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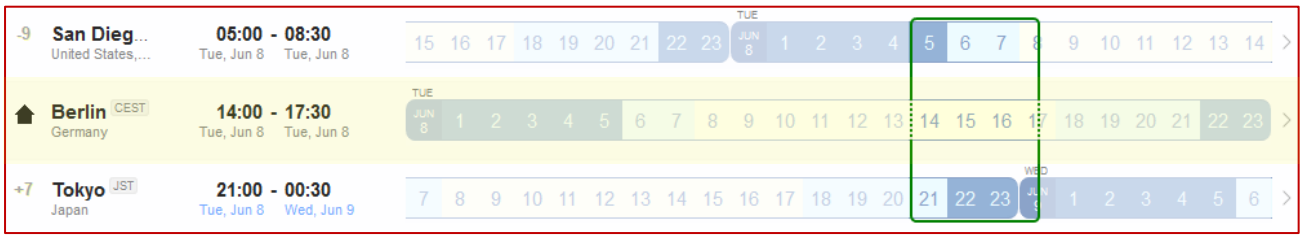

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14:25-14:50	I2	**K. Arakawa:** Quantum de-trapping and transport of heavy defects in tungsten
14:50-15:15	I3	**B. Wielunska:** D retention and dislocation structure of W irradiated by different ions
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I1

New microstructural insights into neutron-irradiated tungsten

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Tungsten (W) is considered as promising plasma facing material for future fusion reactors due to a number of advantages such as high melting temperature, excellent thermal conductivity, high strength and low sputtering yield. Knowledge of its microstructural response to neutron irradiation is important to assess the applicability and lifetime of plasma facing components. The polycrystalline W was irradiated with neutrons up to a damage dose of 1.25 dpa at temperatures 800°C in the BR2 materials testing reactor (Mol, Belgium). The irradiated material was examined with the Talos F200X transmission electron microscope (TEM) equipped with four energy-dispersive X-ray detectors (Super-X).

The microscopic analysis includes the investigation of voids, dislocation loops and precipitates. Their quantitative analysis includes the determination of size distribution, Burgers vector, nature and number density as a function of irradiation temperature. The application of spatially resolved energy-dispersive X-ray (EDX) analysis enables the study of radiation-induced segregation of transmutation induced Re and Os in pure W. Spherical and rod-shaped precipitates with a W-Re-Os composition were identified as σ- and χ-type precipitates, respectively. Formation of Re and Os rich clouds around voids and precipitates was observed and analyzed.

The coherent precipitation of both σ and χ is phases was determined. The [110] direction of σ-phase is oriented along that [110] of W, whereas in-plane the orientation relation is $(1\text{–}10)_W \parallel (1\text{–}12)_\sigma$ and $(002)_W \parallel (-441)_\sigma$. The out-of-plane the W [110] direction is parallel to the [214] direction of the χ-type precipitates, whereas in-plane it is $(1\text{–}10)_W \parallel (2\text{–}40)_\chi$, $(002)_W \parallel (-5\text{–}32)_\chi$.

Previous investigations showed that the accumulation of irradiation defects near the grain boundary and in the grain interior differs, i.e. a so-called denuded zone is formed close to the grain boundary, which is depleted or even completely free of any voids [1, 2]. For this reason, the defect formation and distribution of transmutation elements in the adjacent area was investigated in detail using TEM imaging and EDX analysis.

This study demonstrates a complex microstructural response of W to neutron irradiation.

[1] M. Klimenkov et al., Nuclear Materials and Energy 9 (2016) 480–483
[2] M. Dürrschnabel, et al., Sci Rep 11, 7572 (2021)

I2

Quantum de-trapping and transport of heavy defects in tungsten

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Nuclear-fusion materials are degraded primarily due to the accumulation of lattice defects such as point defects (self-interstitial atoms (SIA) and vacancies) and their clusters, which are produced upon energetic particle irradiation. Therefore, to precisely predict the lifetime of these materials, accurate understanding of the structures and dynamic properties of radiation-produced defects is required.

Defects are unavoidably bound to static trapping centres such as impurity atoms, meaning that their diffusion is dominated by de-trapping processes. We successfully monitored the de-trapping and migration of nanoscale SIA clusters in the form of dislocation loops, strongly trapped by impurity atoms in tungsten, by triggering de-trapping out of equilibrium at cryogenic temperatures, using high-energy electron irradiation and in-situ transmission electron microscopy [1]. We reveal the quantum de-trapping of defects below around 1/3 of the Debye temperature, in contrast to a traditional notion that de-trapping occurs only by thermal activation. In the presentation, we also show the impacts of this intrinsically high mobility of the dislocation loops in the microstructural evolution upon irradiation.

