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Plasma–Wall Interaction for Irradiated Tungsten and Tungsten Alloys in Fusion Devices

Summary Report of the Third Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

27-30 June 2017

Report prepared by

H.-K. Chung, T. Schwarz-Selinger, H.-T. Lee, S. Dudarev, T. Oda, A. Hasegawa, R. Kurtz,

M. Shimada and M. Mayer

September 2017

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ABSTRACT

The Third Research Coordination Meeting of the IAEA Coordinated Research Project on Plasma–Wall Interaction for Irradiated Tungsten and Tungsten Alloys in Fusion Devices held on 27-30 June 2017 at IAEA in Vienna with twenty one participants. Seventeen projects out of nineteen CRP projects were presented. The participants reviewed their work over the period after the last meeting, and reported on the coordinated activities of Thermal Desorption Spectroscopy (TDS) Round Robin Experiments and a comparison workshop on TDS modeling codes. Seventeen groups participated in the TDS Round Robin Experiments including three groups outside the CRP. Current status on fundamental modelling and its connection to experiments, production and characterization of damage, and hydrogen (tritium) retention in damaged tungsten were reviewed. A final report of the CRP was discussed and databases on molecular dynamics calculations of collisional cascades after irradiation and density functional theory calculations of fusion relevant materials were discussed. The proceedings of the meeting are summarized in this report.

September 2017

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1. INTRODUCTION

Fusion energy production relies on the reaction of hydrogen isotopes deuterium (D) and tritium (T) forming helium and releasing 14-MeV neutrons. In the magnetic confinement approach to fusion, D-T plasma at a temperature of around 15 keV (about 150 million K) is trapped in a toroidal magnetic field inside a vacuum vessel. The confinement is not perfect and the plasma interacts with the vacuum vessel wall. This may cause erosion of the surface and may also cause tritium to become trapped in the wall material, making it unavailable for fusion. The plasma-wall interaction issues of erosion and tritium retention are perhaps the most serious impediment to the realization of fusion energy production.

The choice of wall material for a fusion demonstration experiment involves a difficult compromise between the demands of low erosion, low radiation loss as a plasma impurity, high melting point and high thermal conductivity, low nuclear activation and low propensity to absorb tritium. It should be noted that the tritium retention issue is one of safety and nuclear licensing as well as cost; in ITER and in any successor facility there will be strict limits on the amount of tritium that may be trapped in the wall material. For ITER in its nuclear phase these considerations have led to the choice of tungsten as the wall material for the regions of highest heat load and beryllium for the larger main wall surface area that is exposed to less severe heat load. For a fusion demonstration experiment, DEMO, or a reactor the same considerations point to tungsten for the regions of highest heat load and some kind of reduced-activation steel for the main wall, but there are major unresolved issues still.

The most serious complication for these considerations, and the one that leads to the topic of the present CRP, is the very high neutron fluence in DEMO or in a reactor. For DEMO estimates of neutron fluence are around 30 dpa (displacements per atom) per year of full power operation and for a reactor the expected fluence is even higher. For tungsten this level of neutron irradiation will cause many dislocations and will change the composition to an alloy of (primarily) tungsten, rhenium and osmium. Pure crystalline tungsten has an extremely low affinity for tritium, but this good property will be compromised by the neutron fluence in DEMO or in a fusion reactor and erosion properties will also be affected. These issues are critically important for fusion energy development beyond ITER, but investigations into properties of irradiated fusion materials are hampered by the unavailability of an adequate neutron source and by the great difficulty of relevant first principles computations. Therefore the material properties, the resistance to sputtering and ablation, and the behaviour of trapped tritium in tungsten-based materials after neutron irradiation are still poorly known.

The CRP on Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices was established to improve the knowledge base and databases on properties of irradiated tungsten. The most important topic is to understand how tritium retention, tritium migration and ways to extract trapped tritium are affected by radiation damage. The relevant level of neutron damage is so high that it cannot be simulated in present experiments and therefore experiments employ only low levels of neutron irradiation or they employ surrogate irradiation by charged particle beams. The difference between neutron irradiation and surrogate irradiation in their effect on plasma-material interaction properties needs to be much better understood. This leads to the need to characterize the effects upon microstructure due to different kinds of irradiation and to characterize how changes in microstructure influence the tritium retention and tritium transport properties.

The first Research Coordination Meeting (RCM) was held on November 26-28, 2013 at the IAEA headquarters in Vienna, Austria and the second RCM was held on September 8-11, 2015 at Seoul National University in Seoul, Republic of Korea. The third and final RCM was held on June 27-30, 2017 at IAEA in Vienna with twenty one participants. At this meeting, the work over the period after the 2nd RCM was reviewed. Particularly, there was a report on the coordinated activities of Thermal Desorption Spectroscopy (TDS) Round Robin Experiments and a comparison workshop on TDS modeling codes that were proposed at the second RCM in 2015. There were three review sessions on current status on fundamental modelling, damage production and characterization, and hydrogen (tritium) retention in damaged tungsten. A final report of the CRP and databases from the CRP were discussed.

The proceedings of the meeting are summarized in Section 2 and the discussions are summarized in Section 3. The list of participants is in Appendix 1 and the meeting agenda is given in Appendix 2. Presentations are available at the IAEA atomic and molecular data unit web page https://www-amdis.iaea.org/CRP/IrradiatedTungsten/RCM3/ and summaries are presented in Appendix 3.

2. PROCEEDINGS

The Third Research Coordination Meeting was opened with the welcome address by Arjan Koning, the Head of Nuclear Data Section. It was followed by the introduction of all participants and the proposed agenda was adopted. The first part of the meeting proceeded with review presentations of research done by the CRP members and the second part of the meeting was devoted to discussion sessions described in the Section 3 in more detail.

On the first and second day of the meeting, presentations on experimental work were given by CRP members. Prof. Yuji Hatano of Toyama University, Japan updated the current status of research on deuterium behavior in neutron-irradiated tungsten; long-range diffusion, defects responsible for D trapping, neutron-irradiation under hydrogen gas atmosphere and effects of rhenium. Dr. Masashi Shimada of Idaho National Laboratory, USA reviewed the progress on research on the deuterium retention in HFIR neutron-irradiated tungsten under US-Japan PHENIX program and updated on the status of Tritium Plasma Experiment Upgrade, Surface/bulk diagnostics upgrade for low-activation and tritium-contaminated samples at STAR facility and MELCOR-TMAP code integration. Dr Matej Mayer of IPP Garching, Germany reviewed the deuterium retention in tungsten damaged by mechanical work, electrons, and fast ions, particularly using samples with defined specific defects for fundamental understanding. Dr Haishan Zhou of IPP-CAS, Hefei, China, reported on the progress of W-relevant plasma-material interaction studies at ASIPP (Institute of Plasma Physics Chinese Academy Of Sciences) which range from the deuterium retention in ion-damaged tungsten and permeation behavior in tungsten and its alloys and described the new research and development capabilities for tungsten PWI research. Dr Elodie Bernard of CEA, France reviewed the experimental research on the impact of helium irradiation on tritium retention in tungsten and emphasized the significance of in-situ exposure experiments at high temperatures. Prof Akira Hasegawa of Tohoku University, Japan presented the current status of study on damage structure evolution of neutron-irradiated tungsten and its alloys. The first day concluded with the discussion on TDS modelling code comparison exercise, led by Dr Shimada.

The second day proceeded with the presentation of Dr Sabina Markelj of Jožef Stefan Institute, Ljubljana who reviewed the studies on hydrogen retention in self-damaged tungsten, in tungsten simultaneously damaged by high-energy tungsten ions and loaded by deuterium, and on the influence of helium on deuterium retention. Prof Mizuki Sakamoto of University of Tsukuba, Japan described the experimental setup, tungsten samples and the experimental results on the effect of heavy ion irradiation on the deuterium retention in tungsten. Dr Yury Gasparyan of National Research Nuclear University "MEPhI", Moscow, Russia presented the theory of TDS (Thermal Desorption Spectroscopy) for detrapping energy determination and experimental results on comparisons of hydrogen interaction with defects by ions and neutrons as well as on helium retention in tungsten. Dr Marius Wirtz of Forschungszentrum Jülich, Germany presented the work on the behavior of tungsten under thermal and plasma exposure and development of advanced tungsten materials; thermal shock behavior of irradiated and un-irradiated W grades, change of W microstructure under simultaneous heat and particle loads and impact on W erosion and fuel retention in W, Development of advanced materials with improved micro-structure and characterization of commercially available tungsten grades.

In the afternoon, Dr Boris Khripunov of Kurchatov Institute, Moscow, Russia presented the work on production of damage in tungsten by high energy ion, plasma experiment on irradiated tungsten and tungsten erosion in deuterium plasmas as well as the effect of implanted helium accumulation. Tungsten damaged by carbon ions and tungsten irradiated by protons were investigated. Dr Prakash M. Raole and SP Deshpande of IPR, Gandhinagar, India presented molecular dynamics (MD) simulations of interstitial locations and cascade structures for ion-irradiated tungsten and experiments using heavy and light ion irradiation of recrystallized tungsten foils to study various types of defects such as dislocations, point defects and vacancy clusters. Presentations continued on the CRP-coordinated activities on Thermal Desorption Spectroscopy Round Robin Experiments (TDS RRE) by Dr Thomas Schwarz-Selinger of IPP Garching, Germany on TDS round robin samples: Motivation, preparation and pre-characterization and by Heun-Tae Lee of Osaka University, Japan on the review of TDS Round-Robin Experiments.

Presentations on simulations proceeded on the third day with Dr Sergei Dudarev of CCFE, UK who described the non-local real-space diffusion-driven models for microstructural evolution of irradiated tungsten such as self-diffusion of dislocations and vacancy-diffusion-mediated evolution as well as defect production in collision cascades, high- and low-temperature mobility of radiation defects and anomalous phase decomposition of W-Re alloys. Prof Takuji Oda of Seoul National University, Korea presented modeling of tritium trapping effects of vacancy, grain boundaries and vacancy clusters and reviewed the development of a code to simulate tritium behavior in damaged tungsten. Dr Marie-France Barthe of CNRS, France reviewed modeling and experimental validation studies of the vacancy-type defects formation in tungsten crystal due to helium accumulation, damage induced in W by W-ion irradiations and atomic deuterium exposure in self-damaged tungsten. Prof Hong-Bo Zhou of Beihang University, Beijing, China presented computational studies of interstitial-mediated diffusion and aggregation mechanism for transmutation elements rhenium and osmium precipitation in tungsten.

