originate e. g. as a result of sputtering events from the plasma-chamber wall interactions,

ii) sample surface damage: excess damage of the target surface may take place due to heavy elements from the plasma, such as helium and wall impurities, or due to high energy plasma ions or neutrals,

iii) Soret effect: temperature gradient in fusion components may induce a large Soret effect, but is not necessarily an issue when performing PDP research with typical laboratory samples,

iv) multi-layer diffusion: fusion components have a layered structure, such as the divertor W monoblock and hydrogen transport at interfaces is still unknown,

v) steady-state permeation model: experimental permeation results obtained with PDP are challenging to simulate with current models for surface recombination. Therefore, surface conditions used in the models are needed to be modified in order to reach an agreement with experiments. To illustrate, the experimental surface recombination coefficients for W are largely scattered and therefore challenging or even impossible to interpret. Problem arises when choosing the appropriate surface model parameters for the simulations. Restricting the recombination parameter space by modelling using e. g. DFT and MD and comparing with experiments might narrow down the recombination coefficient space,

vi) surface contamination: target surface contamination may take place due to the PWI effects in the plasma device. In-situ surface measurements were proposed for assessing the effectiveness of surface contamination, but these measurements are extremely challenging during plasma exposure. Surface contamination may not play a role when using energetic plasmas, where impinging plasma particles clean the target surface off contamination and the eroded particles could be measured. However, the effect of surface oxygen is still an unknown and important issue.

vii) modelling of the plasma exposure experiments: PDP modelling is crucially important in order to understand all the underlying effects affecting hydrogen permeation. Modelling of the surface is challenging but processes taking place in the bulk, such as lattice trapping and detrapping, are somewhat manageable with the current models. An important feature for modelling is the post-exposure characterization of the sample surface.

PDP can be easily performed on large target surface areas. Further, large fluxes of impinging ion energies and temperature can be easily varied but interpretation of the results requires understanding of details in the experiment, such as plasma composition (see list above).

3.4 Ion-driven permeation

Discussion **Session IV: Ion-driven Permeation** focused on the usefulness of ion-driven permeation (IDP). The method has a simple, controllable source term for selecting the impinging ion type, energy, flux and the sample temperature. This makes IDP experiments fairly easy to model with simulation tools, such as SDTrimSP. However, when compared to PDP a downside with IDP is the low interaction area and low ion fluxes. By varying ion energy in IDP one can vary the resulted implanted concentration gradient, which affects the permeation simply by resulting to implanting at different depths: with higher ion implantation energies, one gains deeper implantation depths. The effect of local modification of subsurface lattice regions to create hydrogen supersaturated layers is not well addressed with IDP. In high flux plasma experiments blistering and other effects at lower temperatures are observed, where the local concentration maximum at the end of ion range plays a crucial effect. RE simulation tools, such as TESSIM, are very important for interpreting experimental IDP data. Assessing the amount of neutral particles in the ion current and flux is important for determining concentration-dependent effects. As an example, modelling recent IDP experiments using TESSIM code, one needs to take into account the ions and a small fraction of neutral particles with high energy. If these neutrals are excluded, modelling shows lower permeation and diffusion takes place more slowly when compared to experimental observations.

3.5 Hydrogen isotope retention

Session V: Hydrogen isotope retention discussions summarized presentations on experiments and modelling of hydrogen in-situ uptake, transport and retention in self-irradiated W; exploitation of X-ray diffraction (XRD) and TDS in the studies of hydrogen induced near-surface effects in fusion materials, such as crystallographic microstructure and lattice constant; deuterium retention in W at high fluences up to 10^{29} m^{-2} and utilization of IBA on fusion materials exposed to hydrogen for permeation experiments.

As discussed previously, a standard recombination coefficient cannot be used in modelling of many materials. Due to the dynamical change of surface hydrogen coverage and the corresponding surface energetics, rate equations describing absorption and desorption processes need to be included in modelling. High flux plasma experiments show fluence dependence for hydrogen retention: high implantation fluxes induce huge strains in the lattice, which promote defect creation near surface and increase retention by acting as trapping sites for plasma particles. Also, the increasing effect of blister formation and the decreasing effect of He contamination to hydrogen retention has been demonstrated with high flux experiments. For the material characterization a collaboration activity was proposed by the CRP participants performing IBA.

Retention data has been created for decades on D for W and Be but to less extent for steels and CuCrZr. Progress for well-defined experiments is only to be expected in close collaboration with theoretical understanding and the corresponding modelling. There is a need for hydrogen depth profile characterization and determination of the desorption kinetics in order to get a solid interpretation of the processes involved in retention and release dynamics. To illustrate, for the TDS interpretation one needs to understand the retention depth profile i.e. where in the lattice hydrogen is located at a given time and temperature.

Experimental sample exposure parameters are critical for the interpretation of hydrogen retention results related to

- i) effect of surface contamination
- ii) blister formation
- iii) effect of intrinsic defects in undamaged W
- iv) defect creation due to build-up of lattice stress in supersaturated sub-surface layers.

3.6 Neutron-irradiated materials

Discussions on **Session VI: Neutron-irradiated materials** summarized the planned round-robin activity using neutron-irradiated fusion materials for hydrogen permeation studies. Main purpose is to execute retention and permeation studies using set of already irradiated samples. Further, an additional irradiation campaign was discussed to be organized, where samples are irradiated with neutrons at predetermined equivalent conditions. Also, the selected materials for irradiations must be well pre-characterized e.g. with IBA methods and positron annihilation spectroscopy.

i) Types of materials to be used in the irradiation campaign are W, EUROFER97 or SS316L and CuCrZr.
ii) Irradiation doses can be varied from 0.025 – 0.5 dpa per irradiation campaign.
iii) The irradiation temperatures can be varied from 50 degC up to 1200 degC (3 – 4 temperatures can be chosen).
iv) Sample geometries need to be agreed in order to prepare the corresponding irradiation capsules.

Call is open for participants joined this CRP and the first plans for irradiation and sample requirements are planned to be discussed before end of the year 2020. In an ideal case, the irradiation campaign would be launched and finished within 2021. This is followed by cooling down of the samples allowing them to be transported to participating laboratories in middle of 2022. Post-irradiation analysis can be done prior shipment of samples and comprise of hardness tests and electron backscatter diffraction (EBSD) in order to ensure that irradiation conditions correspond to the expected ones.

Appendix I: List of Participants

Tommy AHLGREN, University of Helsinki, Finland

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IAEA

Arjan KONING, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, AUSTRIA.

Kalle HEINOLA, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, AUSTRIA.

Christian HILL, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, AUSTRIA.

Sehila GONZALEZ-VICENTE, IAEA Physics Section, Division of Physical and Chemical Sciences, AUSTRIA.

Matteo BARBARINO, IAEA Physics Section, Division of Physical and Chemical Sciences, AUSTRIA.