[1] K. Arakawa et al., Nature Mater. 19 (2020) 508

Deuterium retention and dislocation structure of tungsten irradiated by different ions

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Tungsten is a promising candidate material for the wall of a future fusion reactor due to its low erosion yield and low hydrogen solubility. However, fusion neutron irradiation will induce radiation defects in the material which can strongly increase hydrogen retention. Therefore, it is important to study the mechanism of defect creation and its influence on hydrogen retention in tungsten. Neutron-displacement damage is often simulated by high-energy ion irradiation, but it is not clear to what extent the displacement damage created by the ions resembles that of neutrons. In this study, different ions with different energies are used to study the effect of the primary-knock-on energy spectrum on damage creation and deuterium uptake.

Tungsten samples were polished to mirror-like finish and recrystallized at 2000 K for 5 min. They were damaged with different ion species (H, D, He, Si, Fe, Cu, W) at energies between 0.3 and 20 MeV to two different damage levels of 0.04 dpa and 0.5 dpa (in the maximum of the damage profile), calculated using SRIM.

For studying hydrogen retention in defects, the samples were exposed to a low-temperature D plasma to decorate the defects at 370 K. The D depth distribution was obtained by nuclear reaction analysis (NRA) using the D(3He, p)α reaction. The damage range calculated by SRIM is in good agreement with the region of increased D retention seen in the D depth profiles. Tungsten damaged by heavy ions (Si, Cu, Fe, W) to identical dpa values shows similar D depth profiles, i.e., D retention, is comparable. For tungsten damaged by light ions (p, D, He) the depth profiles show larger differences. In addition to NRA, trapped D was measured by thermal desorption spectroscopy. Tungsten irradiated by heavy ions shows similar deuterium desorption. The desorption spectrum from tungsten damaged by helium shows a significantly different shape. It is assumed that the D retention is influenced to some extent by the microstructure of the samples. Therefore, the dislocation structure was observed by transmission electron microscopy (TEM). For TEM observation lamellas perpendicular to the sample surface were cut with a focused ion beam microscope to image the whole damage depth profile. The damaged samples were observed under four different diffraction conditions. Within the accuracy the dislocation density was very similar at all four diffraction conditions. The evolution from dislocation loops at 0.04 dpa to dislocation lines at 0.5 dpa was observed. The microstructural evolution was similar for heavy ions. Differences in the dislocation loop diameter between the different samples were found.

I4

Vacancy distribution and hardness of high temperature neutron irradiated tungsten

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The aim of the present study is to extend the knowledge about the formation and thermal stability of vacancy-type defects in tungsten under neutron irradiation, thereby mimicking the temperature and neutron flux expected in the ITER divertor. Neutron irradiation of different tungsten grades in the temperature range 600-1200 °C is performed up to 0.1 dpa. Positron annihilation spectroscopy is employed to detect the presence of open volume defects, while hardness tests are applied to relate the irradiation-induced defects with the modification of mechanical properties. Rationalization of the experimental results is enhanced by the application of a kinetic Monte Carlo simulation tool, applied to model the microstructural evolution under the neutron irradiation process. The relation between radiation microstructure and hardness is explained via a dispersed barrier model.

I5

Modelling of the primary damage in Fe and W

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We have built up a large database of displacement cascades using Molecular Dynamics and several empirical potentials for Fe and W. Statistics studies reveal detailed features of the primary damage, particularly from the point of view of the defect production and the distributions of size of the vacancy and SIA defects at the end of the cascades. The potentials differ by their short range part (called "soft" or "hard" potentials) as well as their long range (or equilibrium) part and we have analyzed the sensitivity of the defect distributions to the equilibrium part of the potential as well as its hardened part. In parallel, other simulations of the static non-equilibrium properties (quasi static drag (QSD)), threshold displacement energies (TDE), replacement collision sequences (RCS) along the ⟨110⟩ direction have been realized and correlations between the primary damage and these new properties established. Along the ⟨110⟩ direction, the lower the TDE, the lower the QSD and the more energy is transmitted along the ⟨110⟩ direction during the RCS: the softest potentials are the ones for which the most energy is transmitted from the PKA to the first head-on atom in the direction of the RCS sequence.

To describe the morphology of the individual displacement cascades we use 3 descriptors: the volume, the number of sub cascades and the sphericity, and for the primary damage, 7 descriptors: the total number of defects, the number of SIA and vacancy clusters and their full size distributions. A multivariate multiple linear regression analysis based on these 3+7 descriptors and the choice of the potential indicates that the combination of the volume and the sphericity is meaningful. This analysis highlights several cascade properties, among them, that the large and spherical cascades create less defects and in particular, less mono defects than small and fragmented ones. The multivariate analysis also shows that the choice of potential has a limited influence on the total number of defects but a large one on the number of mono vacancies. On average, soft potentials create cascades of larger volume, smaller sphericity and produce more defects than hard potentials.

Finally, this work demonstrates that the formation of vacancy clusters is different in Fe and in W. In Fe, the fraction of vacancies in clusters is larger than that of SIAs and larger vacancy clusters are created than SIA clusters whereas in W, it is the opposite. The reasons are the differences of nuclear stopping power and threshold displacement energies, which result in different spatial distributions of open volumes that form during the expansion stage of the cascade.