In the afternoon, Dr Rick Kurtz of Pacific Northwest National Laboratory, USA presented an overview of SciDAC- PSI project developing a multiscale - multiphysics approach to simulating tungsten plasma surface interactions from the boundary plasma to the bulk substrate. The presentation of Changsong Liu of ISSP-CAS, Hefei, China was given by Prof Hong-Bo Zhou on the topic of cross-scale self-healing mechanism for radiation damage in nano-crystalline tungsten.

After all the presentations, participants were grouped into three to review the current status and problems addressed in the course of the CRP for three topics: 1) fundamental modelling and its connection to experiments led by Dr Dudarev and Prof Oda, 2) production and characterization of damage: experiments and modelling led by Prof Hasegawa and Dr Kurtz, and 3) hydrogen (tritium) retention in damaged tungsten: experiments and modelling led by Dr Mayer and Dr Shimada.

On the fourth day, presentations on proposed databases of density functional theory (DFT) simulations and molecular dynamics (MD) simulations related to irradiation and plasma-matter interaction were given by Prof Oda and Dr Dudarev. The summaries of three discussion sessions were presented on the three topics by Dr Dudarev, Prof Hasegawa and Dr Mayer. Prof Lee presented the future plans for the TDS RRE project and Dr Shimada discussed the future plans for the TDS code comparison workshops. Finally, participants agreed to produce the volume of Atomic and Plasma-Material Interaction Data for Fusion (APID) with contributions of each group.

3. DISCUSSIONS

3.1 Discussion on hydrogen retention in damaged tungsten: experiments and modelling

M. Shimada, M. Mayer, Y. Hatano, H. Zhou, S. Markelj, M. Sakamoto, Y. Gasparyan

Current status of various topics related to hydrogen retention phenomenon in damaged tungsten was reviewed and summarized in this section.

Modelling of trapping/diffusion/TDS:

- Good progress during the period of the CRP –
- Development of new codes (MHIMS, DIFFTRAP, HIDT, TMAP), extension of codes by new models such as fill-level dependence of traps (TESSIM, MHIMS Reservoir), isotope exchange - Classical codes are often sufficient (except isotope exchange)
- Close connection between modelling and experiment
- All available input data are taken into account (depth profiles, TDS spectra, damage profiles, input from DFT)
- Input data for modelling remain uncertain (Diffusion coefficient, pre-exponential factor) require clarification
- Code-code comparison of 3 codes within EUROfusion, code-code comparison within CRP ongoing
- Variation of heating rate can give precise detrapping energies.

Damaging at elevated temperatures in the presence of H:

- Good progress during the period of the CRP
- Data about damaging at elevated temperatures became available from a number of groups
- Data at elevated temperatures with presence of H are still very scarce: More data are required
- Re and transmutation element effects: Some data for Re are available, no data for Os, some data for Ta

Diffusion in the presence of a temperature gradient:

- No data available
- No data on Soret constant

Diffusion code with time-dependent trap density and microstructure change:

- Can be included in some codes, but not widely used

Relation between microstructure and hydrogen trapping:

- Good progress within the CRP
- Correlation of TEM and PAS/PALS investigations with D depth profiles and TDS
- Work in progress

Different methods of sample loading:

- Good progress within the CRP
- Data for different types of loading conditions (gas, atom, ion beam, plasma) are available
- More data for low energy particles are required

Effect of He:

- Good progress within the CRP
- Data available for pure He and H/He plasmas
- Only few data available for He in bulk W

Effect of impurities (C, N, O):

- Some data available for C, N
- Generally only scarce data

Extrapolation of surrogate irradiation to neutrons:

- Some data for fission neutrons available
- Surrogate irradiation for different (heavy) ion species give comparable results
- Discrepancy for measured damage rate dependence
- Work ongoing

3.2 Discussion on production and characterization of damage: experiments and modelling

A. Hasegawa, R. Kurtz, M. Barthe, B. Khripunov, P. Raole, M. Wirtz

Knowledge inventory of tungsten microstructure following exposure to various damage production processes (e.g., neutron and ion irradiation, plasmas, thermo-mechanical loading, etc.) has been achieved as following:

- Currently used damage processes represent a simulation of the actual fusion environment.
- Erosion, tritium retention and transport properties depend strongly on tungsten microstructure.
- A database of experiments performed to explore tungsten microstructure evolution will be prepared.
- The database will summarize relevant features of exposure conditions employed, the resulting microstructure obtained, and properties measured.
- A spreadsheet will be circulated to CRP participants to collect their information.

- The database would provide greater value if its content could be expanded to include all known work being done worldwide – but this will be difficult to accomplish with the limited resources available.

Brief reports will be prepared summarizing work performed since the inception of the CRP by participants performing experiments and modeling of damage production and characterization.

Integration of the brief reports would be desirable to conserve space, but how this will be accomplished is uncertain due limited resources.

3.3 Discussion on fundamental modelling and its connection to experiments

S. Dudarev, T. Oda, H.-B. Zhou, E. Bernard, S. Deshpande, C. Hill

The work on threshold displacement energies for defect production in tungsten is in progress. Lately, a large scale of DFT calculations were performed which is in good agreement with experiments by P. Olsson, et al. Mater. Res. Lett, 4, 219 (2016) for Iron, and A. De Backer, et al. (Phys. Scr. T167, 014018 (2016) for tungsten. There is a HVEM (high voltage electron microscopy) experimental data by Prof Lee where displacement energy is less than 70 eV for (110) direction. Binding and trapping energies, involving not only single defects but also defect complexes – e.g. vacancy clusters are investigated with simulations and DFT simulations will be useful.

Interpretation of macroscopic TDS experimental data necessarily requires the use of rate theory type, or kinetic Monte Carlo simulations, or both approaches. There is a progress in the study of defect, dislocation and grain boundary microstructure as in the model by A. De Backer et al. (submitted to Nuclear fusion, 2017). Relating TDS measurements to microstructure is probably a reasonable overall objective for the modelling effort, however, it has not been achieved due to lack of funding.

Comparison of TDS experiments, accompanied by comparison of interpretations using various codes (TMAP, kMC) is in progress, particularly with the proposed code comparison exercise. Comparison of software for the interpretation of TDS experiments is also in progress.

Potentials for MD of tungsten, comparison of potentials with DFT, have been achieved for various configurations by M.-C. Marinica et al. (J. Phys: Condens. Matter 25, 395502 (2013)).

Two databases, one for DFT simulations on tungsten and tungsten containing materials, and the other for MD simulations of collisional cascades after irradiation will be developed at the IAEA.

3.4 Coordinated Activities of Thermal Desorption Spectroscopy Round Robin Experiments

T. Schwarz-Selinger and H.-T. Lee

A summary of the analysis of total D retention values is as follows:

- ❑ Measure of accuracy determined by comparison to NRA (Nuclear Reaction Analysis) data.
    - Mean is ~12% lower than NRA

    - Standard deviation is ~30%

- ❑ Measure of consistency determined by ability to differentiate D amount between outer- and inner- ring samples (2-3)×10^{15} D atoms/cm^2.

    - Both mean and standard deviation values are ~2×10^{15} D atoms/cm^2

- ❑ System base pressure or ratio of mass 3 and 4 are insufficient parameters to evaluate the quality of the system.

A summary of the analysis of the shape of the TDS release curves is as follows:

- ❑ Inner ring samples show better agreement between groups vs. outer ring

- ❑ Peak shifts and distortion of the leading and trailing edge of the profiles observed – effect of system parameters.

    - The peak shifts could occur due to systematic error in temperature or phase differences arising from finite pumping speed
    - Distortion of the peak shapes can arise from finite pumping speeds or nonlinear temperature ramping
    - The observed distortions are more significant at 1 K/s vs. 0.1 K/s

- ❑ The shift in desorption spectra with varying ramping rates arising from kinetic parameters could not be determined

    - Likely due to the fact that the system dependent parameters and their convolution dominate the release spectra over any kinetic parameters
    - More analysis underway examining the Mass 3, 19, 20 signals

It was decided that the RRE can only be finalized if the observed discrepancies can be explained. In the worst case, the reason for the scatter of values and distortion of TDS curves cannot be given. In this case, the reported variation amongst a wide number of systems can still be deemed valuable information. In the best case, all discrepancies and their reasons can be explained. In such a case, such information gained can be distilled down to provide a recommended guideline or practice to perform quantitative TDS work. Such work would be highly valuable to both experimentalists and modelers and have the potential to have wider impact in other fields using TDS or residual gas analysis (RGA) methods. It is anticipated that the outcome will fall somewhere between such two extremes. Nevertheless, TSS and HTL believe there is a basis for a journal article that can be published following peer review.

Further information is required to proceed with the analysis. The next step will consist of a query in the form of a standardized questionnaire that will be distributed to participants by the middle of July, with the deadline being the end of July 2017. The questionnaire will broadly consist of the following categories (which substitutes as possible reasons for the observed discrepancies): (1) Background; (2) Temperature; (3) Pumping speed; (4) Q-mass linearity; (5) Calibration leak

With respect to the release of TDS data, it was proposed that the submitted excel files would be uploaded and made available to all participants. The estimated timeline is by end of July 2017. It is recommended to set up a user-friendly interface at IAEA, but it is anticipated that this will take at least 6 months to realize.

One possibility of further work is additional characterization of the calibration samples. Since we have "fixed" the kinetic parameters, the identification of such parameters has the potential to lead to the establishment of a "standard" set of kinetic parameters in tungsten. It of course remains to be seen whether thin film traps and bulk tungsten traps are equivalent. Nevertheless, if properly executed, such "standard" data will be highly valuable as benchmark data for backwards calculation using various modeling codes. At a minimum, the parameters to evaluate are the sample porosity and microstructure. It is anticipated that the workload can be distributed among participants under this CRP depending on the interest.

4. Future Plans

As an output of a CRP, final reports from the CRP should be produced. Participants agreed to produce the volume of Atomic and Plasma-Material Interaction Data for Fusion (APID) from individual group. Submitted manuscripts from each group will be peer-reviewed and published by the Agency as an IAEA publication. The scope of the final report is the summary/review of each group's activities during the CRP on the topic of plasma-interaction data of irradiated tungsten. It is recommended that the group-compiled data sets in the course of the CRP should be published in the final report for dissemination to member states. The word template of the IAEA publishing style can be found at https://nucleus.iaea.org/sites/iaeastyle/SitePages/Home.aspx

Once the contributions from the group are assembled, participants will review the possibility to write review articles for a journal publication. Potential topics for review articles are 1) comparisons of hydrogen retention for neutron-damage and surrogate ion beam damage, 2) review of thermal desorption spectroscopy round robin experiments, and 3) review of thermal desorption spectroscopy code comparisons.