Appendix II: Meeting Agenda

Monday 23 November 2020

Welcome (14:00-14:20)

-Conveners: Hill, Christian (IAEA); Heinola, Kalle (IAEA); Koning, Arjan (IAEA)

time	title	presenter
14:00	Opening	KONING, Arjan (IAEA) HEINOLA, Kalle (IAEA) HILL, Christian (IAEA)
14:10	Activities of the IAEA Atomic and Molecular Data Unit in support of nuclear fusion research on hydrogen permeation	HEINOLA, Kalle (IAEA)

Atomistic modelling I (14:20-15:00)

Atomistic modelling and experiments

-Conveners: Kalle Heinola

time	title	presenter
14:20	Hydrogen diffusion at surfaces, defects and interfaces	FERRO, Yves (Aix-Marseille University)
14:40	Modeling and Experimental Investigation of Hydrogen Permeation in Fusion Materials	WIRTH, Brian (University of Tennessee)

virtual coffee break (15:00-15:20)

Atomistic modelling II (15:20-16:00)

Atomistic modelling and experiments

-Conveners: Kalle Heinola

time	title	presenter
15:20	DFT Studies on Diffusion and Permeation of Hydrogen Isotopes in Iron (Fe) and Tungsten (W)	ALI, Musharaf (Bhabha Atomic Research Centre)
15:40	Interatomic potential development for H permeation in critical components	LEE, Byeongchan (Kyung Hee University)

Gas-driven permeation I (16:00-16:20)

GDP and corresponding modelling activities

-Conveners: Anne Houben

time	title	presenter
16:00	Permeation and trapping in Eurofer97: a wide-angle approach	LEBLOND, Floriane (CEA)

Discussion (16:20-17:00)

Tuesday 24 November 2020

Gas-driven permeation II (14:00-15:00)

GDP and corresponding modelling activities

-Conveners: Anne Houben

time	title	presenter
14:00	Hydrogen permeation studies on fusion materials and the influence of interfaces on the permeation: Gas-driven permeation measurements on bulk and layered substrates and hydrogen retention studies	HOUBEN, Anne (Forschungszentrum Juelich GmbH)
14:20	Diffusion and permeation of hydrogen isotopes in tungsten and F82H steel near room temperature.	BRUZZONI, Pablo (CNEA)
14:40	GDP permeation of bronzes and other structural materials for fusion	GOLUBEVA, Anna (NRC "Kurchatov institute")

virtual coffee break & group photo (15:00-15:20)

Plasma-driven perm. I (15:20-16:20)

PDP and corresponding modelling activities

-Conveners: Haishan Zhou

time	title	presenter
15:20	Experimental validation of H permeability models for Be, W and RAFM steels	ZALOZNIK, Anze (THE PISCES TEAM, UCSD)
15:40	Plasma driven permeation of hydrogen isotope for W	OYA, Yasuhisa (Shizuoka University)
16:00	Influence of the permeation barrier oxide layers on hydrogen permeation of W and RAFM steel	QIAO, Li

Discussion (16:20-17:00)

Wednesday 25 November 2020

Plasma-driven perm. II (14:00-14:20)

PDP and corresponding modelling activities

-Conveners: Haishan Zhou

time	title	presenter
14:00	Plasma-Driven Permeation of Hydrogen through Materials and Components	ZHOU, Haishan (Institute of Plasma Physics, Chinese Academy of Sciences)

Ion-driven permeation (14:20-14:40)

IDP and corresponding modelling activities

-Conveners: Wolfgang Jacob

time	title	presenter
14:20	Ion-driven Permeation Experiments and Modelling	JACOB, Wolfgang (IPP Garching)

Retention I (14:40-15:00)

Retention in plasma & ion beam experiments and corresponding modelling

-Conveners: Kalle Heinola

time	title	presenter
14:40	Experiments and modelling of in-situ uptake, transport and release studies of hydrogen isotopes in irradiated tungsten	MARKELJ, Sabina (Jozef Stefan Institute)

virtual coffee break (15:00-15:20)

Retention II (15:20-16:20)

Retention in plasma & ion beam experiments and corresponding modelling

-Conveners: Sabina Markelj

time	title	presenter
15:20	Development of the X-Ray Diffraction and Thermal Desorption Spectroscopy Techniques for Investigation of Proton (Deuterium/Helium) Induced Near-Surface Effects in Fusion Relevant Materials	DANILCHENKO, Sergii (Institute of Applied Physics National Academy of Sciences of Ukraine)
15:40	Deuterium retention in tungsten under fluences up to 10^29 m-2	CHENG, Long (Beihang University)

16:00	Analysis of materials exposed to hydrogen isotopes (H,D,T) in permeation experiments: surface pre-characterization and post-exposure depth profiling of steel, tungsten, and Cu-Cr-Zr.	PRIMETZHOFER, Daniel (Uppsala University)

Discussion (16:20-17:00)

Thursday 26 November 2020

Neutron-irradiated materials I (14:00-15:00)

-Conveners: Dmitry Terentyev

time	title	presenter
14:00	Recent irradiation experiments involving baseline and advanced tungsten materials performed at SCK CEN	TERENTYEV, Dmitry (SCK CEN)
14:20	Plasma- and gas-driven tritium permeation in fusion materials	SHIMADA, Masashi (Idaho National Laboratory, USA)
14:40	Deuterium and helium retention and corresponding modifications of W-based materials under transients	OGORODNIKOVA, Olga (National Research Nuclear University "MEPHI" (Moscow Engineering Physics Institute))

Discussion (15:00-15:30)

virtual coffee break (15:30-15:50)

Neutron-irradiated materials II (15:50-16:30)

-Conveners: Dmitry Terentyev

time	title	presenter
15:50	Hydrogen diffusion, retention and irradiation-induced damage in fusion-relevant materials	AHLGREN, Tommy (University of Helsinki)
16:10	Combined experimental and theoretical studies of the retention and permeation of hydrogen isotopes in fusion-relevant materials	LAVRENTIEV, Mikhail (UK Atomic Energy Authority)

Discussion (16:30-17:00)

Friday 27 November 2020

Discussion (14:00-15:00)

-Conveners: Kalle Heinola; Dmitry Terentyev; Sabina Markelj; Haishan Zhou; Wolfgang Jacob; Anne Houben

virtual coffee break (15:00-15:20)

Discussion (15:20-16:00)

-Conveners: Kalle Heinola; Sabina Markelj; Dmitry Terentyev; Anne Houben; Haishan Zhou; Wolfgang Jacob

Appendix III: Summaries of Presentations

Activities of the IAEA Atomic and Molecular Data Unit in support of nuclear fusion research on hydrogen permeation

Author: Kalle Heinola[1]

[1] IAEA, Austria

This presentation briefly summarises the history of the IAEA's Atomic and Molecular Data (AMD) Unit, its activities and place in the organisation. The nature and purpose of IAEA Coordinated Research Projects (CRPs) is described and the procedure for initiating one outlined. Typical activities related to the CRP on Hydrogen Permeation, such as requirement for experimental materials pre-characterisation, benchmarking activities, and experimental and computational cross-comparison activities are discussed. Currently active and recently completed CRPs as well as previous CRPs related to Hydrogen Permeation are briefly described.