I6

Multiscale simulations of defects in irradiated materials

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Understanding the effect of radiation damage on materials is critical to the design of fusion power plants. The choice of materials and their resistance to irradiation affects the expected performance and lifetime of reactor components. The change of thermal and mechanical properties due to the evolution of a radiation-induced microstructure can have significant implications for safety, maintenance, and the cost of constructing a reactor. Predicting strain, stress and swelling of components during operation requires knowledge about how microstructure changes under irradiation, where the local deformation of lattice structure stems from the volumes of irradiation defects. The microstructure of an irradiated material contains many defects and defect clusters that are too small to be observed by means of even high-resolution experimental methods, making modelling and simulation a vital tool in the context of fusion materials research.

The elastic field of a localised defect can be described by its elastic dipole tensor, and the long-range interaction between defects can then be treated using elastic Green's function formalism. Elastic dipole tensors of defects can be calculated using *ab initio* density function theory and/or molecular dynamics simulations. It represents the source terms for radiation induced stresses and strains in a material. This information can be transferred and adopted in continuum models, which are many orders of magnitude, in both length and time scales, larger than electronic and atomistic scale simulations. We will present the fundamental theory and numerical techniques for calculating the elastic dipole tensors of defects, with examples of large-scale *ab initio* calculations of mesoscale dislocation loops. It bridges the gap between electronic scale calculations and linear elasticity limit, where the defect core effect is prominent. The direct link between elastic dipole tensor and relaxation volume provides critically significant information about swelling of materials. We also show the possibility of developing a dynamic model, coupled to the finite element method that treats the evolution of an ensemble of nanoscale defects in a finite size sample, including the effect of interaction between migrating defects and surfaces of the sample.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No. 633053 and from the RCUK Energy Programme [grant number EP/T012250/1]. To obtain further information on the data and models underlying this paper please contact PublicationsManager@ukaea.uk. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

I7

Machine learning for atomistic materials science

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Multi-scale approaches in materials science face a traditional dichotomy in the choice of the atomistic force fields: robust, accurate and numerically expensive *ab initio* methods against less transferable but fast empirical methods. The ML methods propose a third avenue that allows control of the balance between the accuracy and numerical efficiency. Moreover, the ML-based vision of fundamental concepts in materials science, such as structural defects, can augment and revise traditional interpretations.

In metals, the interaction and transformation of crystal defect networks gives rise to an extraordinarily diverse range of defect morphologies [1]. Using the recently developed package MiLaDy (Machine Learning Dynamics) [2]: (i) we redefine the concept of defects in materials science [3]; (ii) we provide reliable force fields for complex defects such as interstitial, dislocation loops, dislocations; (iii) we are able to explore the atomistic free energy landscape of point defects in metals with *ab initio* accuracy up to the melting temperature [4], and, finally, (iv) we are able to propose surrogate models that bypass the traditional approaches [5]. We exemplify and discuss in the framework of experimental findings the case of energetic landscape of defects in body centered and face centered cubic metals.

[1] K. Arakawa , M.-C. Marinica *et al*. Nature Mat. **19**, 508(2020) ; R. Alexander *et al*. Phys. Rev. B **94**, 024103 (2016)

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[3] A. M. Goryaeva *et al.* Nature Commun. **11**, 4691 (2020)

[4] C. Lapointe *et al.* (to be submitted). , T.D. Swinburne, M.-C. Marinica, Phys. Rev. Lett. **120**, 135503 (2018)

[5] C. Lapointe, T. D. Swinburne *et al.* , Phys. Rev. Materials **4**, 063802 (2020); F. Bruneval *et al.* J. Chem. Theory Comput. **16**, 4399 (2020)

I8

Progress of tungsten spectral modeling for ITER edge plasma diagnostics and NIFS atomic and molecular databases

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Strong radiative cooling by tungsten ions in the core plasma is one of issues in fusion reactors. Quantitative analysis of tungsten density in divertor plasma, scrape-off layer, and main plasma relies on accuracy of spectroscopic model of tungsten ions. We have developed a collisional-radiative (CR) model for tungsten ions to calculate line intensities of tungsten ions [1]. We also have measured tungsten spectra from W to W^{46+} ions in wide wavelength region from extreme ultraviolet (EUV) to visible wavelengths simultaneously in the Large Helical Device (LHD) with tungsten pellet injection [1-6] and in the compact electron beam ion trap (CoBIT) [7] to validate the CR model for tungsten ions. So-called unresolved transition array (UTA) measured in EUV spectra at 4.5-7 nm are commonly seen in fusion plasmas with electron temperature of around 1 keV, which corresponds to edge temperature in ITER. The UTA is strong and largely contributes to the radiation power at this temperature. This feature is produced with numerous lines from W^{25+} - W^{34+} ions [1], but two-wide-peak spectral profile has not been reproduced yet, especially for 6nm-peak, by the CR model. We have developed the CR model to include recombination processes which were not considered before for tungsten ions. We find recombination and cascade processes enhance spectral features around 6nm, but not enough to reproduce the measured 6 nm-peak. The CR model for lower charged tungsten ions should be developed. Spectral peaks at 2-4 nm due to n=4-5 transitions can be used to examine tungsten behaviour in fusion plasmas [8].