Nuclear Fusion also accepts the conference summary paper. A short summary paper on the CRP of plasma-wall interaction data for irradiated tungsten and tungsten alloys in fusion devices should be considered for publication.

A database will be assembled and available through the CRP website on damage production & characterization by Prof. Hasegawa on spreadsheet.

A database on DFT simulations proposed by Prof. Oda and a database on MD simulations proposed by Prof. Dudarev will be developed with atomic and molecular data unit to be available at the Unit's web site.

The TDS code comparison exercise will be organized by Dr. Shimada and the Unit staff will help meeting and discussion of participants in the conferences on plasma-surface interaction.

The TDS RRE exercise will produce a database of TDS results in collaboration with the Unit staff to be available at the Unit website. The TDS RRE exercise will be completed by Prof. H. Lee, Dr. W. Jacob and Dr. Schwarz-Selinger.

Appendix 1: List of Participants

Marie-France Barthe, CNRS, 3A rue de la Férolerie, 45071 Orleans cedex 2, France

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Hyun-Kyung Chung, International Atomic Energy Agency, Vienna, Austria

Appendix 2: Meeting Agenda

Tuesday 27 June 2017 **Meeting Room: M0E75**

09:30 – 09:45 Opening, Adoption of Agenda

09:45 – 10:00 **H. Chung** "Meeting Objectives"

Session I: Experiments (Chair:H. Chung)

10:00 – 10:45 **Yuji Hatano**, Toyama University. "Update on deuterium behaviours in neutron-irradiated tungsten"

10:45 – 11:00 *Coffee break*

11:00 – 11:45 **Masashi Shimada**, Idaho National Laboratory. "Deuterium behavior in HFIR neutron-irradiated tungsten under US-Japan PHENIX program"

11:45 – 12:30 **Matej Mayer**, IPP Garching. "Deuterium retention in tungsten damaged by mechanical work, electrons, and fast ions"

12:30 – 14:00 *Lunch*

Session II: Experiments (Chair: Y. Hatano)

14:00 – 14:45 **Haishan Zhou**, IPP-CAS, Hefei, "Progress of W-relevant plasma-material interaction studies at ASIPP"

14:45 – 15:30 **Elodie Bernard,** CEA. "Impact of helium irradiation on tritium retention in tungsten"

15:30 – 15:50 *Coffee break*

15:50 – 16:35 **Akira Hasegawa**, Tohoku University. "Current status of study on damage structure evolution of neutron irradiated tungsten and its alloys"

16:35 – 17:15 Discussion on TDS modelling code comparison exercise (**M. Shimada)**

19:00 Dinner

Wednesday 28 June 2017

Session III: Experiments (Chair: C. Grisolia)

09:00 – 09:45 **Sabina Markelj**, Jožef Stefan Institute, Ljubljana. "Hydrogen retention in self-damaged and He-irradiated tungsten for PFC - update on the recent results"

09:45 – 10:30 **Mizuki Sakamoto**, Plasma Research Center, University of Tsukuba. "Deuterium retention in tungsten irradiated by heavy ions"

10:30 – 10:50 *Coffee break*

10:50 – 11:35 **Yury Gasparyan**, National Research Nuclear University "MEPhI", Moscow. “Quantitative characteristics of H and He interaction with radiation defects in tungsten”

11:35 – 12:20 **Marius Wirtz**, Forschungszentrum Jülich “Behavior of tungsten under thermal and plasma exposure and development of advanced tungsten materials”

12:20 – 13:40 *Lunch*

Session IV: Experiments (Chair: S. Markelj)

13:40 – 14:25 **Boris Khripunov**, Kurchatov Institute, Moscow. “Deuterium plasma effect on tungsten irradiated with high-energy ions”

14:25 – 15:10 **Prakash M. Raole,** IPR, Gandhinagar. “Ion-Irradiation of Tungsten: Modeling & Experiments”

15:10 – 15:30 *Coffee break*

15:30 – 16:15 **Thomas Schwarz-Selinger**, IPP Garching. “TDS round robin samples: Motivation, preparation and pre-characterization”

16:15 – 17:30 **Heun-Tae Lee**, Osaka University, “Review of TDS Round-Robin Experiments”

<u>Thursday 29 June 2017</u>

Session V: Simulations (Chair: M. Shimada)

09:00 – 09:45 **Sergei Dudarev**, CCFE, Abingdon. “Non-local real-space diffusion-driven models for microstructural evolution of irradiated tungsten”

09:45 – 10:30 **Takuji Oda**, Seoul National University. “Modeling of tritium trapping effects of vacancy, grain boundaries and vacancy clusters”

10:30 – 10:50 *Coffee break*

10:50 – 11:35 **Marie-France Barthe**, CNRS

11:35 – 12:20 **Hong-Bo Zhou**, Beihang University, Beijing. “Interstitial-mediated diffusion and aggregation mechanism for transmutation elements rhenium and osmium precipitation in tungsten”

12:20 – 13:40 *Lunch*

Session VI: Simulations (Chair:S. . Dudarev)

13:40 – 14:25 **Rick Kurtz**, Pacific Northwest National Laboratory, “Overview of SciDAC - PSI: A multiscale - multiphysics approach to simulating tungsten plasma surface interactions from the boundary plasma to the bulk substrate”

14:25 – 15:10 **Changsong Liu**, ISSP-CAS, Hefei.” Across-scale self-healing mechanism for radiation damage in nano-crystal tungsten”

15:10 – 15:30 *Coffee break*

15:30 – 16:00 Review of CRP objectives that were addressed in the course of the CRP

- To inventorise knowledge about effects of neutron irradiation and charged particle surrogate irradiation on the microstructure of tungsten-based plasma-facing materials.
- To inventorise knowledge about the relation between tungsten microstructure after irradiation and plasma-material interaction properties for erosion, tritium retention and tritium migration.
- To perform coordinated experiments and computations (based on quantum theory and molecular dynamics) to improve the knowledge base on effects of irradiation upon tungsten microstructure.
- To perform coordinated experiments and computations to improve the knowledge base on the influence of tungsten microstructure on tritium retention and tritium transport properties.
- To synthesize new information, extrapolate to relevant fusion neutron fluence, and provide best expert estimates and uncertainties for plasma-material interaction properties (especially tritium retention and tritium transport) for tungsten-based materials in a fusion reactor environment.

16:00 – 17:30 Group discussions (3 groups)

<u>Friday 30 June 2017</u>

Session VII: Discussions

09:00 – 09:50 Discussion on fundamental modelling and its connection to experiments. Review of main problems that were addressed in the course of the CRP. Discussion on the current status of simulations and proposed code comparisons

09:50 – 10:40 Discussion on production and characterization of damage: experiments and modelling. Review of main problems that were addressed in the course of the CRP.

10:40 – 11:00 *Coffee break*

11:00 – 11:50 Discussion on hydrogen (tritium) retention in damaged tungsten: experiments and modelling. Review of main problems that were addressed in the course of the CRP**.**

11:50 – 13:30 *Lunch*

13:30 – 15:00 Future Work and Plans for the Final Report

15:00 *Adjournment of Meeting*

Appendix 3: Summary of Presentations

Impact of helium irradiation on tritium retention in W

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The WHIrr (W under Helium Irradiation) project focuses on the study of He impact on W and its consequences for the material properties, using various irradiation techniques and controlled irradiation temperature (300 to 800ºC). Transmission Electron Microscopy (TEM) was used to evaluate the evolution of W microstructure, coupled with complementary analysis (Positron Annealing Spectroscopy (PAS) and Grazing Incidence Small Angle X-ray Scattering (GISAXS)). We presented the most recent results of the WHIrr project, notably on W samples exposed to He in the linear plasma device PSI-2 (with 10^{20}-10^{22} $s^{-1}.m^{-2}$ flux and 10^{23}-10^{26} m^{-2} fluence ranges). W fuzz was not observed, nevertheless He irradiation led to major changes in the material morphology, rising concerns about properties such as H retention. Tritium (T) inventory was evaluated through T gas loading and desorption at Saclay Tritium Lab, and impact of He irradiation temperature, flux and fluence on the subsequent H trapping and release were investigated.

First, we observed that the material preparation prior to He irradiation was crucial, with a major reduction of the D/T trapping when pristine W had been annealed at 1500ºC for 2h. This was confirmed by the PAS preliminary study, which validated that our annealing procedure had annihilated pre-existing defects existing in as-received W, therefore allowing an initial material for irradiation similar to an ideal W structure.

The PAS study of defects created by He in the W structure showed that the great majority of free volume traps created are detected under 2 keV, which corresponds to a 0 to 10 nm deep layer: it is in good agreement with the heavily damaged layer formed at the surface as observed by the TEM study. PAS also highlighted that all He irradiated samples exhibit a free volume of traps that is close to the one of the monovacancy. Yet, we know from the TEM and GISAXS studies that much larger cavities are present in the material: if their electronic density is higher than if they were void, it means those bubbles are indeed filled with helium, as expected.

The T loading study highlighted that increasing the He fluence leads to higher T inventory. Also, for a given fluence, increasing the He flux reduces the T trapping: for the same 800ºC and $3x10^{23}$ m^{-2} He exposure, retention is almost twice higher for the $3x10^{20}$ $s^{-1}.m^{-2}$ case compared to the $2x10^{22}$ $s^{-1}.m^{-2}$ one, suggesting a diffusion-like process. At fixed He flux and fluence, a temperature increases from 200 to 750 °C consistently increases the T trapping sites present in the W sample.

It is important to point out that PAS results exhibit similar trends: when He flux increases, a thinner surface layer is impacted by traps creation; when He fluence increases, the free volume of defects increases and the latter are located deeper; and as temperature increases from 200 to 750°C, the free volume of defects increases and extends to a deeper portion of the sample. Therefore, traps for positrons and for tritium created by He irradiation both increase when one of those three parameters (the irradiation time, He fluence and temperature) increase, pointing out a probable diffusion-like process for He damaging impact in W.

Deuterium retention in tungsten damaged by mechanical work, electrons, and fast ions

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Hydrogen isotopes are trapped in lattice defects (dislocations, vacancies, vacancy cluster, …) in tungsten. Irradiation by neutrons or fast ions results in the formation of many different types of defects: This renders the interpretation of these results difficult. For a fundamental understanding of the interaction of hydrogen isotopes with various kinds of defects samples containing one dominant defect type are highly wishful.