Atomistic modelling I

Hydrogen diffusion at surfaces, defects and interfaces

Author: Yves FERRO[1]

[1] Aix-Marseille University, France

The presentation will summarize the work we recently achieved and is currently going on regarding the surface of tungsten. The title of the presentation reflects our full project to the CRP. However, this meeting presentation will only focus on the role of oxygen on tungsten and how it modifies the interaction of hydrogen.

We will start by presenting the work we carried out on the adsorption of hydrogen on both the W(110) and W(100) surfaces without oxygen. This way, we will present the methodology we follow; it is made of Density Functional Theory (DFT) calculations, thermodynamics and kinetics, with which we attempt to produce macroscopic data that can be compared with experimental results. In particular, we recently developed a model that determines the surface coverage in hydrogen of both the W(110) and W(100) surfaces depending on the pressure and the temperature. Thanks to the Low Energy Ions Scattering (LEIS) and Direct Recoil Spectroscopy (DRS) measurements from Rob Kolasinski at SANDIA National Lab, Livermore, we are now able to confront the predictions from the model to experimental measurements. The agreement will be presented and discussed. Then we adsorbed oxygen on the bare W(110) surface. Despite many configurations were investigated, only the three-fold (TF) adsorption site was shown to be relevant for the rest of the study.

The adsorption pattern we calculated at various coverages are in good agreement with experimental observations. The adsorption energy is nearly constant at -4.5eV per O atom up to saturation of the surface, which is obtained for 1 Mono-Layer (ML) of oxygen. Beyond saturation, oxygen still absorbs below the surface up to the formation of a WO2 layer that is very weekly bonded to the surface.

When hydrogen is added to the tungsten surface with oxygen, it is shown that oxygen blocks the TF sites and prevents the adsorption of hydrogen. Again, saturation is achieved for 1 ML of adsorbent, but regardless of the concentration of oxygen and hydrogen. It is also shown that the adsorption energy of hydrogen on the surface decreases with increasing coverage in oxygen. In the end, a brief summary of the work we intend to do in the one or two coming years will be provided.

Modeling and Experimental Investigation of Hydrogen Permeation in Fusion Materials

Author: Brian Wirth[1]

Co-authors: Ze Chen[1]; Wendy Garcia[1]; Xunxiang Hu[2]; Gui-yang Huang; Ane Lasa[1]; Li Yang[1]

[1] University of Tennessee, USA
[2] Oak Ridge National Laboratory, USA

The recycling of hydrogen isotopes in the plasma (fuel) is self-regulated through processes involving near-surface diffusion, trapping, and gas bubble formation, coupled to the ionization that results from interactions with the plasma. The multitude of time and length scales controlling material evolution and device performance requires the development not only of detailed physics models and computational strategies at each of these scales, but also experimental validation. Similarly, the permeation of tritium through first wall structural materials and the components within the breeding blanket is critically important for assessing the tritium breeding ratio and sustainability of the fusion fuel cycle, and involve a hierarchical, multiscale set of phenomena.

This project seeks to integrate computational simulations of materials evolution under fusion relevant exposure conditions with microstructural characterization and focused mechanism-based experiments to provide improved understanding of fusion materials behavior. This program addresses several critical questions associated with PFC and first wall/blanket materials performance in materials systems ranging from model alloys to tungsten-based PFC/divertor materials, in addition to iron-based first wall and blanket structural materials and a fundamental investigation of radiation effects in model alloys, and the impact on hydrogen permeation and trapping inventory.

The first year will focus on expanding our experimental measurements of deuterium permeation through tungsten and ferritic-martensitic alloys as a function of initial microstructure, to include different grain sizes, radiation damage and helium bubble distributions. These experimental studies will also involve different microstructure characterization techniques, and be complemented by multiscale modeling studies, ranging from ab initio density functional theory assessments of hydrogen diffusion and interaction with microstructural features, large-scale molecular dynamics simulations of hydrogen permeation and continuum level reaction-diffusion cluster dynamics modeling of the permeation and thermal desorption experiments.

DFT Studies on Diffusion and Permeation of Hydrogen Isotopes in Iron (Fe) and Tungsten (W)

Author: Musharaf Ali[1]

Co-authors: Anil Boda [1]; KT Shenoy [1]

[1] Bhabha Atomic Research Centre, India

The fundamental understanding of H isotopes behaviour in metallic systems vis-a-vis its adsorption, absorption, diffusion and permeation is of great technological importance. This will help in controlling the hydrogen induced embrittlement and also very helpful in the selection of structural materials for reactors with minimum permeability of these gases. Steels with 9–12 wt% Cr are considered as potential structural materials in nuclear power and fusion reactors having hydrogen diffusion coefficients one order of magnitude lower than those of pure Fe. Further, Tungsten (W) has shown promise to be the most favored plasma withstanding material in nuclear fusion with deuterium (D) and tritium (T) as fuel. In order to identify a better material, atomistic understanding of the behavior of D/T with W is highly desirable. In view of that, plane wave based density functional theoretical calculations were conducted to investigate the interaction and dynamical behaviours of hydrogen isotopes in pure bcc Fe and W systems. The adsorption and dissociation pathways for hydrogen isotopes were predicted on both Fe(100) and W(100) surfaces. Further, the activation barrier energy for H atom to diffuse from one interstitial void to nearest interstitial void has been computed using nudge elastic band (NEB) method. Zero point energy was incorporated using phonon calculations to capture the isotope effects. The most favourable diffusion path of H atom was observed from one tetrahedral site to the nearest tetrahedral site in both Fe and W systems. The calculated diffusion coefficients, rate constants, permeability constants and solubility are found to be higher for H compared to its heavier isotopes D and T for W system. The calculated diffusion coefficients and permeability constants are found to be higher for lighter H compared to heavier D and T. In addition, the effect of vacancy is also studied. Further, the diffusion and permeability coefficients of H, D and T are found to be increased with increase in the temperature, which is of first of its kind prediction from DFT studies. Further, the calculated diffusion coefficients are shown to be two order of magnitude lower than Fe and thus might be the basis for considering W as plasma facing materials. The findings will be useful in modeling the behavior of tritium in Fe and W metals for which data is either scattered or least available.

1. A. Boda, Sk. M. Ali, K. T. Shenoy, S. Mohan, Adsorption, Absorption, Diffusion and Permeation of Hydrogen and Its Isotopes in bcc Bulk Fe and Fe(100) Surface: Plane Wave based Density Functional Theoretical Investigations, J. Phys. Chem. C 2019, 123, 23951-23966.
2. A. Boda and Sk. M. Ali, K. T. Shenoy, S. Mohan, Diffusion, Permeation and Solubility of Hydrogen, Deuterium and Tritium in Crystalline Tungsten: First principles DFT Simulations, Int. J. Hydrogen Energy, 2020, 45, 29095-29109.