NIFS Atomic and Molecular numerical databases has been developed since the 1980s and the database is opened for public at http://dbshino.nifs.ac.jp/. Numerical data for electron-impact ionization, excitation, and recombination cross sections and rate coefficients for atomic ions, charge exchange cross sections for ion-atom collisions, cross sections and rate coefficients of electron-molecule and atom-molecule collision processes, sputtering yields and backscattering coefficients for atom-surface collisions are stored in the database. They are retrievable and graphic display is available and useful for users [9].

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[2] S. Morita et al., AIP Conf. Proc. 1545 (2013) 143
[3] T. Oishi et al., Phys. Scr. 91 (2016) 025602
[4] Y. Liu et al., Japanese J. Applied Phys. 57 (2018) 106101
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[6] T. Oishi et al., Phys. Scr. 96 (2021) 025602
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[9] I. Murakami et al., Atoms 8 (2020) 71

I9

Erosion and impurity transport modelling with ERO2.0:
Introduction to the code; recent improvements; examples of data needs and validation

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ERO2.0 is a Monte-Carlo code for three-dimensional (3D) simulations of plasma-material interactions (PMI) and impurity transport in a fusion reactor or fusion-relevant plasma device [1]. The code uses the realistic 3D wall geometry of a give plasma device and a corresponding steady-state plasma background as input to simulate the gross erosion of plasma-facing surfaces, as well as re-deposition of sputtered wall elements. Sputtering yields used for this purpose are typically obtained from binary-collision approximation (BCA) or molecular dynamics (MD) simulations.

PMI-related data and validation needs are discussed in detail in this contribution on the example of sputtering yields for deuterium (D) impact on beryllium (Be). Presence of D in the Be surface layer not only leads to dilution effects and changes the Be surface binding energy, but also induces chemically assisted physical sputtering (CAPS) as an additional erosion channel besides physical sputtering [2]. Sputtering yield data obtained from both BCA and MD, as well as their application in ERO2.0 simulations and validation via JET experiments were discussed in [3].

As another example, effects of micro-scale surface roughness on PMI processes are addressed. To investigate such effects, micro-scale simulations with an arbitrarily defined initial surface geometry with representative roughness can be performed in ERO2.0 [4]. It is shown that with increasing roughness, the effective sputtering yield is reduced, which is confirmed by experiments at the linear plasma device PSI-2. Comparison with JET experiments suggests that a higher surface roughness may be the reason for the lower net erosion rate observed at certain divertor areas [5]. Furthermore, the roughness model of ERO2.0 is compared to the analytic Skeren model for benchmarking reasons [6].

To describe the formation and evolution of mixed material layers and surface concentrations by erosion and deposition, the recently implemented homogeneous mixing model (HMM) is used in ERO2.0 [7]. Since the HMM was already available in the predecessor code ERO, a detailed code-code-benchmark study is presented using a JET case with Be/W layers in the divertor.

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[3] D. Borodin et al., Nucl. Mater. Energy 19 (2019) 510–515
[4] A. Eksaeva et al., Nucl. Mater. Energy 19 (2019) 13–18
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I10

A new interpretive model for W erosion in EAST divertor during type-I ELMs

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Tungsten has been widely used as the plasma-facing material (PFM) in current tokamak devices, and is also foreseen for the future fusion reactors. Erosion of tungsten PFM is a critical issue, which can not only limit the material lifetime, but also lead to tungsten impurity degrading the plasma performance. Previous studies show that tungsten erosion is mainly due to physical sputtering by incident impurity ions at steady state [1]. During transient events such as edge-localized modes (ELMs), tungsten erosion by the main ion species become more important because of the high incident energy [2]. The intra-ELM tungsten erosion rate is normally much higher than the inter-ELM erosion rate. The physics process of ELM-induced tungsten erosion is also much more complicated and validated modelling is essential.

During EAST type-I H-mode discharges, a unique double-peaked intra-ELM tungsten erosion phenomenon was observed with high time resolution WI spectroscopy. To study this unique phenomenon, an analytic model of plasma expansion into vacuum is used to investigate the ELM parallel transport along the magnetic field line to the divertor target. During ELM transport, a self-consistent electric field is established to ensure the quasi-neutral approximation. Under this electric field, the kinetic energy of electrons will be transferred to ions thus accelerate the ions to a higher speed. A semi-analytic one-dimensional Monte Carlo tracing code is developed dedicatedly to model the particle transport during ELMs, and modelling results reveal that the C^{6+} particles transport slower than the main ions due to a lower initial thermal speed.