Dislocations were introduced into recrystallized tungsten (recrystallized at 1873 K for 1 hour in vacuum) by tensile deformation at temperatures above the ductile-to-brittle transition temperature (DBTT) at temperatures of 573 K and 873 K to strains from 3% to 39%. The dislocation density was measured using transmission electron microscopy (TEM) and increases with increasing strain level. Positron annihilation Doppler broadening spectroscopy (DBS) shows an almost linear correlation of *W* vs. *S* with the amount of plastic deformation: The nature of positron-trapping defects, therefore, does not change with increasing deformation level. Higher deformation levels lead to higher concentrations of positron-trapping defects. Samples loaded with D at 370 K to a fluence of 2.4×10^{25} D/m^2 from a low-temperature plasma showed blistering. Increasing deformation levels resulted in an increase of the number density of blister-like structures, the D depth profiles and TDS spectra were probably affected by the presence of the blisters. Plasma exposure at 450 K did not lead to the formation of blisters. The trapped D concentration was below 40 ppm, i.e. dislocations have only a small influence on D retention at 450 K

Mainly single vacancies were created by irradiation of W (100) single crystals with 200 keV protons and 4.5 MeV electrons to low damage levels (below 10^{-3} dpa_{KP}) at 295 K. The damaged samples were post-annealed in vacuum for 15 min at temperatures in the range of 550-1800 K for studying the annealing and clustering behavior of single vacancies using positron annihilation lifetime spectroscopy (PALS) and DBS. At temperatures above 600 K vacancies become mobile and start to agglomerate in clusters. Annealing at temperatures above 1300 K results in partial annealing of vacancy clusters, complete recovery of the defects is observed after annealing at 1800 K.

Tungsten was damaged with different ion species (D, He, Si, Fe, Cu, W) at energies between 0.3 and 20 MeV to 0.04 dpa_{KP}[1] and 0.5 dpa_{KP} in the damage peak maximum. The energies were chosen to get similar damage ranges up to 2 µm. For the small dpa level comparable D concentrations are observed in the damaged range for all heavy ion species using nuclear reaction analysis (NRA), the TDS spectra are also comparable. At the high dpa level identical D concentrations and identical TDS

[1] All dpa values were calculated using the SRIM Kinchin-Pease (KP) model with displacement energy of 90 eV.

spectra are observed for all heavy ions, only He-damaged sample shows a somewhat different behavior.

Damage rate dependence is not observed at 0.23 dpa from $5x10^{-6}$ to $5x10^{-3}$ dpa_{KP}/s average damage dose rate (corresponding to 1 – $6x10^{-3}$ dpa_{KP}/s peak damaging dose rate).

Quantitative characteristics of H and He interaction with radiation defects in tungsten

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Hydrogen accumulation in the bulk of W is very sensitive to presence of radiation defects. Therefore, knowledge of trapping sites parameters is essential for predicting H isotope transport and retention in W plasma-facing components.

It was shown that rough estimations of the detrapping energy from vacancies and vacancy clusters can be done using a simple "adsorption model" (see details in [1]). More precise numbers have been derived from thermal desorption experiments with different heating rates after keV ion irradiation. (for a single vacancy - E_{dt} = 1.56 eV [2] and for vacancy clusters - $E_{dt} = 2.1$ eV [3]).

The results have been compared with the data derived from ion-driven permeation experiments and from TDS experiments with tungsten damaged by MeV heavy ions and neutrons. In spite of possible significant differences in defect microstructure produced by different species, hydrogen detrapping energies were found to be in the range from 1.4-2.2 eV.

Helium desorption from radiation damaged tungsten has been also analyzed by means of thermal desorption spectroscopy. It was shown, that in the case of irradiation by MeV particles, helium can stay in tungsten above 2500 K. He desorption temperature decreased in the case of smaller He implantation range and smaller concentration of defects. This is explained by a high detrapping energy from radiation defects and effective re-trapping process on the way to the surface.

In the case of high fluence irradiation by low energy ions, a part of implanted He can release at very low temperatures, starting almost from room temperature. Low temperature release was observed even in the case of exposure at 1300 C. This is different from H desorption behaviour, where desorption usually started above irradiation temperature.

[1] O.V. Ogorodnikova. JAP 118 (2015) 074902.
[2] M.Zibrov et al., JNM, 477 (2016) 292.
[3] S.Ryabtsev et al., NIMB, 382 (2016) 101.

Current Status of Study on Damage Structure Evolution of Neutron Irradiated Tungsten and Its Alloys

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To construct a database of Tritium behaviour of irradiated Tungsten(W), data collection and integration of neutron irradiated tungsten materials are required. Material response by irradiation depends on irradiation conditions and microstructure of the examined specimen introduced by its fabrication process. In the case of neutron irradiation, neutron energy spectrum, fluence (number/m2) and its dose rate (number /m2/s) are required parameters to quantify the amount of produced displacement damage and transmutation elements by the neutron irradiation. Temperature, irradiation period and environments such as vacuum, inert gas or liquid sodium are also important parameters to understand the irradiation response of the examined material. Considering about point defect behaviour, defect sinks such as dislocation, sub-boundary, grain boundary, surface, precipitates are required parameters to understand material response of mechanical properties, size stability (volumetric change), corrosion, erosion and hydrogen retention.

Neutron irradiation and ion-beam irradiation to W and W alloys have been conducting by many researchers but the data is not much as other nuclear materials such as stainless steels and ferritic steels. To construct the irradiated W database, overview of microstructural development of neutron irradiated W was conducted based on the previously obtained data in fission reactors. It is well known that Rhenium(Re) is a major transmutation element of W due to its (n, γ) reactions in fission reactors. The Re effect on microstructural evolution in W was also summarized based on microstructural observation by TEM. Mechanism of the Re effects was also studied by computer simulation. Current status of the effects of Re and Osmium(Os) on defects migration in W were presented.

New neutron irradiation experiments in a fission reactor was planned under the Japan-USA joint project PHENIX(2013-2018). The reactor irradiation was carried out in 2016. Brief summary of the irradiation and post irradiation experiments were introduced.

Irradiation level (dpa) of current fission reactor data is lower than that of fusion power reactors. In order to extrapolate the data of lower dpa region to higher dpa region, W-self ion irradiation experiments were also conducted. Microstructural observation and hardening behaviour were examined. Some results of the accelerator irradiation works were introduced and subjects of the data correlation between the accelerator irradiation and neutron irradiation was presented.

Hydrogen retention in self-damaged and He-irradiated tungsten for PFC - update on the recent results

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On the way to understand the recycling and HI retention in plasma facing materials at particle fluxes up to 10^{24} $s^{-1}m^{-2}$ we need to understand the basic processes such as transport in a material with lattice defects, the effect of interstitial impurity atoms on defect evolution and the role of surface on HI uptake and release. Lattice defects act as trapping sites for HIs with high de-trapping energy as compared to the energy of diffusion between solute interstitial sites. For this purpose benchmark experiments are needed where D atoms are only a tool to detect and pin down the nature of defects:

their de-trapping energy for HI and evolution with sample temperature with and without presence of HI.

For this purpose we used the specific installation of JSI laboratory where samples are exposed to low energy (0.3 eV) HI atoms with typical fluxes of $5x10^{18}$ - $3x0^{19}$ at.$m^{-2}s^{-1}$, that populate the traps induced by 20 MeV W ion irradiation. In contrast to ion or plasma exposures with high flux density this does not create any additional damage or lattice stress. Moreover, the ability of performing studies *in-situ* by ion beam methods, i.e. measuring D depth profile during a specific study, minimizes the ambiguities that might occur with sample change or transfer through air. We have presented recent advances on the field of *in-situ* studies on the dynamics of HI retention and transport, isotope exchange and D outgassing in self-damaged W [1]. By the help of rate equation models these experiments [1,2] enabled us to pin down the nature of traps and detrapping energies [3,4], parameters for the surface processes and energy barrier for inward diffusion [4]. In order to further study the influence of energy barrier for D atom inward diffusion additional benchmark experiments where performed as a function of loading temperature and grain size distribution. Namely, recrystallized self-damaged W samples were loaded at different temperatures from 450 K to 600 K by D atom beam [5] or samples with different grain size distribution were D loaded at the same temperature (600 K). The studies showed that there are difference between loading by D atoms with thermal energy of 0.3 eV and plasma loading with ion energy of <5 eV. The studies will help us to explain the differences between low energy atom loading versus few (ten) eV ion/plasma exposure and set the basis to predict the influence of neutrals on HI retention at orders of magnitude higher fluxes as well as in remote areas in future fusion applications. A major step forward in *in situ* studies was performed with simultaneous W ion irradiation and D loading which was performed for the first time and the effect of presence of D on evolution of lattice defects was studied [6]. Simultaneous exposures were compared with sequential ones such as W irradiation and post defect annealing and W irradiation at elevated temperature. As a result synergistic effects have been identified [6]. The effect of He as an analysing beam and its influence on HI retention and transport was also presented where accumulation of deuterium around helium was observed [7].

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[2] A. Založnik et al. Phys. Scr. T167, 014031 (2016).
[3] O. V. Ogorodnikova et al. J. Appl. Phys. 119, 054901(2016).
[4] E. Hodille et al., Nucl. Fusion. 57, 056002 (2017)
[5] A. Založnik et al. Submitted to JNM
[6] S. Markelj et al. Nucl. Mater. Energy (2017) in press.
[7] S. Markelj et al. Nucl. Fusion letters 57, 064002 (2017)

Deuterium plasma effect on tungsten irradiated with high-energy ions

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Radiation damage induced in PFMs by 14 MeV-neutrons during long operation of D-T fusion reactor is supposed to be relevant to high levels and is estimated from 1 to a few tens *dpa*. The recent results of experimental investigation of plasma effect on damaged tungsten undertaken at Kurchatov Institute a few years ago are presented.

Experimental procedure includes two stages. At the first stage, the damage was produced by fast ions accelerated on the cyclotron at Kurchatov Institute (1-60 MeV) to simulate neutron radiation effect. The experiments were conducted on tungsten W (99.95% wt.) (Russian grade) and W Plansee - ITER candidate grade. The ion species used in these experiments to produce damage were fast helium ions He^{2+} accelerated to 3.5-4.5 MeV, carbon ions C^{3+} at energy of 10 MeV at fluences of 10^{21}-$3\cdot10^{22}$ ion/m^2 and protons of 3.7 MeV in average, 10^{22} m^{-2}. The primary damage in a few micron surface layer of the material fell into the interval from 0.1 to several tens *dpa* thus covering the whole range supposed to be of interest for fusion research. Analysis of the resulting radiation damage was performed by calculation (SRIM) providing primary defect profiles in the surface layer in dependence on irradiation dose and ion energy. Swelling effect was observed on irradiated tungsten by surface profiling on irradiated samples. Profilometry has shown 0.1-2 % swelling for C-irradiated tungsten and 2-3 % for He-irradiated material.