Future Work Plan (2021-2022)

A. Recombination of H and its isotopes to form diatomic molecules at the surface of the collectorside (Fe and W surface)

- Energy barrier for recombination of H atom using nudge elastic band (NEB) method and DFT
- Kinetics (rate constant) of recombination using TST(transition state theory) and DFT
- Effect of H coverage on the recombination and kinetics using NEB, TST and DFT
- Desorption of molecular hydrogen from the surface using NEB and DFT

B. Dissociation, adsorption, diffusion and permeation of H isotopes through bulk and surface Cr.

- Dissociation pathway of H2 molecule on the Cr surface using DFT
- Absorption H isotopes in surface and bulk Cr using DFT
- Diffusion and permeation of H isotopes through bulk and surface Cr using NEB, TST and DFT

Interatomic potential development for H permeation in critical components

Authors: Byeongchan Lee[1]; Takuji Oda[2]; Keonwook Kang[3]; Duho Kim[1]

[1] Kyung Hee University, Korea
[2] Seoul National University, Korea
[3] Yonsei University, Korea

A broader range of materials that are relevant in fusion power generation is studied. Each fusion-relevant material, whether in plants or operators, requires an extensive study of hydrogen permeation due to either safety or efficiency, which is critical to the success of DEMO plants. Here we propose a 5-year coordinated research project in which many different materials ranging from plasma-facing components to concrete shielding to human tissues are reviewed from the perspective of urgent needs and readiness for molecular dynamics simulation. Critical systems for which no (accurate) potential models are identified in the first two years, and interatomic potentials for large-scale molecular dynamics in these material systems are developed in the subsequent years.

Gas-driven permeation I

Permeation and trapping in Eurofer97: a wide-angle approach

Authors: Floriane Leblond[1]; Christian Grisolia[1]

[1] CEA, France

Assessing the tritium inventory in the walls of fusion reactors is of paramount importance to comply with the promise of a safe energy with low impact of the environment. This evaluation requires a better understanding of tritium permeation in plasma-facing components. The multi-layer design of DEMO PFCs (tungsten, Eurofer and a function graded material in-between) includes several internal interfaces, which behaviour regarding permeation remains unknown. The surface processes on both sides (plasma and cooling loop) also require more investigation.

Properties of the bulk regarding diffusion and trapping are also required to reach a full understanding of tritium permeation in plasma-facing components. To that end, we have undertaken gas-driven permeation experiments. The materials to be studied are tungsten, Eurofer and DEMO-like multi-layer samples. It is also foreseen to study the efficiency of permeation barriers such as alumina. The purpose of the presentation is to introduce the experiment as well as our most recent results on the study and modelling of deuterium permeation in tungsten and Eurofer. In particular for the latter, surface state turns out to be determining in permeation behaviour, as shown by the evolution of permeation flux as a function of upstream pressure.

In parallel, we have performed thermal desorption spectroscopy on deuterium-loaded Eurofer. The peaks on the resulting spectrum reveal that the main trapping site corresponds to a low trapping energy. These results altogether feed our home-made finite element code in order to fully simulate permeation, in the plasma-facing components and up to the coolant.

The ongoing developments to carry out the same measurements using tritium as a driving gas will also be presented.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

Gas-driven permeation II

Hydrogen permeation studies on fusion materials and the influence of interfaces on the permeation: Gas-driven permeation measurements on bulk and layered substrates and hydrogen retention studies

Author: Anne Houben[1]

Co-authors: Dmitry Matveev [1]; Liang Gao [1]; Sören Möller [1]; Bernhard Unterberg [1]; Christian Linsmeier [1]

[1] Forschungszentrum Juelich GmbH, Germany

Fuel retention and permeation in the wall of future fusion devices are among crucial factors for the reactor safety and its economical operation. For the prediction, evaluation and calculation of hydrogen permeation and retention in fusion reactor walls, it is essential to know fundamental parameters of hydrogen transport and retention.

In order to obtain such basic parameter for hydrogen isotopes, gas-driven permeation measurements have to be performed. For hydrogen retention studies, thermal desorption spectroscopy (TDS) measurements have to be carried out on relevant gas loaded materials. With nuclear reaction analysis (NRA) the hydrogen depth distribution can be quantified. In order to investigate the influence of the microstructure and sample conditions, sample characterization is crucial before and after permeation and retention measurements by surface analysis techniques.

Various fusion relevant bare substrate materials, such as steels, tungsten and CuCrZr will be studied. Especially for the prediction of the hydrogen retention and permeation through fusion reactor components, the influence of interfaces on the permeation and retention of magnetron-coated substrates will be investigated. For a deeper understanding of the permeation and retention processes in fusion materials, a reaction-diffusion model will be applied. With these studies combining complementary methods, the prediction, evaluation and calculation of hydrogen permeation and retention in fusion reactor wall materials and components will be enabled.

In this presentation, the work plan and methods of our group related to this CRP will be discussed and first results will be shown.

Diffusion and permeation of hydrogen isotopes in tungsten and F82H steel near room temperature.

Authors: Pablo Bruzzoni[1]; Carolina Hurtado-Noreña[1]

[1]CNEA, Argentina

Experimental data on hydrogen permeation (P) and diffusion coefficient (D) of H isotopes in tungsten and F82H at service temperatures (i.e. 500-1000 K) is already available. The aim of this project is to add data at room temperature. This is important since hydrogen damage is likely to occur at room temperature, i.e. during plant stops. We plan to measure P and D of hydrogen and deuterium in tungsten and F82H by a method of permeation with gas phase charging and electrochemical detection at the temperature range 30-90 °C. For the measurements on F82H steel we will use massive permeation membranes. Either hydrogen or deuterium will be generated in situ by a hydrogen generator fed with light or heavy water, respectively. For the measurements on ungsten we will use thin tungsten coatings deposited on a F82H substrate. This implies the development of a PVD deposition method and the characterization of the tungsten coatings. We will attempt to rationalize the literature data and the data obtained in the present project in the frame of a model that includes quantum effects which are usually observed in H diffusion.

GDP permeation of bronzes and other structural materials for fusion

Author: Anna Golubeva[1]

[1] NRC "Kurchatov institute", Russia

Fusion reactor is a very complicated system. Hydrogen isotopes interaction with fusion materials includes hydrogen diffusion from gas and plasma through plasma facing and structural (SM) materials into coolant and also diffusion from coolant. A lot of opened questions remain around hydrogen isotopes transport trough materials of fusion reactor. The work planned will be focused on permeability of ITER-grade CuCrZr bronzes and on oxides influence on permeability of SMs. Hydrogen diffusion in bronzes is very slow at temperatures below 350 C. In low temperature region measurements are very time demanding, up to several months per one experimental curve. For performing such long experiments a GDP installation is under construction. The installation will allow register permeating flux during months at stable conditions of gaseous D2 interaction with membrane surface at pressures up to 1 atmosphere.