Based on the particle flux density and energy obtained from the Monte Carlo modeling, a Li-C-W mixed-material tungsten sputtering model is developed to calculate the intra-ELM tungsten erosion rate. A Li-C overlayer will dramatically reduce the tungsten erosion, meanwhile, it can make the heavier impurity contribute comparatively more effective than the main ions on causing tungsten erosion. By adjusting the thickness of the Li-C enriched layer, the tungsten gross erosion rates are well reproduced. Modelling results suggest that the second tungsten erosion peak during ELMs is caused by the energetic C^{6+}. The key physics governing the intra-ELM tungsten erosion in EAST has been revealed by the interpretive modelling.

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I11

Modelling of hydrogen isotopes outgassing from the strike-point vicinity in edge-plasma transport code

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Outgassing of hydrogen isotopes (HI) retained in the wall of nuclear fusion reactors represents a serious threat for the operation of future devices, both in terms of discharge control and reactor performance. Indeed, such phenomenon can lead to a loss of the plasma density control and a confinement degradation as it was observed in the long and high-power-heated discharges in JT-60U [1]. The Tore Supra long-pulse operation has also demonstrated that the plasma density increase can ultimately cause the abrupt termination of the plasma discharge [2]. Such events could be observed even in a full tungsten machine like WEST, where low HI retention is expected. Indeed, the existence of a HI Super-Saturated Layer (SSL) at the subsurface of tungsten with HI density of up to 0.1 at.fr, experimentally evidenced by nuclear reaction analysis [3] and predicted theoretically [4], could lead to the outgassing into the plasma of a HI quantity which is of same order of magnitude as the plasma HI content.

The Dynamics of Wall ElemEnts (D-WEE) module [5] aims to study the impact of the dynamics of retention and outgassing on the operation of nuclear fusion reactors. To this end, D-WEE incorporates a thermal model and the Reaction-Diffusion code MHIMS [6]. It is interfaced with the edge-plasma code SolEdge3X-EIRENE [7] by considering the HI implantation quantities and the net heat flux density on each element composing the wall. We exemplify the capability of this module to simulate dynamic retention on the full vacuum vessel during a plasma discharge in the JET tokamak, assuming as first approximation a full-tungsten wall. The simulation shows a depletion of the traps at both divertor strike-points during the H-mode phase of the discharge.

In the second part, we introduce an analytical version of D-WEE with the aim to study HI outgassing from the strike-points vicinity due to material heating and its effect on the divertor SOL. This model is applied to three SolEdge3X-EIRENE simulations with increasing input power (1.5, 3.0 and 4.5 MW) in the WEST tokamak. A full-tungsten wall with SSL at the subsurface is considered. The estimation of the quantity of outgassed HI for the three cases shows that only the 4.5 MW case exhibits outgassing of a HI quantity similar to the one in the plasma within few seconds. Retroaction of the model on the plasma within the SolEdge3X-EIRENE code is ongoing.

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I12

Coupled DFT-rate equation model for understanding H in W

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The interaction of hydrogen isotopes (HI) with tungsten (W) plasma facing material is an important concern for safety (retention and permeation of tritium) and control issue (outgassing from the wall to the plasma). Thus, modelling of HI uptake in and release from W is important to assess these points. Such modelling can be done from the atomic scale to the macroscopic scale. Atomic scale calculations determine the fundamental processes of trapping, diffusion and desorption of H from W. Macroscopic scales calculations allows to determine how the H inventories and desorption fluxes evolves at the scale of an experiment or a plasma discharges. Thus, it is important to be able to couple both scale in a multi-scale approach.

Here, we present the code MHIMS (Migration of Hydrogen Isotopes in MaterialS) which can simulate the migration of HI in plasma facing materials at macroscopic scale. The code takes input from DFT calculations such as the detrapping energies of HI from defects (vacancy, vacancy clusters, dislocations, etc.) or the energy barriers at the surface. It allows to compare the simulation results to experimental data from thermal desorption spectrometry (TDS) or ion beam analysis (IBA).

We first present simulations of HI gas or low energy atoms/ions exposure of single crystalline W for which the uptake is limited by the surface. The energy activation of HI on the surface are taken from Ajmalghan et al. [1] and Bergstrom et al. [2]. Then, we move toward simulations of more complex systems accounting for HI super-saturated layer observed experimentally [3] and predicted theoretically [4]. In this super-saturated layer, the HI are trapped in the mono-vacancies for which the detrapping energies are taken from Fernandez et al. [5], Heinola et al [6] or You et al. [7]. After that, we initiate the simulations of HI trapping in vacancy-like defects relevant for neutron and self-damaged W based on the DFT calculations from Hou et al. [8].

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Effect of elevated temperature and D presence on defect creation in W

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The effect of D presence on the amount of displacement damage created in W during self-damaging is investigated. We have employed a macroscopic rate equation (MRE) model to analyse the results obtained in experiments where W was sequentially or simultaneously irradiated by high-energy W ions and exposed to low-energy D ions [1]. The model includes fill-level-dependent D atom trapping in different defects and a novel damage creation and stabilization model [2] based on spontaneous recombination of Frenkel pairs and on stabilization of traps that are occupied by D atoms.