The irradiated samples were then subjected to steady-state deuterium plasma on the LENTA linear plasma divertor simulator. The plasma ion energy on the surface chosen to obtain erosion condition (250 eV) and relevant to divertor plasma condition in tokamak. The loss of material by sputtering was detected from the tungsten surface, the surface microstructure suffered important modification as it has been shown by surface analysis. The plasma processing of the damaged samples was performed in an exposure sequence: multiple exposures resulted in the surface progress to depth finally reaching the depth of the fast ion range. D-ion fluence of 10^{25}-10^{26} ion/m^2 was collected on the W surface. Erosion yield of the damaged tungsten was evaluated at Yd-w $\cong (2\text{-}4)\cdot10^{-3}$ at/ion. No correlation of damage and erosion rate was found so far for the ITER relevant levels.

Surface microstructure modification was observed by Scanning Electron Microscopy technique and comparative analysis was made with unirradiated material.

Gas uptake in the ion-irradiated and plasma exposed tungsten was measured by nuclear methods and by **TDS** spectroscopy. **E**lastic **R**ecoil **D**etection **A**nalysis was applied to measure concentration of the trapped deuterium and hydrogen content. Increased content of the retained deuterium (1.8-20%) was found in the surface layer of irradiated tungsten (100-150 nm deep) Significant D uptake was found in He-irradiated tungsten at the ion range depth ($2\cdot10^{21}$ D/m^2)

The implanted Helium concentration accumulation in tungsten to depth of ~6 micron was found by **R**utherford **B**ack**S**cattering and that was compared with the calculated He distribution profiles.

The experiments performed as well as the results obtained to date showed the high potential of the developed approach in the research of PFMs as to their service life and tritium hazardous effects in a fusion reactor.

Deuterium behavior in HFIR neutron- irradiated tungsten under US-Japan PHENIX program

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The recent progress on deuterium retention in HFIR neutron-irradiated single crystal tungsten was presented. The (100) single crystal tungsten (SCW) samples (4x4x0.5 mm^3) were irradiated at High

Flux Isotope Reactors at Oak Ridge National Laboratory to neutron dose of 0.1 dpa ($0.5x10^{25}$ n/m^2, E_n>0.1 MeV) at three-different temperature (360, 690, and 760 ^{o}C).

The neutron-irradiated tungsten samples were exposed to high flux deuterium plasma at Tritium Plasma Experiment at Idaho National Laboratory to deuterium ion fluence of $5x10^{25}$ m^{-2} at the temperature similar to neutron-irradiation temperature (400, 600, and 700 ^{o}C). Two samples were exposed to similar plasma conditions for thermal desorption spectroscopy (TDS) and nuclear reaction analysis (NRA) measurement. The results shows enhanced D retention in SCW, indicating deep migration.

The modeling by the INL's Tritium Migration Analysis Program (TMAP) confirms the deep migration and agrees well with experimental TDS spectrum. The TMAP simulated the TDS spectra and D retention for extremely high ion fluences for DEMO application.

The update on the status of TPE upgrade, TMAP integration MELCOR code, and PHENIX project was reported. The unique neutron-irradiation under PHENIX will provide valuable samples and database for this CRP, and the initial results will be obtained in the spring of 2018.

Update on deuterium behaviors in neutron-irradiated tungsten"Summary of presentation

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In the beginning, the history of neutron-irradiation studies on hydrogen isotope retention in tungsten (W) was reviewed. The main activities were initiated in Japan-US collaboration project TITAN (2007–2012), in which significant increase in hydrogen isotope retention in W after neutron irradiation was confirmed using samples irradiated at relatively low temperature (> 100 ºC). The activities have been continued in Japan-US collaboration project PHENIX (2013–2018) and collaboration program of International Research Center for Nuclear Materials Science, Institute for Materials Research (IMR-Oarai), Tohoku University. In these programs, hydrogen isotope retention in tungsten and tungsten alloys is examined after neutron-irradiation at elevated temperatures.

Recent results were reported on the IMR-Oarai collaboration program for plasma-surface interaction studies. In this program, tungsten specimens irradiated in High Flux Isotope Reactor (HFIR), Oak Ridge National Laboratory at 300 ^{O}C, and those irradiated in Belgium Reactor 2 at 290 ^{O}C were exposed to D_2 gas in quartz capsules or D plasma in the linear plasma device called Compact Divertor Plasma Simulator (C-DPS). Characterization of vacancy-type defects was performed using positron annihilation spectroscopy before and after D loading. The main messages derived from the experiments were as follows:

- ✓ Neutron irradiation induces vacancy and vacancy clusters in various sizes, and those act as strong trap sites with detrapping energy of 1.8–2 eV.
- ✓ Penetration depth of D was proportional to square root of plasma exposure time.

- ✓ Re significantly reduces trap concentration at irradiation temperatures ≥ 500 ^{O}C. Post-irradiation annealing did not provide similar effects. Dynamic processes under high temperature irradiation play key-roles.

- ✓ High temperature neutron irradiation (800 and 1100 ^{O}C) of W-Re alloy in HFIR has been completed in PHENIX Project. Specimens are waiting PIE.

It was also reported that neutron irradiation under H_2 gas atmosphere (400 ^{O}C, 0.1 dpa) is in progress under the framework of IMR-Oarai–ORNL collaboration to understand effects of hydrogen on microstructure development under irradiation.

Progress of W-relevant plasma-material interaction studies at ASIPP

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1. D retention studies have been done for high energy Ne/He ion irradiated W by gas absorption, plasma exposure and thermal desorption spectroscopy.

- The ^{20}Ne ion (122 MeV) irradiation was performed at HIRFL, with an energy degrader to produce a quasi-homogeneous distribution of atomic displacement damage to 0.16 dpa within a depth of 50 μm. Results of PAS indicated the formation of intermediate-sized vacancy clusters (~12 vacancies) in the irradiated W. Thermal desorption spectra for the D_2 gas exposed samples showed a broad D desorption temperature range (730-1173 K) with a high release peak at ~1010 K for the irradiated W, and the amounts of D retained in the irradiated W were significantly larger than the un-damaged ones. Further TEM characterization showed a large amount of voids with a diameter of ~1 nm in the irradiated W.

- W was pre-damaged by 80keV He^+ to peak dpas of 0.054, 0.54 and 5.4. The irradiated samples were then exposed to EAST D plasma for ~2000 s. The electron density and temperature were ~1×10^{18} m^{-3} and 5-10 eV, respectively. TDS results showed that the retained amount of D in irradiated W increased with the increase of irradiation fluence and no sight of retention saturation can be found.

2. D permeation has also been studied with the newly built gas-driven permeation (GDP) and plasma-driven permeation (PDP) setups at ASIPP.

- Effects of intrinsic defects (mainly dislocations), irradiation defects (e.g. voids) and second phase additions on D permeation behavior were systematically investigated with GDP at 730-1000 K, using various W materials, including rolled/annealed/recrystallized W, heavy-ion (Au^{3+}) irradiated W and ZrC/La_2O_3-dispersion strengthened W. Results showed that the permeability of D was not sensitive to the intrinsic defects, irradiation defects or ZrC/La_2O_3 phases in W. The diffusivity of D, however, was microstructure dependent.

- Preliminary PDP study of D through W has also been performed within a temperature of 690-770 K. With a new sealing stage adapted from GDP facility, further study on H isotopes PDP behavior through W will be carried out soon.

3. New facilities are under development to support further W-relevant PWI research at ASIPP.

- In EAST tokamak, a multichannel spectroscopy system with 22 lines-of-sight (LOS) in outer divertor and 17 LOSs in inner divertor has been built. A poloidal resolution of 13 mm on the surface has been achieved.

- To understand the hydrogen isotopes behavior in W, a new linear plasma device, Permeation and Retention Evaluation FACility for fusion Experiments (PREFACE), has been constructed at ASIPP. The typical electron temperature and density are T_e = 2-6 eV and $n_e = 10^{16}$-10^{17} m^{-3}, respectively.

- Another new linear facility: HPPX (Helicon Physics Prototype eXperiment) has been built at ASIPP to achieve divertor-relevant plasma parameters in a laboratory environment and to conduct W-relevant PWI studies. The total plasma heating power is ~150kW and a steady-state electron density of >$1x10^{19}$ m^{-3} is expected.

Deuterium retention in tungsten irradiated by heavy ions

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Deuterium retention in tungsten (W) samples irradiated by 2.4 MeV Cu2+ ions has been investigated to study effects of the damage on hydrogen isotope retention in W. TEM observation revealed that most of the dislocation loops (ILs) were nucleated by cascade collisions and additional loops were formed in the vicinity of pre-existing dislocation loops and dislocations and aligned to coalesce with each other. Nano-voids (d<1nm) are also observed in 1 dpa case and they formed densely.

Recrystallized W samples irradiated by 2.4 MeVCu2+ ions were exposed to high flux and low energy D plasma in APSEDAS and then D retention in the sample was evaluated by thermal desorption spectroscopy (TDS). There exists three desorption peaks in the TDS spectra. The desorption peak around 850 K newly appeared due to Cu2+ ions irradiation. This peak must be related to voids. TDS spectrum was reproduced by using the HIDT code using experimental data. The binding energies of three desorption peaks are 0.83 eV, 1.22 eV and 1.46 eV.

When the Cu^{2+} ion flux decreased by 5 times, D retention decreased by 3.5 times, indicating clear flux dependence. In the case of higher ion flux, D retention increased with the damage level but it saturated around 0.4 dpa, suggesting that newly introduced defects may be cancelled by already existing vacancies and voids with high density. In the case of low flux irradiation, on the other hand, D retention increased with the damage level up to 2 dpa and no saturation was observed. As for dependence of D retention on sample temperature during Cu^{2+} irradiation, D retention in W sample that had been irradiated at higher temperature became lower. It is necessary to know effects of the number of defects and their size on D retention.