Keywords: structural materials, RAFMS, bronzes, oxidation, neutron damage, hydrogen isotopes, permeation

Plasma-driven permeation I

Experimental validation of H permeability models for Be, W and RAFM steels

Author: Anze Zaloznik[1]

Co-authors: the PISCES Team

[1] UCSD, USA

Accurate models for plasma-driven permeation play an important role in predicting the fuel retention and tritium recovery from plasma-facing components of future fusion devices. Only with an in-depth understanding developed from such models can we plan for safe and successful operational campaigns. In order to develop new models, capable of describing newly observed physical and chemical processes and/or non-equilibrium conditions, as well as validate the existing ones, a large database of experimental results is required.

With a focus on ITER, we have experimentally investigated D retention and release from Be co-deposits and bulk Be samples. Bulk samples were exposed to D plasma and Be/D co-deposits were deposited at different experimental conditions, varying D neutral pressure, sample temperature, and energy of the impinging particles. With the use of a standard rate-equation diffusion/trapping model, we were able to recognize four Arrhenius-type traps and study the influence of implantation/deposition conditions on trap densities and D retention. In addition to the four traps, we observed the appearance of a sharp low-temperature release peak in the TDS spectra, but only under certain experimental conditions. The simple diffusion/trapping model was unable to reproduce such a peak nor the release behavior under ramp-and-hold types of desorption. The model was modified by incorporating the physics of decomposition of beryllium deuteride precipitates, which allowed us to accurately reproduce our experimental results. However, the modified model showed possible uncertainties of the widely used surface recombination coefficient, therefore additional work is needed to verify the new model and determine the validity of the newly determined recombination coefficient.

With a focus on burning plasma operations, our work on W includes studying the non-equilibrium conditions that exist during D plasma implantation into bulk W. Laser-induced breakdown spectroscopy (LIBS) allows us to measure D concentrations in the near-surface region during plasma exposure. It has been shown that a super-saturated layer exists in the near sub-surface region, exhibiting extremely high concentrations of hydrogen isotopes. The standard diffusion/trapping model is not capable of reproducing such non-equilibrium phenomena, therefore, modifications to the model are needed. In addition, calibrated high-resolution SIMS will provide ex-situ measurements of D depth profiles resulting from different plasma exposure conditions, which will be used to validate the modified model. Retention measurements have also been made in RAFM steels, however modelling the release from these materials is complicated and needs some further attention.

This talk will focus on our recent and future attempts to develop better and more accurate models capable of describing and predicting hydrogen isotope interaction with fusion relevant materials. Our plans for future experimental work producing results needed for validation of such upgraded models will be presented and discussed.

Plasma driven permeation of hydrogen isotope for W

Author: Yasuhisa Oya[1]

[1] Shizuoka University, Japan

Tungsten (W) is one of candidate plasma facing materials for future fusion reactors due to its favorable properties such as high melting point, low physical sputtering yield and low solubility for hydrogen (H) isotopes. During the operation of fusion reactor, W will be exposed to high flux deuterium (D), tritium (T) and helium (He) particles in addition to 14 MeV neutron under elevated temperature. The energetic T ions will impinge on W surface and migrate toward the coolant, leading to the loss of T and contamination of coolant. Therefore, it is crucial to evaluate T permeation through W from the view of fusion reactor safety and T self-sufficiency. In the present work, the influence of He or irradiation defects on the plasma driven permeation behaviour in tungsten material are studied.

The D_2/He mixture plasma driven experiment (PDP) is performed to evaluate the He effect on the D plasma driven permeation behaviour. The He emission is detected in the D_2/He mixture plasma by a spectrometer. The reduction in steady state D permeation flux is observed as the presence of He ions in plasma. To understand the effect of irradiation defects on the D plasma driven permeation behaviour, PDP experiment is carried out with the iron ions (Fe^{2+}) irradiated W with the maximum damage level of 1 displacement per atom (dpa). The results show that the steady sate D permeation flux for damaged W sample is lower than that for undamaged one. The lower permeation flux at back surface in the case of D_2/He PDP or PDP for damaged W indicates a lower D in solution near the front surface. In addition, recently, PDP experiment by H/D mixed plasma has started. In this presentation, recent progress of the H/D PDP experiment will be explained.

Influence of the permeation barrier oxide layers on hydrogen permeation of W and RAFM steel

Authors: Li Qiao[1]; Hong Zhang; Peng Wang; Liqiang Chai

[1]Lanzhou Institute of Chemical Physics, China

In fusion reactor, the interaction between plasma and fusion reactor materials caused by D-T reaction discharge directly determines the operation safety, selection of related materials and service life of fusion device. In particular, the diffusion, penetration and retention of hydrogen isotopes usually reduce the ductility of the material, resulting in hydrogen embrittlement and cracking. For the sake of safe operation, it is important to know as much as possible about the behaviour of these materials with respect to permeation of hydrogen isotopes. Thus, we can assess the suitability for containing and isolating the radioactive T fuel of a fusion reactor from the surrounding components, then understand and mitigate the potential damage that could be caused to key components in a fusion reactor.

Tungsten (W) and reduced-activation ferritic martensitic (RAFM) steels are the primary candidate materials for the first wall and structure materials respectively due to their excellent physical and mechanical properties, and have been successfully tested on some tokamak devices. In the process of operation, hydrogen isotopes have obvious diffusion, penetration and retention in W and RAFM steel, which not only affect the mechanical properties of materials, but also have potential harm to plasma quality and discharge safety. So, it is urgent to develop and master the hydrogen permeation data of W and RAFM steel. At the same time, some studies have found that the retention and diffusion of hydrogen isotopes in W or steels with oxide coatings were much lower than that in materials without oxide coatings. Therefore, the hydrogen-impermeable oxide barrier layer can be studied to provide basic theoretical data and safe service support for the use of W and RAFM steel as the fusion-relevant materials.

Therefore, on the basis of mastering the deuterium permeation behaviour in W and RAFM steel, the influence of surface oxide coating on the deuterium permeation behaviour of the materials will be investigated. The oxide coating, e.g. Al_2O_3, Y_2O_3, Er_2O_3 and Cr_2O_3, will be prepared on the surface of W and CLAM steel by magnetron sputtering deposition combined with thermal annealing treatment. Based on the linear experimental plasma system (LEPS) of the laboratory in LICP, the deuterium permeation behaviours of W and CLAM steel with and without surface oxide coatings will be studied. Finally, it will evaluate the effect of material surface and microstructure on hydrogen permeation behaviour. The experimental results will provide basic data for hydrogen permeation behaviour in the fusion-relevant materials and provide reference for development of anti-hydrogen permeation materials and material treatment schemes suitable for the reactor.