The MRE model was first applied on the sequential experiment where the samples were first irradiated by high energy W ions at elevated temperatures to create displacement damage and afterwards loaded with deuterium ions. Such an experiment serves as a comparison with other experiments that simulate damage evolution at high temperatures by employing room temperature damaging and subsequent damage annealing [3]. This distinction in damage creation is important to consider, as displacement damage in future tokamaks will be created at elevated temperatures and not at room temperature. By simulating the experimental results, we deduced that three different defect types with several fill levels retain the majority of D in the sample. The defect densities show a linear decrease with rising temperature in the entire 300-1000 K damaging temperature range with slightly different slopes for defects one and two. Defect three is independent of temperature.

The new stabilization model was developed to understand the simultaneous experiment, where damaging was done at the same temperatures as in the sequential experiment but with the addition of a simultaneous D ion exposure. To consider the effect of the W ion irradiation, kinetic de-trapping was also included as it was shown [4] that it could play an important role in the dynamics of D diffusion and trapping. A clear effect of the D presence was observed as the defect densities were higher than the values obtained in the sequential case in the region where D was present during the damaging. This effect was reproduced in our simulations by introduction of stabilization parameter, which defines the new defect saturation value due to the presence of D during defect creation. The effect of D presence on additional damage created is very large when damaging at 450 K, as a two-fold increase in created defect fraction is observed, while at 800 K almost no increase is observed. This is expected as less and less defects are occupied by D with rising temperatures and therefore stabilization by trapped D becomes less and less efficient.

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Co-deposition model for hydrogen isotopes with metals

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Tritium accumulation is a serious safety concern in future fusion devices, such as ITER. Co-deposition of tritium with eroded first wall materials is one of the main channels of tritium accumulation. Co-deposition parameters, such as hydrogen isotope fluxes and surface temperature during deposition can vary significantly from device to device and even within one machine from one area to another.

This means that a way to predict hydrogen isotope content in co-deposited layers in fusion devices depending on co-deposition conditions is desired. Because parameters of future devices will exceed those of currently existing machines, including in ways that are hard to experimentally model in laboratory setups, a model for which the range of applicability exceeds the experimentally verified parameter range is needed. For this, the model should have an established physics basis.

A model based on diffusion-convection equations with trapping and detrapping of hydrogen was developed [1] and verified for W-D, and Mo-D layers [2,3] using data obtained in MD-2 device [4], and for Be-D layers using literature data [5]. The model does not take into account hydride formation. It was observed that the developed model provided very good agreement with experimental data for D/Me vs. T curves, but not for D/Me vs deuterium implantation curves. The difference is attributed to the influence of implantation energy on the layer structure and the number of available traps, which is not taken into account in the model. In order to improve the agreement between the model and the experimental data, an energy empirical scaling factor was added for the total number of available trapping sites. As a result, a significant improvement was observed. The resulting half-empirical model provided an agreement with the experimental data of the same quality as G. De Temmerman's empirical scaling equation.

Currently, further work is underway in order to study the role of isotope competition in individual hydrogen accumulation in co-deposited layers.

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I15

Multi-scale modelling of the behaviour of gases in the nuclear fuel

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The Fuel Department of the CEA (Commissariat à l'Energie Atomique et aux Énergies Alternatives) develops a multi-scale approach to simulate the nuclear fuel behaviour during normal condition irradiation, incidental conditions, or storage. The panel of simulation tools is shown with a focus on the fission gas and helium issues. Then, two examples are presented, where modelling at different scales has been involved.

The first one is about the "annealing paradox" for fission gases. For annealing conditions above 1600°C, the large measured fission gas release implies that there is a significant transport of gases out of crystallographic grains, despite the presence of nano-bubbles acting as traps. A multi-scale approach helped assessing the efficiency of different scenarios for explaining these measurements. DFT calculations of xenon in a Schottky defect, then used in the calculation of the equilibrium concentration of dissolved xenon at the vicinity of a xenon bubble, allowed to eliminate the thermal resolution scenario. Then a mesoscale model named BEEP, was developed and used to assess a second scenario: bubble movement in a vacancy gradient. This phenomenon turned out to be insufficient to explain the measured fission gas transport out of the grain. Then random movement of bubbles was added in the model but was also insufficient. Finally, a mechanism involving coupled edge dislocation climbing and bubble movement and growth was proposed and tested. This mechanism seems to be the best candidate to explain fission gas release measurements in these conditions, and needs in turn new low scale studies to confirm its existence.

The second example is about the helium behaviour in storage conditions. After irradiation, helium production continues due to the presence of alpha emitter actinides in the fuel. We show how low scale studies help predicting the long-term location of helium in the fuel (intra or intergranular, dissolved or in bubbles).