Behavior of tungsten under thermal and plasma exposure and development of advanced tungsten materials

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The thermal fatigue performance of metallic materials and full components is one of the major concerns for any application, which exposes materials/components to repetitive high thermal loads. Tungsten as a plasma facing material (PFM) for future power reactors has to withstand severe environmental conditions especially in terms of stationary and transient heat loads. For the qualification but also for subsequent lifetime analyses of tungsten candidate materials and components for an application as PFM in the divertor region, standardized testing procedures were established to characterize the thermal shock and fatigue performance.

Mechanical strength was found to be the main influencing factor for the formation and evolution of damage. Especially, recrystallization and melting/solidification will make the material more prone to thermal shock and fatigue, accelerating the evolution of damages. The combination of different material modifications/damages accompanied by the degradation of mechanical properties will have a strong impact on the plasma performance and lifetime of plasma facing materials/components. Based on the performed tests, damage mappings were prepared. This enabled us to determine damage and cracking thresholds for all materials and it became obvious that high pulse number test are indispensable to estimate the impact of thermal shock damages on the long-term operation of future power reactors and allow determining the high cycle fatigue of materials. Furthermore, the interaction between the damage behavior/response and the material properties is essential for new material developments and design improvements of plasma facing components

The lifetime of the divertor and plasma facing components is also determined by synergistic effects of the highest thermal and particle flux densities as well as neutron induced material damages. The linear plasma device PSI-2, located at the Forschungszentrum Jülich, was utilized to perform experiments combining transient thermal loads with deuterium and helium plasma particle exposure to investigate the influence of “Edge Localized Modes (ELMs)” on tungsten.

The results showed – in dependence on the microstructure and grain orientation of the material – even after 1000 transient heat pulses, a drop of the damage threshold for the combination of thermal and plasma loading in contrast to pure thermal loading. This outcome was related to the embrittlement of the material due to hydrogen absorption/implantation. The retention of hydrogen in tungsten for a combined thermal and plasma exposure is significant larger (up to a factor of 10) in comparison to plasma loading with the same particle fluence but no transient thermal loading. A higher uptake at thermal shock induced defects as well as a higher mobility of hydrogen along induced cracks in conjunction with the higher thermal gradients present during the combined exposure could contribute to the observed effect.

Ion-Irradiation of Tungsten: Modeling & Experiments

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<u>Modelling</u>

MD simulations have been carried out to study the cascade and the defect structuring for both low and high energy tungsten PKA using EAM type interatomic potentials coded in ParCas code. Single crystal bcc tungsten lattice was created up to 7 million atoms and relaxation at 300 K was carried out using temperature and pressure control using Berendsen thermostat. Periodic boundary conditions were used to simulate the lattice and a tungsten PKA atom of desired energy has been initialized at the middle of the simulation cell.

Interstitial and vacancy clustering has been observed during the 'cooling down' phase of the thermal spike generated due to the cascade. The size of the clusters increases with the PKA energy and at energies below 30 keV, smaller defect clusters are formed did not lead to the formation of ordered clustering or dislocations. However, above 30 keV PKA energy, the ordered clustering of interstitials was observed even in single bombardment events which appeared to form dislocations while dislocation analysis was carried out using ovito. Interstitial atoms clustered at the cooler end of the cascade whereas vacancies were observed at the core of the cascade. The cooling down of the cascade shows 3 distinct time-scales. The fraction of single-vacancy and interstitial reduces with PKA energy and the consequently the cluster size increases. At 1-4 keV almost all vacancies and interstitials were single, whereas at 100 keV only 58 % of the total interstitials were of isolated ones.

At energies above 150 keV, the cascades were found to split into sub-cascades originating from the secondary knock-on atoms of the initial cascade. At 375 keV, we have seen 3 distinct sub-cascades and associated thermal spikes. The number of surviving Frenkel pairs at the end of the cascade were found to scale linearly with the PKA energy. The thermal spike volume, which is calculated from the physical extent of thermal spike at its peak, was also found to scale linearly with the PKA energy. The dynamics of clustering of interstitials and subsequent dislocation analysis show that there were both ½ <111> and <100> type dislocations, with roughly 90 % of the studied ones, were of ½ <111> type. We have also observed dislocation reactions of ½ [1-11] and ½ [11-1] type leading to [100]. The analysis was done 100 ps after PKA initiation and we have not observed any vacancy dislocation formation during this time scale.

MD simulations were also carried out with electronic loss by assuming a fraction of the energy of moving atoms in the lattice is absorbed by the electrons in the lattice which is modelled using a frictional loss term in the equation of motion. A cut-off energy for the loss implemented in ParCas code was used in such a way that any atoms moving below this energy cannot contribute to the electronic energy loss. It has been observed that cascade structure and the subsequent defect structure depends on the electronic loss energy.

Surface cascades have been carried out to study the effect of free surfaces in collision cascade and defect structure. Two distinct types of cascades and defect structures were observed with cascades with free surface. A large number of cascades (50 out of 71 trials) showed a PKA dissipating its energy all throughout its range with small multiple cascades and defect-clustering and dislocations were formed at the end of the trajectory far below (~20-25 nm) the surface. In another set of cascades, the PKA dissipated its energy in a thermal-spike in the near-surface region forming distinctly separated interstitial and vacancy clusters. The interstitial atoms moved to the free surface and formed ordered structures on the top surface.

Experiments

Ion-irradiation experiments have been carried out to study the defect formation for different ion-energy and ion-mass on 100 µm-thick tungsten foils recrystallized (99.96 % pure, procured from Princeton scientific corp. USA) at 1838 K under 10^{-3} mbar pressure in Ar+H2 environment. From XRD analysis, it was found that after recrystallization the average crystallite size was more than 700 nm and SEM analysis shows that the average grain size is about 35 µm. The residual-resistivity-ratio of the samples increased from 11 to 163 after recrystallization, indicating the annealing of defects. Positron life-time measurements show a bulk life-time of 107 ps with 70 % intensity indicating a nearly defect free-samples with vacancy-clusters (corresponding life-time of 237 ps). TEM has also shown that the average grain-size has increased with nearly defect-free grains. The average dislocation density was found to be 3.6×10^{8} cm^{-2}.

The recrystallized foils were bombarded with 80 MeV Au^{7+} ions for a fluence of 1.3×10^{14} cm^{-2}. The implantation profile of the gold was measured using SIMS and found to have a mean range of 4.06 ± 0.5 µm which is in agreement with the projected range from SRIM simulations (4.49 ± 0.73 µm). The positron Doppler broadening measurements showed a saturation of S-parameter (showing annihilation from valance electrons from the lattice) within the positron-beam penetration range of 500 nm. The positron life-time measurements indicated three lifetimes, one corresponds to the tungsten bulk life-time (t1 = 107 ps) with an intensity of 18 % (reduced from 70 % of un-irradiated sample), second measurement of 154 ps and the third of 260 ps with 41 % and 37 % intensity respectively, which might correspond to dislocations as well as vacancy clusters. TEM micrographs shows enlarged dislocations with length varied between 0.4 µm to 3 µm. The dislocation density of the sample is reduced to 2.9×10^{8} cm^{-2} within the observational depth of 200 nm. TEM micrographs taken at 2 µm depth from the top-surface (near the peak of damage zone) has also shown long dislocation lines with similar lengths as found near the surface region. No dislocation-loops were observed either in the surface region or in the bulk. The dislocation density at the bulk was about 6.1×10^{8} cm^{-2}.

The recrystallized foils were also bombarded with low mass boron (B^{3+}) ions of 10 MeV for two different fluence values: 1.3 x 10 14 cm^{-2} and 1×10^{15} cm^{-2}. The 10-MeV boron-ions have a similar penetration range (4.1 ± 0.3 µm) as of 80-MeV Au. The point defect analysis using positron beam and bulk life-time showed that defects are created due to bombardment and showed an increase in the S-parameter with the ion-dose. The TEM micrographs showed different type of dislocations: (1) dislocation lines with size varying between 50 nm – 900 nm and (2) loops with diameter varying from 35 nm to 80 nm. The average dislocation density was found to be 7.9×10^{8} cm^{-2} which is higher than that of gold-irradiated sample as well as recrystallized foil.

Low-energy, low-mass implantation experiments were carried out using 100 keV deuterium as well as 250 keV helium ions. The defect depth profile measured using positron DB studies indicated a broad peak between 100 nm – 300 nm deep into the foil. The deuterium depth profile analyzed using SIMS also showed that the D-concentration was closer to the surface than predicted by SRIM (427 ± 139 nm), a deuterium-peak was observed around 230 nm. The S-W curve obtained from positron-DB measurements also showed a different slope in the annihilation curve, which might be indicating deuterium-rich defects in the beam penetration range. The bubbles observed in SEM images of deuterium irradiated samples also indicate this. TEM images of 100 keV deuterium showed dislocation lines, network of dislocations and loops with dislocation line length ranging from 120 nm to 1900 nm and loop diameter within a range of 50 to 100 nm. The dislocation density was $9.7x10^8$ cm^{-2}, higher than what is observed in boron and gold irradiated sample. Deuterium bombardment was carried out on Au irradiated sample and the deuterium depth profile was measured using SIMS. It has been observed that the deuterium penetration was found to be deeper into the sample in the case of "Au+D".

On samples that are bombarded with 250 keV He ions, small dislocations are found with line-length varying between 40 nm – 1000 nm. No dislocation-loops were observed and the average dislocation was about $1x10^9 cm^{-2}$ which is the highest observed among any of the irradiated samples. Helium ions were also bombarded on samples that are pre-irradiated with gold. Further deuterium bombardment was carried on those samples and the preliminary SIMS analysis shows that the helium bombardment reduces the deuterium content in "Au+He+D" samples.

Modeling and experimental validation of Hydrogen behaviour in tungsten for Tokamak

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The main objective of the project is to better understand the behaviour of hydrogen in W submitted to the extreme conditions of a tokamak environment and be able to better quantify the H retention. The H retention in W mainly relies on its trapping and detrapping rate in traps such as grain boundaries, or defects existing in the material. In the tokamak the microstructure of W is expected to evolve severely due to plasma interactions (He, H, heat fluxes) and to neutrons irradiation. In the last 4 years we studied what would be the impact of He plasma and W ions irradiations on recrystallized W. To do that, we associate modeling and experimental validation. Furthermore a new code has been developed to model the H retention in self damaged W.