Plasma-driven perm. II

Plasma-Driven Permeation of Hydrogen through Materials and Components

Authors: Haishan Zhou[1]; Haodong Liu[1]; Lu Wang[2]; Xuechun Li[2]; Guang-Nan Luo[2]

[1] Insitute of Plasma Physics, Chinese Academy of Sciences, China

[2] University of Science and Technology of China, China

To understand fuel migration behaviour in ITER and the Chinese Fusion Engineering Testing Reactor (CFETR), plasma-driven permeation of hydrogen isotope (H) through plasma-facing materials and components are being extensively investigated at the Institute of Plasma Physics, Chinese Academy of Sciences (ASIPP). Permeation parameters of H through tungsten (W), reduced activation ferritic/martensitic steel (RAFMs), copper alloy and vanadium alloy are measured in a systematic manner. Considering reactor operation scenario, various surface condition effects on permeation behaviour are investigated. Plasma impurity and neutral H irradiation are taken into account as well. For components, first-of-a-kind experiments of enhanced permeation through plasma-facing component mock-ups are demonstrated and H retention at the W/Cu interface are studied. Permeation barriers to reduce permeation flux are being developed. In near future, Further measurements of permeation parameters for fusion-relevant materials will be continued under various plasma irradiation conditions. Permeation experiments using a new high flux plasma device and a permeation probe in EAST tokamak are proposed.

Ion-driven Permeation Experiments and Modelling

Author: Wolfgang Jacob[1]

[1] IPP Garching, Germany

Basic permeation and retention data are required for the following materials: Tungsten, RAFM steels, copper alloys (CuCrZr), doped tungsten materials or tungsten alloys, and functionally graded materials foreseen to be used in first-wall or divertor components. Apart from the data for pristine materials, data for radiation-damaged materials need to be determined because permeation and retention of hydrogen isotopes will be strongly affected by lattice damage and transmutation due to neutron irradiation. In addition, the influence of interfaces on diffusion and permeation is a topic that deserves further attention, because those will be present between W and CuCrZr in divertor components, or between W and RAFM steels at the first wall.

This proposal aims at determining, assembling, and evaluating data needed for a sound assessment of hydrogen permeation in fusion-relevant materials. It further aims at expanding our knowledge of parameters affecting hydrogen permeation in fusion-related materials, including temperature, temperature gradients, microstructure and irradiation-induced defects.

Ion-driven permeation (IDP), which will likely dominate permeation at plasma-facing surfaces in a fusion device, requires a dedicated set-up with a well-characterized, monoenergetic, mass-selected, high-current ion beam. The ion-driven permeation experiment PERMEX-II has been commissioned at IPP Garching at the beginning of 2020. After thorough testing and further qualification, it will be available for IDP measurements in the second half of 2020.

Measurement will focus on the materials EUROFER97 and tungsten. EUROFER97 samples will be prepared following the identical sample preparation procedure as used in Forschungszentrum Jülich, Germany (FZJ) for GDP measurements and ion-driven permeation of deuterium will be studied as a function of incident ion energy and sample temperature. Permeation experiments will be complemented with measurements of D retention after ion loading at SIESTA (Second Ion Experiment for Sputtering and TDS Analysis) followed by in-vacuo thermal desorption spectroscopy (TDS) or ex-situ nuclear reaction analysis (NRA), respectively. These experiments will be performed in close coordination with FZJ (A. Houben) to allow comparison of GDP and IDP in EUROFER. In addition, IDP in tungsten and in radiation-damaged tungsten are planned.

If time allows and samples become available, it is conceivable to perform IDP experiments with EUROFER foils covered with tungsten surface layers. This will provide additional data for studying (also theoretically) the influence of specific material interfaces on permeation. Experimental data of D permeation in EUROFER97 and tungsten will be compared to modelling from the diffusion-trapping code TESSIM and/or TMAP. Further modelling activities aim at a description of permeation across material interfaces and calculation of trapping cross-sections for continuous Trap-Diffusion Models from first principles.

Retention I

Experiments and modelling of in-situ uptake, transport and release studies of hydrogen isotopes in irradiated tungsten

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Implantation of energetic hydrogen, charge exchange neutrals and helium (He), as well as displacement damage creation by neutron irradiation will occur simultaneously during operation of a real fusion reactor. All this is leading to consequences on crystal structure, hydrogen isotope (HI) retention and transport which we do not understand sufficiently in order to predict tritium retention in future fusion devices. Basic processes that occur in the plasma-facing wall material, such as hydrogen transport in a material with lattice defects, the effect of interstitial impurity atoms (HI and He) on defect evolution, and the role of the surface on HI uptake and release need to be studied. For this purpose, well-defined experiments with in-situ measuring the D depth profile are proposed to study transport and permeation through tungsten.

We will present recent advances on the field of in-situ studies on the dynamics of hydrogen isotope retention and transport, isotope exchange and D outgassing in displacement damaged tungsten. I will give an overview of our in-situ studies that we have performed on tungsten by the use of a hydrogen atom beam source delivering atoms with kinetic energy of 0.3 eV [1,2]. By the help of rate equation models the experiments enabled us to determine the de-trapping energies, parameters for the surface processes and the energy barrier for inward diffusion [2,3,4]. I will discuss also how the microstructure and He can affect transport and retention. Plans for further studies performed within the project will be presented.

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Retention II

Development of the X-Ray Diffraction and Thermal Desorption Spectroscopy Techniques for Investigation of Proton (Deuterium/Helium) Induced Near-Surface Effects in Fusion Relevant Materials

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Experimental simulations of ITER-like events in which hydrogen, helium and heavy ion irradiation causes ion-induced radiation damages in the near-surface region of a metal target is a common method; and XRD is widely used for assessment of the structural alterations in the targets after such irradiation. To get the reliable data, the damage depth (irradiated layer) and penetration depth of X-rays in the XRD analysis (the layers from which the information is collected, the “information depth”) should be of the same order of magnitude. The reactor wall materials have quite different X-ray absorption rates: tungsten in the conventional analysis in reflective mode may be probed in depth of few (0.5-2.5) micrometres, while beryllium is almost transparent for X-rays of any commonly used tubes (the penetration depth in it is up to several thousand micrometres). For alloys based on Fe (like RAFM steels) or based on Ni, Cr and Fe (like Inconel), the information depth of XRD analysis (τ) depends on their composition, ranging from few micrometres to dozen micrometres. To reduce X-ray penetration depth inside the material down to few hundreds or even tens of nanometres, we are planning to apply the grazing incidence XRD (GIXRD), where τ depends on the grazing incidence angle (α). Additional advantage of GIXRD is that τ in this case is almost independent from the diffraction angle θ (in contrast to the conventional mode), that allows the microstructure analysis (crystallite sizes, microstrain, dislocation density, etc.), since the volume of the material participating in the formation of total diffraction pattern does not change for reflections (peaks) with different hkl indices.

We performed the calculation of τ for several materials of interest (W, Be, Inconel690, F82H steel, Li_2TiO_3) at a number of incidence angles α, and for several selected X-ray sources (tubes). The appropriate graphical material is given in the presentation. These evaluations show that XRD experiment can be adapted to certain materials and conditions of their ion irradiation. The use of GIXRD may provide selective analysis of the near-surface regions in order to measure the structural features of affected layers, eliminating the contribution of the non-irradiated volume to the measured diffraction pattern. As τ depends not only on the material’s properties (density and absorption coefficient), but also on instrumental factors (mainly detection system), the calibration should be done to estimate the part of total X-ray radiation, which comes from the subsurface layer at the depth tau; (I_0/I_τ). For this the model samples with the coating of known thickness (two-layer systems) will be examined.