Machine learning assisted ab initio thermodynamics of multi-component alloys

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Recent developments in machine learning techniques has immensely benefited ab initio modeling of materials. Interatomic potentials such as the moment tensor potentials (MTPs) (Shapeev, 2016) that are trained to high-temperature density-functional theory (DFT) data are able to predict energies and forces of various atomic configurations highly accurately, thereby enabling them to statistically sample a much wider part of the phase space in a fast and efficient manner. Such interatomic models can hence be used to accurately simulate and analyze the behavior of novel multicomponent alloys such as high entropy alloys (HEAs) and explore various compositional spaces of these alloys. In combination with a systematic thermodynamic integration method (Two-Stage Upsampled Thermodynamic Integration using Langevin Dynamics (TU-TILD), Duff et al., 2015), the MTPs can be used to calculate total free energies of HEAs to 1 meV accuracy (Grabowski et al., 2019, Ferrari et al., 2020) up to the melting point with far lesser computational cost. Apart from static and electronic energies, the total free energy also includes vibrational contributions including anharmonicity coming from phonon-phonon interactions in the system, which significantly affect thermodynamic properties such as specific heat capacity and bulk modulus at high temperatures in certain refractory HEAs.

Two studies are described in this talk. Firstly, we demonstrate the accuracy of MTPs for a bunch of refractory BCC systems ranging from unaries to five-component alloys. The individual anharmonic contribution to the vibrational free energy for these alloys are compared. Interestingly, certain BCC unaries have a small positive anharmonic contribution to the total free energy (beyond quasi-harmonic) whereas the other set of unaries have a large negative anharmonicity, which is also reflected in the alloys that constitute them. We narrow this feature down to the density of states (DOS) and the first- and second- neighbor forces and illustrate a difference in bonding behavior between the two sets of BCCs. Secondly, the full free energy surface and the thermodynamic properties of a TaVCrW alloy calculated using this methodology are also presented. The effectiveness of the methodology is promising and can be easily extended to other compositions of this system that are known for their high radiation resistance.

I17

SIA Defect Morphologies in W Collision Cascade Simulations

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The morphology of defects is an essential aspect of the evolution of crystal micro-structure and its response to stress. While reliable and efficient standard computational algorithms exist for finding defect concentration and size distribution in a crystal, algorithms for defect morphology identification are still nascent. The need for an efficient and comprehensive algorithm to study defects is becoming more evident with the increase in the amount of simulation data and improvements in data-driven algorithms. We present a method to characterize a defect's morphology precisely by reducing the problem into graph theoretical concepts of finding connected components and cycles. The algorithm can identify the different homogeneous components within a defect cluster having mixed morphology. The algorithm gives details of the internal structures within the defect and can therefore help understand the mechanism of morphological transitions and defect interactions. We apply the method to classify morphologies of over a thousand point defect clusters formed in high-energy W collision cascades. The method's comparative advantage for its completeness, computational speed, and quantitative details are highlighted. The defect morphologies obtained with three widely used interatomic potentials for W are compared using this method. It is seen that the disagreement between predictions of the different potentials regarding defect morphology is much stronger than the differences in predicted defect numbers. We briefly discuss the thermal stability and diffusion of dislocations with <100> Burgers vector and show the dependence of stability on size, morphological details, and choice of interatomic potential.

I18

Collaborative motion of helium and self-interstitial atoms enhanced self-healing efficiency of irradiation-induced defects in tungsten

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Tungsten (W) and W alloys are considered as the most promising candidates for plasma facing materials (PFMs) in future fusion reactors. However, as a PFM, W will be irradiated by high-energy fusion neutrons causing severe displacement damage and performance degradation, which should be originated from the evolution of irradiation-induced defects. Helium (He), as a typical impurity element, plays a crucial role on the microstructure and mechanical properties of W. Generally, the presence of He is expected to aggravate the irradiation damage, due to the strong attractive interaction between He and vacancies. However, recent experiments found that the He addition may also reduce the number of surviving defects in W under high-energy particles irradiation, indicating the enhancing effect of He on self-healing efficiency, while its underlying mechanism is still unclear so far.

In present work, we systematically investigate the energetics and kinetics of He-SIAs complexes as well as their influences on the evolution of irradiation-induced defects in W using first-principles method and object kinetic Monte Carlo calculations. We found that there are strong attractive interactions between He and SIAs in W, and the attraction is enhanced with the increasing of SIA numbers. More importantly, the presence of He significantly affects the kinetic behaviors of SIAs, in which the one-dimensional (1D) migration energy barriers are substantially increased, while the corresponding rotation energy barriers are reduced. Therefore, the migration patterns of SIA1/SIA2 change to 3D from 1D with the presence of He. Such unexpected collaborative 3D motion of He-SIA complexes increases the probability of Frenkel pairs recombination and reduces the number of surviving defects. Consequently, our calculations reveal the enhancing effect of He on the self-healing efficiency in W, governed by the concerted 3D motion of He-SIA complexes. These will improve our fundamental understanding of the influence of He on the evolution of irradiation defects in nuclear materials.