1. Study of the vacancy-type defects formation in tungsten crystal due to helium accumulation

This study means to observe the first steps of the vacancy-type defects formation in the tungsten crystal subjected to low ion flux of low kinetic energy in order to understand the influence of the accumulation of helium in W. For the experiments, an ICP-RF plasma source was developed and characterized to perform helium implantations under controlled conditions. He implantations were performed under various conditions of fluence, energy and substrate temperature on polycrystalline tungsten samples. Positron annihilation spectroscopy (PAS) was used to characterize vacancy-type defects, nuclear reaction analysis (NRA) to quantify implanted He and thermal desorption mass spectrometry to characterize the interactions of He in the crystal. For implantation with a kinetic energy of 320 eV at room temperature, a saturation of the He implanted quantity is reached for an incident fluence threshold and large vacancy defects starts to form [L. Pentecoste, et al., NIM B 383 (2016) 38–46]. Study of the influences of the kinetic energy of He ions and of the surface temperature shows the importance of the depth distribution and of the mobility of He in the crystal on the size and the diversity of the created defects. Molecular dynamic simulations have been carried out using LAMMPS. The numerical results have been compared to experimental ones in order to get a better understanding of the atomic scale mechanisms [L. Pentecoste, et al., JNM 470 (2016) 44-54]. More recently we show that the He-vacancy complexes distribution depends on the He flux [E Bernard et al, PFMC 2017 (CEA IRFM)].

2. Study of damage induced in W by W ions irradiations.

Neutrons irradiations induced predominantly transmutation and nuclear collisions in materials. M Gilbert et al [M.R. Gilbert et al, Nucl. Mat.& Ener. 9 (2016) 576] showed that the predominant recoils in a tokamak are W atoms with a large energy distribution up to 1 MeV and a fraction of less than 1% of PKA with energy higher than 300keV. To try to approach the characteristics of the damage induced by neutrons irradiation we performed W ions irradiations using different conditions (energy, flux, fluence and temperature). We use PAS and TEM to characterize the induced damage. The main conclusions can be drawn. V-clusters and dislocation loops are observed even for irradiations performed at low dpa and temperature. When the irradiation temperature increases from -185°C to 700°C, the V-cluster size increases from 0.5 to 1.4 nm and their densities remain in the range of a few 10^{23} m^{-3} and the $\frac{1}{2}$<111> loops becomes predominant with respect to the <100> loops. In samples irradiated with damage dose of 0.02 dpa and at temperatures of 700°C the V-Clusters/ $\frac{1}{2}$<111> loops densities ratio is ~ 10. Number and size of V-clusters observed by TEM increases with annealing temperature in the range from room temperature to 700°C due to their growth. A large increase of the V-clusters size and decrease of their density is observed when temperature increases from 1100°C to 1500°C.

3. Simulations of atomic deuterium exposure in self-damaged tungsten

A new code called MHIMS (Migration of Hydrogen Isotopes in MaterialS) has been implemented to describe the interaction of D in W. It has been parametrized and used to simulate TDS spectra and implantation depth profiles obtained in W after D atom exposure at 500 K and isothermal desorption at 600 K after D atom exposure at 600 K. These data can be reproduced quantitatively with three bulk-detrapping energies, namely E_{t1}=1.65±0.01 eV, E_{t2}=1.85±0.03 eV and E_{t3}=2.06±0.04 eV, in addition to the intrinsic detrapping energies known for undamaged tungsten (0.85 eV and 1.00 eV). Thanks to analyses of the amount of traps during annealing at different temperatures and *ab initio* calculations, the 1.65 eV detrapping energy is attributed to jogged dislocations and the 1.85 eV detrapping energy is attributed to dislocation loops. Finally, the 2.06 eV detrapping energy is attributed to D trapping in cavities based on literature reporting observations [E.A. Hodille *et al*, Nucl. Fusion **57** (2017) 056002].

Non-local real-space diffusion-driven models for microstructural evolution of irradiated tungsten

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The presentation described recent progress in the development of models for microstructural evolution of materials, and in particular tungsten, occurring under bombardment by energetic ions or neutrons.

The first part of the presentation is focused on the treatment of production of irradiation defects in cascades. It has been known since the early 1990s that defects in cascades form clusters, but until relatively recently the statistical laws of clustering had not been established. Work by Andrea Sand and colleagues published in EPL **103** (2013) 46003 showed that the distribution of defects produced in cascades as a function of defect size follows a power law with a characteristic exponent close to 1.6. This finding has now been confirmed experimentally by X. Yi et al., EPL, **110** (2015) 36001. More recent, and yet unpublished, calculations appear to confirm that the power law of defect clustering applies to a broad variety of materials, and not just tungsten.

Since the broad methodology of cascade simulations is now relatively well established, the personal view of the first author (S L Dudarev) is that it is essential to focus on the topic that has so far proved elusive, namely the treatment of thermal evolution of defect configurations formed in cascades. This is a difficult and highly challenging issue, where it is necessary to explore the link between the discrete microscopic defects, and the notion of macroscopic dislocations. First significant steps in the mathematical treatment of these phenomena have just been made, particularly those involving the treatment of diffusion-mediated evolution of dislocations and vacancy-type objects. For the latter case, it appears critical to use a new method, based on the application of Green’s theorem, which makes it possible to treat dislocation climb and evolution of ensembles of voids on equal footing.

Finally, the presentation describes recent work on vacancy-mediated clustering of rhenium in tungsten occurring under irradiation. The work explains the fundamental origin of clustering as resulting from many-body collective interaction between vacancies and rhenium in the tungsten matrix.

Interstitial-mediated diffusion and aggregation mechanism for 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 [1]. Re and Os will precipitate under irradiation, and form new Re/Os-rich phase, which has significant effect on the microstructure and mechanical properties of materials. However, the formation mechanism of Re and Os precipitates phase 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 and thermodynamic models. It is 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, and form W-Re/Os complex dumbbell. The diffusion energy barrier of W-Re/Os is much lower than that of Re/Os diffusing via mono-vacancy or even vacancy clusters. Further, the

W-Re/Os can be easily trapped by the substitutional Re/Os atoms, and form high stable Re-Re/Os-Os dumbbell structure. Most importantly, 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 for the irradiation-induced Re/Os clustering in W [2].

[1] M. R. Gilbert and J. -Ch. Sublet, *Nucl. Fusion* **51**, 043005 (2011).
[2] Yu-Hao Li, Hong-Bo Zhou, Shuo Jin, Ying Zhang, Huiqiu Deng and Guang-Hong Lu, *Nucl. Fusion* **57**, 046006 (2017).

Modeling of tritium trapping effects of vacancy, grain boundaries and vacancy clusters

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In this CRP, we have been performing multi-scale modeling aiming to establish a computational method/code to simulate the tritium behavior in irradiated tungsten which contains radiation defects. For this aim, we made a plan to work on the following 3 subjects at the beginning of this project: (1) to construct a high-quality potential model for W-H systems to simulate behaviors of tritium and defects in W, (2) to establish kinetic models relevant with tritium behaviors in damaged W, and (3) to develop a code to simulate tritium release/pile-up behaviors in damaged W. In the 3rd RCM held in June, 2017, we presented the progress for each subject

For (1), we have developed an embedded-atom method (EAM) potential for W-H systems. The potential model was constructed by fitting to energies, forces, and stresses obtained by quantum mechanical calculations based on the density functional theory (DFT). These data were acquired over 70,000 configurations including perfect bcc-W crystals, deformed crystals, defective crystals containing self-interstitial atom (SIA), vacancy or vacancy clusters, surfaces models, and those with hydrogen atoms. In the potential model construction process, we put a large weight on the reproductivity of V-H interaction energies. And we gave up reproducing hydrogen solution energy, which means the developed potential model does not work appropriately in systems where H_2 molecules may be formed. Although the developed potential model has this limitation, it can better reproduce V-H interaction energies of DFT calculations than other potential models previously reported. Using the developed potential model, we calculated H binding energy to vacancy clusters (up to a large cluster like V_{137}) as a function of the number of trapped H atoms and the size of vacancy cluster.

For (2), we have developed kinetic/thermodynamic models for effects of vacancy [1], grain boundary (GB) [2] and vacancy clusters on hydrogen solution and diffusion behaviors. For each model, we referred to DFT calculation results and/or molecular dynamics (MD) calculation results in the model construction step and in the determination step of kinetic/thermodynamic parameters such as defect-hydrogen interaction energy and activation energy for trapping/detrapping processes. For a vacancy, the interaction with hydrogen is relatively simple and the constructed model gives good agreement with available experimental results [2]. For GBs, the interaction with hydrogen is intrinsically more complicated and thus we introduced a large assumption in the model. Specifically, we assumed that there are sole interaction energy and sole activation energy for trapping/detrapping processes in GB-hydrogen interactions although these energies should have a larger variety depending on the structure of GB. In spite of this approximation, the present model can reasonably reproduce previous experimental results on diffusivity, solubility and permeability of hydrogen in bcc-W [2]. For vacancy clusters, we constructed a model based on results of MD calculations performed with the developed W-H potential model. In this model, we can estimate how the capacity and the strength of hydrogen trapping by vacancy are changed by clustering of vacancies. The model can treat vacancy clusters of a wide range of size and nicely reproduces the MD calculation results.

For (3), we have recently started to construct a code for this purpose. The code is based on rate theories, where the kinetic/thermodynamic models constructed in the subject (2) are employed. Currently, the code can treat the following processes: hydrogen desorption, hydrogen migration between the surface and the bulk, hydrogen diffusion in the bulk and along GB, and hydrogen-defect interactions for vacancy, vacancy clusters and GB. For a benchmark test, we have gathered experimental data of single-crystal and poly-crystal W specimens, which were first irradiated by 2.8 MeV W^+ ions for radiation defect production, then were exposed to 1 keV D_2^+ irradiation for deuterium implantation, and finally was used as a sample for a thermal desorption experiment for deuterium release. The developed code reproduced some key features of the deuterium release profiles although there are still non-negligible discrepancies quantitatively and qualitatively. One of the important research tasks to improve the accuracy of the code is to clarify the deuterium reflection coefficient when deuterium atoms are densely accumulated in the surface.

This research has been supported by the national research foundation (NRF) of Korea.

Reference

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Across-scale self-healing mechanism for radiation damage in nano-crystal tungsten

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Nano-crystalline metals have been demonstrated to exhibit radiation-resistance. In this presentation, we introduced the across-scale self-healing mechanisms for radiation damage in nano-crystal tungsten. The simulation techniques at different scales e.g., molecular statics, molecular dynamics, and Kinetic Monte Carlo methods were combined to reveal the diffusion, segregation and annihilation near the grain boundary (GB). We found that, the self-healing mechanism depends on several structural and defect properties parameters, e.g. the local density of the GB, the binding energy of the interstitial and vacancy with the GB, the interaction range, the diffusion energy barrier for the interstitial and vacancy in the grain interior and along the GB.