In the project GIXRD method for structural study of thin irradiated layer will be combined with thermal desorption spectrometry (TDS) to study hydrogen (helium) trapping and retention in these layers. For this we have constructed and tested two laboratory setups allowing to examine gaseous species (including hydrogen and helium) released from metallic materials under programmed heating. First one uses a mass spectrometer as the detector (TD-MS setup), and the second is based on a gas chromatograph (TD-GC setup). From our own experience and the available literature, it seems that the quantitative assessment of hydrogen content by TD-GC is more realistic than by TDMS. Moreover, TD-GC technique has some other advantages compared to TD-MS, such as: lesser discrimination effects in quantitative analyses of gas mixtures; the ability to detect separately ^4He and D_2 in contrast to conventional MS; TD-GC technique does not need high vacuum equipment and is easier in calibration than TD-MS. At the same time, TD-GC has several limitations, some of which are mentioned in the presentation and can be partially compensated by applying TD-MS. The general restrictions for any TDS approach should be taken into account aware as well. Nevertheless, in our opinion, the combined application of TD-MS and TD-GC may give certain benefits in investigation of gas impurities in fusion materials.

The work plan describing the near-future work (1-2 years).
- GIXRD calibration using model samples with coatings with the known thickness (two-layer system) to get information about the dependence of effective penetration depth vs. the grazing incidence angle for metals of interest;
- to study the possibility to apply unfiltered X-ray radiation (containing Kα and Kβ components) exploiting the K-absorption edge effect for simultaneous structural examination of surface and bulk by using the same X-ray tube; e.g., for steels the CoKα radiation can provide “bulk” information due to low absorption, while the CoKβ radiation may represent “surface” information owing to rather big absorption;
- to perform calculations and preliminary experiments to evaluate the possibility of depth controlled GIXRD structural analysis of samples with the coatings, e.g., copper-coated, tungsten-coated and beryllium-coated RAFM steel; the aim is the structural study of near-interface layers of the substrate;
- further development of the TDS methods (equipment and protocols) to determine the total content of the gas-forming impurities (hydrogen, helium etc.) in irradiated metals (alloys), getting the information on the relative amount of hydrogen trapped into different internal sites of the materials, and for evaluation of the kinetic parameters (the activation energy and frequency factor) associated to each detrapping event;
- calibration of the TDS setups (the mass spectrometric system and the gas chromatography system) using reference materials (some hydrides, gaseous mixtures).

Deuterium retention in tungsten under fluences up to 10^{29} m^{-2}

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Hydrogen retention in tungsten is an important topic for fusion energy, which involves both tritium safety and the lifetime of wall components (therefore plasma operation). The topic is also of scientific interest considering the uncertainty in hydrogen behaviours in metals such as trapping and diffusion, and the impact on material’s properties. So far, the study of hydrogen retention in tungsten is limited by plasma parameters such as plasma fluence and exposure time. The highest accumulated plasma fluence in ITER and CFETR divertor is predicted to reach 10^{30}-10^{31} m^{-2}, which is far beyond the accessible fluence (~10^{28} m^{-2}) in laboratory by linear plasma devices.

To provide as much data as possible in terms of ITER- and CFETR- relevant fluences, the main objective of this research is to study deuterium retention in tungsten under fluence up to 10^{29} m^{-2} using the linear plasma device STEP at Beihang University, China and Magnum-PSI at DIFFER, the Netherlands. The relationship between deuterium retention and plasma fluence will be measured in different conditions, such as tungsten microstructure (rolled, recrystallized tungsten and so on), sample temperature (500 K~1200 K), pre-damage conditions (up to 2 dpa by ion beam) and special surface modifications (blister).

At present, preliminary experiments have been done using STEP and Magnum-PSI. A fluence of 1×10^{28} m^{-2} after a single continuous exposure at a sample temperature of ~500 K has been achieved in both devices. Surface morphology changes and thermal desorption spectroscopy were measured. In the STEP experiment using recrystallized tungsten samples, a saturation of deuterium retention is not achieved at fluence up to 1×10^{28} m^{-2}, and the analysis of thermal desorption spectrum indicates a possible relationship between deuterium trapping and blister-induced defects. While in the Magnum-PSI experiment, it is quite interesting to find that blisters were rarely observed though the exposure fluence and temperature were quite similar to those in STEP. The difference in the sample biasing voltage is proposed to explain the difference.

The following experiments are on-going. And the project is expected to establish a database of hydrogen retention in tungsten under ITER- and CFETR- relevant plasma fluences and reveal the mechanism of trapping and diffusion in tungsten. These activities will contribute to the evaluation of tritium safety and the lifetime of wall components.

Analysis of materials exposed to hydrogen isotopes (H,D,T) in permeation experiments: surface pre-characterization and post-exposure depth profiling of steel, tungsten, and Cu-Cr-Zr.

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The aim of this contribution is to present a) the available instrumentation for characterization of plasma-facing components from fusion devices at Uppsala University and b) an overview of our intended contributions to the CRP.

At Uppsala University, a 5 MV pelletron with 6 beamlines, a 350 kV high-current implanter with 3 beamlines as well as a Low-energy ion scattering system have been used for research related to nuclear fusion. In the presentation the available instrumentation and complementary facilities as well as highlight basic capabilities for hydrogen depth profiling using Nuclear Resonance Analysis and different elastic recoil techniques will be introduced. Recent developments will also be discussed:

a) a new chamber for in-situ thin film growth and modification while performing ion beam analysis and a new low-energy ion beam analysis chamber for Rutherford Backscattering Spectrometry (RBS), low-energy particle induced X-ray emission (PIXE) as well as low-energy nuclear resonance analysis (NRA).

b) a new chamber for in-situ thin film growth and modification for the medium-energy ion scattering system

c) a new-low energy implantation facility

We will also introduce our intended contributions to the present CRP on hydrogen permeation of fusion relevant materials, which specifically are:

1. Surface pre-characterization of materials (reduced activation steels, W, Cu-Cr-Zr alloys) by ion beam methods: nuclear reaction analysis and heavy ion elastic recoil detection analysis, to determine H and low-Z impurities: oxygen, carbon, sulphur.
2. Preparation of samples loaded with H or D by implantation and ion beam pre-characterization of such samples.
3. Preparation of ion-implanted (H, He, high-Z ions) targets to simulate transmutation products in neutron-irradiated materials; for instance, steel implanted with H, He and Mn.
4. Determination of diffusivity and permeation rate by analysis (with high-resolution quantitative depth profiling) of H, D, T in materials used in permeation experiments. The laboratory has capabilities for handling T-containing samples.
5. Contribution to the selection and qualification of materials, and to the unification of experimental set-ups/conditions in order to enable comparison of results obtained in different laboratories.