I19

A molecular-dynamics study of the diffusion of small He bubbles in tungsten

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Fusion reactor environments inevitably lead to the formation of helium bubbles whose nucleation, growth, and diffusion strongly impact the performance of plasma-facing components. We describe a diffusion mechanism of bubbles via a sequence of Frenkel pair nucleation, self-interstitial migration, and Frenkel pair annihilation. Molecular dynamics was used to characterize their diffusion dynamics and its dependence on helium content, vacancy cluster size, and number of attached self-interstitials. These bubbles are shown to diffuse relatively quickly, at least in the regime where Frenkel pair nucleation and annihilation proceed at similar rates when the bubbles nucleate and annihilate a single self-interstitial. We also characterize the temperature dependence of the diffusivity in the range 800 to 2000K, which we find to be relatively weak for the peak diffusivity. Peak diffusivity however shifts to higher helium content as the temperature drops. We find that the main features of bubble mobility can be captured by a coupled interstitial nucleation/diffusion/annihilation kinetical model that can be used to predict mobility in a wide range of conditions. The output of this model was used to inform cluster-dynamics simulations implemented in the Xolotl code. Results show that He bubble diffusion strongly reduces the predicted retention by providing an additional channel for outgassing. These results provide valuable insight into the mobility of He bubbles in plasma-facing components and input for higher-order modeling of the near-surface region of materials during plasma-surface interactions.

Molecular dynamics simulations of sputtering of rough tungsten surfaces

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Nuclear fusion is a promising concept for future energy production, due to the almost endless source of fuel and the lack of greenhouse effects during operation. To successfully construct a fusion reactor, the development of new materials and knowledge of their behaviour are needed. One important structural part of the reactor vessel is the wall facing the plasma. The wall will be eroded by the products of the nuclear reaction, which will degrade its performance. In this work, we study the sputtering of different tungsten surfaces under various conditions, obtaining a deeper understanding of the process using molecular dynamics simulations.

It is known that the sputtering yield of surfaces depend on several different factors, including incoming particle energy and type, incoming particle angle, surface orientation and surface roughness. However, even though these factors are known to affect the sputtering, detailed investigations of the phenomenon are lacking. To remedy this, we have thoroughly investigated the sputtering phenomena by molecular dynamics simulations. We started by investigating the effect of surface orientation of atomistically flat surfaces and extended the study to investigate the effect of different surface features and surface morphologies on the sputtering yield.

We observed that, indeed, all the before-mentioned parameters will affect the sputtering, including the surface roughness. We observed that already a roughness of a single atomic layer will affect the sputtering in an observable manner. Other larger surface features, like fuzz and hills, were also seen to dramatically affect the sputtering yields at different energies and incoming angles.

To better understand the formation of possible surface features, we have on a related topic investigated the bubble formation and growth. If a bubble is formed close to the surface, the possible increase in bubble pressure, which can destroy the bubble, may form dislocations leading to surface roughness. We studied several NiFe-alloy compositions and investigated the factors leading to a better stability of He-bubbles in some of the alloy compositions compared to others.

Surface structure characterization of plasma facing materials with impact-collision ion scattering spectroscopy

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Plasma facing materials in magnetic confinement fusion devices are subject to extreme temperatures, neutron irradiation, and exposure to hydrogen and helium plasma. These harsh conditions are known to drive defect nucleation and evolution within the surfaces of plasma facing materials [1], which in turn can affect key material properties like the retention of tritium [2]. In-situ characterization of defect nucleation and evolution in the surface during plasma exposure is challenging, due to the plasma's electromagnetic fields. These fields greatly influence the motion of electrons, which are often relied upon by surface science techniques as either a probe or the signal. One technique less sensitive to electromagnetic fields is impact-collision ion scattering spectroscopy (ICISS), as it characterizes surface structure using ions rather than electrons. As a step towards using ICISS to elucidate defect nucleation and evolution during in-situ plasma exposure, we performed experimental ICISS measurements to demonstrate its capability in characterizing the surface structure of a W(111) single crystal under UHV conditions [3].

ICISS was performed by scattering a pulsed 3 keV He+ beam off a W(111) single crystal and measuring the time-of-flight for backscattered He to reach a micro-channel plate (MCP). A multi-angle scattering intensity map was constructed by counting the number of detected backscattered He for thousands of pairs of crystalline orientations ϕ and incidence angles α. The detected count for a given pair of angles (ϕ, α) depended on the likelihood for the He to either channel into the tungsten (uncounted) or undergo a direct backscattering event and reach the MCP (counted). This multi-angle map provides a straightforward visualization of the W(111) surface structure, which can be strengthened with analytical calculations based on shadow cones. Our experimental measurements were then modeled with MARLOWE [4] with sufficient precision to allow for quantitative comparisons, such as quantifying changes to the map in response to strain. An improved ICISS instrument is currently under assembly, with a higher-energy ion source and extended flight tubes to provide superior spatial and energy resolution. This instrument will also allow for plasma exposure during measurements so plasma-driven changes to the surface structure can be monitored in-situ and in real time.

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