For the interstitial and interstitial cluster of parallel <1 1 1> crowdions, their behavior near the GB, segregation or reflection, is determined by the local GB density. As the density is below a certain value, the corresponding region will reflect interstitials. Otherwise, the region acts a sink for interstitials. The annihilation of bulk vacancies was enhanced due to the reflection of an interstitial-cluster of parallel <1 1 1> crowdions by the GB.

After the interstitial segregates to the local loose GB region, the annihilation mechanism at the GB is determined by the relative value of the interstitial diffusion energy barrier along the GB and that for the bulk vacancy diffusion. As the ratio is below a certain value, the interstitial that segregates to the GB moves along the GB, gets clustered therein, and then annihilates the vacancy via the coupled motion of the cluster along the GB and the motion of the vacancy towards the GB. Otherwise, the

annihilation proceeds via the coupled motion of the interstitial along the GB and the segregation of the vacancy nearby.
Finally, we found the potential well for the interstitial at the GB exhibited a triangle shape and could be approximated by a triangle one. The slop for the triangle potential has a physical meaning of the energy barrier that an interstitial overcomes as migrating over the distance of one Å. The interstitial emission mechanism at a defect sink is determined by the ratio of the interstitial binding energy with the sink to the potential half width. As the ratio is below a certain value, the annihilation could be induced by a direct interstitial emission. Otherwise, the annihilation has to be started by a vacancy-induced interstitial emission.
In the future, we will model the accumulation of radiation defects under continuous irradiation so as to evaluate an impact of the described healing mechanism.

References:

X. Li, et al., Annihilating vacancies via dynamic reflection and emission of interstitials in nano-crystal tungsten, **Nucl. Fusion**, 2017(To be published); On the possibility of universal interstitial emission induced annihilation in metallic nanostructures, **J. Nucl. Mater**. 2017 (under review); **Acta Mater**, 2016, 109: 115-127; Data Brief 2016, 7: 798; **J. Nucl. Mater**., 2014, 444 : 229-236; **J. Nucl. Mater**., 2013, 440: 250-256; **Nucl. Fusion**, 2013, 53: 123014.

Overview of SciDAC-PSI: A multiscale approach to simulating tungsten plasma surface interactions from the boundary plasma to the bulk substrate

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The performance of plasma-facing components (PFC) is one of the main issues facing ITER and future magnetic fusion reactors. Tungsten will be used in ITER as the PFC material and is considered to be one of the primary candidates for future reactors. However, recent experiments that exposed tungsten to He plasma exposure or He ion irradiation with ion energy less than about 100 eV (well below the threshold energy for physical sputtering or Frenkel pair production in tungsten) reveal significant surface modification, including the growth of nanometer-sized “fuzz”, and formation of a layer of nano-bubbles in the near-surface region [1, 2]. It is widely accepted that He atoms in tungsten, like in other metals, are insoluble and tend to form small clusters, which serve as the nucleating event for the formation of larger gas bubbles. It is also clear from atomistic simulations [3, 4] that the processes of trap mutation produce W interstitial atoms that lead to surface morphology modification as the interstitials diffuse to and annihilate at the surface, in addition to plastic flow and dislocation loop punching processes driven by high compressive stresses caused by over-pressurized clusters, or nanometer-sized bubbles, and these processes can alter both the tungsten surface morphology and the He clustering dynamics. Further, it is becoming evident that the nanometer-sized high pressure helium bubbles can trap hydrogen isotopes, although many questions remain to be resolved on the trapping energetics.

One of the challenges with describing these effects for the large-extrapolations in performance required for the PFCs in next-step devices beyond ITER is the large span of spatial and temporal scales of the governing phenomena and, therefore, the theoretical and computational tools that can be used. Fortunately, recent innovations in computational modeling techniques, increasingly powerful high performance and massively parallel computing platforms, and improved analytical experimental characterization tools provide the means to develop self-consistent, experimentally validated models of plasma-materials interactions that govern the performance and degradation of the divertor and PFCs in the fusion energy environment. This presentation will describe the challenges associated with modeling the performance of divertor PFCs in a next-step fusion materials environment, the opportunities to utilize high performance computing and present examples of recent progress to investigate the dramatic surface evolution of tungsten exposed to low-energy He and H plasmas, as well as the coupled He-defect evolutions in bulk structural materials exposed to high-energy He and neutron irradiation before laying out a vision for developing a computational materials modeling framework for fusion materials behavior.

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TDS round robin samples: Motivation, preparation and pre-characterization

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During the second RCM meeting in Seoul it was decided to plan a TDS Round Robin experiment. The basic aim is to compare TDS spectra measured with different TDS set-ups. For this a set of identical reference samples was necessary. IPP Garching volunteered to prepare and pre-characterize these samples and to distribute it to all participants. Initially it was suggested to produce these reference samples by plasma loading but the production of up to 50 samples in this way was considered to be unpractical. As an alternative magnetron sputtering of tungsten thin films on tungsten substrates in argon deuterium atmosphere was chosen following the work of De Temmerman and Doerner (De Temmerman, G., and R.P. Doerner. “Deuterium Retention and Release in Tungsten Co-Deposited Layers.” Journal of Nuclear Materials 389, no. 3 (June 2009): 479–83. doi:10.1016/j.jnucmat.2009.03.028.)

First tests were made in March/April 2016. Final deposition was performed in October 2016. Polycrystalline, hot-rolled W with 99.97 wt.-% purity (Plansee SE Austria) was used as substrate. 44 substrates with the size of $10\times10\times0.8\ mm^3$ were prepared (“standard sample”). Ten “special size” samples were requested by participants (three $10x6mm^2$ in size, four with Ø5 mm, three with Ø6mm). All substrates were prepared from the very same material batch. XRD was applied to identify the (110)-orientation dominated surface. This surface side was mechanically polished to mirror finish and electropolished in 1.5% NaOH. After polishing, substrates were annealed at 1200 K for two hours for stress relief and to degas hydrogen.

Deposition of the deuterium containing tungsten film was conducted in an Ar/D_2 atmosphere with a commercial magnetron-sputtering device (Denton, Discovery®18, Denton). A liquid nitrogen trap was used to minimize water vapor/oxygen contamination. The base pressure was $< 5\times10^{-5}$ Pa. Surface etching in Ar with -410V rf bias for four minutes was applied before deposition. Film deposition was done in Ar/D_2 atmosphere (1:1 gas flow) at a total pressure of 0.6 Pa with -100V rf substrate bias for 30 min. Additionally to the tungsten substrates, six silicon substrates were placed for later film characterization. All 60 samples were prepared in one deposition run. Substrates were placed on a rotating substrate holder to minimize layer inhomogeneity. Samples were positioned on this holder in two rings.

Rutherford Backscattering Spectroscopy with 1.2 MeV ^{3}He revealed a tungsten areal density on the central silicon substrate of 2.3 x 10^{22} W/m^2, corresponding to a thickness of around 300 nm. The expected density is about 95 % of the tungsten bulk density. Nuclear reaction analysis was performed with 1.2 MeV ^{3}He on three spots of every standard sample before shipping. The analysis of this data revealed that the D content is roughly 1-2 x 10^{20} D/m^2: The inner ring samples show on average 15.7 % less D content than the outer ring samples. The spread of the D content within one ring is less than 10%. Each sample shows a gradient along the radial direction of less than 10%. NRA analysis of seven samples in March 2017 revealed the very same absolute amount and gradient than the measurements in October 2016 proofing that there is no outgassing but D content is stable.

Thermal desorption analysis of six samples in October 2016 and March 2017 showed identical shape for the TDS spectra as well as total amounts within the expected range stated above and hence samples are identical and can be distributed for this round robin study.

Review of TDS Round-Robin Experiments

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Thermal desorption spectroscopy (TDS) is a useful experimental method to determine the kinetic parameters of hydrogen trapping in materials (e.g. binding energies). The experiments are relatively simple to implement and can be set up at relatively low cost. However, in practice, the interpretation of the data is not straightforward due to system-dependent parameters or several assumptions used in fitting or modeling the desorption spectra.

At the second RCM in Seoul, South Korea (Sep. 8-11, 2015), a consensus was reached that reference experiments were needed to establish a common measure for various devices. To meet this need, TDS round robin experiments using identical reference samples was proposed. T. Schwarz-Selinger (TSS) has summarized the details of such reference samples in the above report. During the 2nd RCM, Bas Braams asked H.T. Lee (HTL) to coordinate the exercise. Wolfgang Jacob (WJ) kindly volunteered that IPP, Germany would consider providing the reference samples.

A timeline of key events between the 2nd and 3rd CRM follows: First, HTL with IPP colleagues (WJ, TSS, and Liang Gao (LG)) set upon finalizing the experimental details of the RRE and sample production. To establish common experimental conditions, information on the participants' system parameters were queried. In June 2016, a mini-meeting was held during the PSI conference in Rome, Italy. Here, it was proposed that each participant would receive 2 samples produced by IPP, and the preferred ramping rate would be 0.1 or 1 K/s. All participants accepted this proposal. The samples began shipping to participants in October 2016. The deadline for data submission was March 2017. The RRE had participation by 17 groups in total, including groups outside CRP. 14 groups responded with submission of data for standard samples and 3 groups with non-standard samples. In May 2017, a second mini-meeting was held at the PFMC conference in Neuss, Germany. Here a brief update on the progress of the RRE was given. Two key facts were revealed to participants – (1) The existence of

NRA measurements for all samples, and (2) Slight difference in total D amounts between the two samples. Following this meeting, NRA data was released to the participants.

The main purpose of the RRE is to evaluate the system-dependent parameters. TDS data is affected by parameters related to the kinetics of desorption and system-dependent parameters. Typically the system-dependent parameters are ignored, leading to the assumption that the observed TDS spectra represents the kinetics of desorption. By fixing the kinetic parameters via reference samples, it allows for evaluation of the system-dependent parameters and the magnitude of such effects on TDS data. Such work can only be accomplished by comparison of multi-systems.

The overview of the goals of the exercise can be summarized as follows: (1) Provide a standard for absolute calibration for total retention values; (2) provide clear evaluation criteria for TDS data to arrive at a quality factor; (3) further our understanding underlying the analysis of TDS data; (4) provide input for TDS using neutron irradiated samples; (5) documentation and dissemination of the knowledge gained.

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