Recent irradiation experiments involving baseline and advanced tungsten materials performed at SCK CEN

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To reduce uncertainty on the scarce information available on neutron irradiation damage in tungsten and to support the development of advanced tungsten-based alloys, SCK-CEN has recently executed the neutron irradiation programme. The irradiation programme lasted for about 2 years and covered a large range of irradiation temperatures and doses. The primary types of post irradiation experiments (PIE) are mechanical testing and microstructural investigation. Next to the main irradiation programme, SCK-CEN has executed the irradiation programme for internal studies, where a number of samples for advanced characterization such as hardness testing and tritium permeation experiments. The irradiation was performed inside the fuel elements to ensure that the transmutation of tungsten into Re and Os would be minimized and achieve the rates comparable to DEMO/ITER conditions.

Six tungsten grades were selected for the irradiation programme due to specific relevance for the application in plasma-facing components of ITER and/or DEMO. These tungsten grades included: Plansee (Austria) ITER specification tungsten, ALMT (Japan) ITER specification tungsten, two products from KIT (Germany) produced by powder injection molding and strengthened by 1% TiC and 2% Y_2O_3 dispersed particles, and rolled tungsten strengthened by 0.5% ZrC from ISSP (China). The materials were irradiated face-to-face at three temperatures equal to 600, 1000, and 1200 °C to the dose of ~1 dpa. The Vickers hardness tests under 200 gf (HV0.2) were performed at room temperature. The Vickers hardness increases as the irradiation temperature increases from 600 to 1000 °C for all materials, except for the ZrC-reinforced tungsten, for which the increase of hardness does not depend on irradiation temperature. The irradiation-induced hardness decreases after irradiation at 1200°C. This is a result of defect annealing enhanced by thermally activated diffusion. However, even at 1200 °C, the impact of neutron irradiation on the hardness increase remains significant; the hardness increases by ~30 to 60% compared to the non-irradiated value. In the case of TiC-strengthened material, the irradiation hardening progressively raises with irradiation temperature, which cannot be explained by the accumulation of neutron irradiation defects solely. The samples irradiated in the above specified programme and in an extra campaign (irradiated to lower dpa) are now available for the advanced post irradiation characterization. The sample irradiated in extra campaign up to 0.2 dpa exhibit the activity of less than 2 mSv/hour on contact – i.e. can be handled in fume hood. These samples could be used for this CRPs to perform dedicated experiments to investigate permeation and retention of hydrogen isotopes.

Plasma- and gas-driven tritium permeation in fusion materials

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Deuterium and helium retention and corresponding modifications of W-based materials under transients

Author: Olga Ogorodnikova[1]

Co-authors: Alexander Poskakalov [1]; Andrey Kaziev [1]; Dmitry Kovalenko [2]; Konstantin Gutarov [1]; Maxim Kharkov[1]; Nikolay Klimov [2]; Vitaly Efimov [1]; Yuri Gasparyan[1]

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Tungsten and dense nano-structured tungsten (W) coatings are used as plasma-facing materials (PFMs) in current tokamaks and suggested to be used for future fusion devices. The high particle and heat loads occur during transients that lead to major damage in PFMs. In this regard, a study of accumulation of deuterium (D) and helium (He) in advanced W materials and corresponding material modifications under transient events appears necessary for assessment of safety of fusion reactor due to the radioactivity of tritium and material performance and for the plasma fuel balance. Therefore, sequential and simultaneous (with 10% of He seeding) D/He plasma exposure of W-based samples in quasi-stationary high-current plasma gun QSPA-T below and above the melting threshold with a pulse duration of 1 ms and number of pulses from one to thirty was performed. Material modification was investigated using an electron microscope equipped with a focused ion beam for in-situ cross sectioning and an x-ray diffractometer. The D and He retention in irradiated samples was measured by a method of thermal desorption spectroscopy using high resolution quadrupole mass spectrometer to separate signals of He and D2. The D retention already after 10 pulses of the D plasma gun exposure was higher than that after stationary plasma exposure even at sample temperature of 600 K indicating the dominate influence of ELM's-like events on the D retention compared to normal operation regime. This effect occurs for both pure D and mixed D/He plasma exposure. As modelling results show, the increased D diffusion into the bulk due to high temperature gradient during the ELMs is one of the reasons of the enhanced D retention after ELMs. A formation of a layer of a thickness of ~10–30 µm with columnar crystal structure oriented perpendicular to the irradiated surface was observed for all W grades after the exposure of samples to both pure D and mixed D/He plasmas with the heat flux exceeded the melting threshold. After irradiation with D/He plasma in QSPA-T above the W melting threshold, spherical cavities in a layer of columnar crystals, containing a lot of D, were observed. It is shown that the synergetic effect of D, He and high heat flux leads to completely different particle retention and material modification compared to separate/sequential irradiation.

Neutron-irradiated materials II

Hydrogen diffusion, retention and irradiation-induced damage in fusion-relevant materials

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The presentation will outline the proposed research to the CRP. The experimental work will focus on studying hydrogen isotope mobility and trapping in W and MoNbTaVW materials, while the simulations will concentrate on hydrogen isotope diffusion, isotope exchange, and the effects of plasma edge-localized modes during fusion plasma operation in tokamaks.

The suitability of the new class of materials called High Entropy Alloys (HEAs) as first wall for fusion reactors is studied. The most promising refractory HEA material MoNbTaVW, which is classified as a complex, concentrated alloy refractory metal is chosen for this study. Hydrogen isotope diffusion and trapping is studied using ion implantation, and TDS, SIMS, and ERDA techniques. The H isotope exchange in the HEA material (relating to diffusion and tritium removal) is studied using the annealing in hydrogen atmosphere method. The second proposed task will focus on determining the H trapping vacancy type defects formed in neutron irradited W using PAS. The third task uses rate equation (RE) simulations to elucidate H isotope exchange experiments and the H isotope retention, vacancy clustering and microstructure change due to plasma edge-localized modes (ELM) during fusion plasma operation in tokamaks.

Combined experimental and theoretical studies of the retention and permeation of hydrogen isotopes in fusion-relevant materials

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We present an overview of experimental facilities available at UKAEA-CCFE, as well as modelling studies that will be used in the course of the CRP. Hydrogen isotope ion exposure facility together with thermal desorption spectroscopy apparatus are already used at UKAEA to study deuterium retention in plasma-facing materials, such as Eurofer steel, Fe-Cr alloys [1], tungsten [2], and molybdenum. In the course of Tritium Retention in Controlled and Evolving Microstructure (TRiCEM) enabling research project, a collaboration has been established with several European research laboratories, that allowed us to perform self-ion irradiation of samples (University of Helsinki, Finland) and post-exposure characterization using SIMS (VTT, Espoo, Finland), TEM (CEA, Université ParisSaclay, France), and PAS analysis (CEMHTI/CNRS, Université d'Orléans, France). This collaboration will be continued during the CRP.

Modelling efforts will be along two lines. On a small scale, similarity in saturation of vacancy content as function of damage, as observed in tungsten [2] and theoretically found by Derlet and Dudarev [3], will be investigated further. Parameters of tritium capture by defects, such as number of atoms and the depth of potential well, will be studied in ab initio and molecular dynamics calculations, as already done for dislocation loops in tungsten [4]. On a larger scale, tritium transport will be modelled under conditions of elastic stress field and temperature gradients.

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