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Book of Abstracts

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Opening words

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Event opening by Deputy Director General Mr Juho KORTENIEMI (Ministry of Economic Affairs and Employment of Finland).

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Overview of the status of Fusion Technology: Progress and Deployment

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Recent years have seen a significant, quickly accelerating dynamic on the path towards making fusion a real option to meet net zero carbon emissions targets. International and national Government-funded programs are assisting the development of fusion technologies with a longer-term deployment window, with private fusion technology developers are focused on the commercialization of fusion over the next decade. Governments are establishing enabling programs to help progress these enterprises in parallel to the traditional public R&D programs. The technological development of fusion spans the three areas: (i) maturing fusion science, (ii) new enabling technologies (iii) private investment in fusion.

Fusion has already been demonstrated on a small scale, with a noted recent energy breakeven at LLNL in December 2022, with the expected scaling up in the next few years lead by the private sector' s demonstration machines. It is the scaling up of the process that presents the key challenge to the commercialization of fusion technology, which require facilities reviewed in this webinar.

There is a significant gap in the availability of engineering data on the effects of intense fluxes of high energy neutrons on materials and components, a gap that both public and private programs must address. International cooperation and access to facilities, to enable their integration into the overall international effort, to help identify the optimum technological choices, will define the success of fusion as a power-generating option. Regulatory uncertainty and standardization also need to be addressed, where the development of global codes and standards, coupled with the harmonization of regulations, is a necessary requirement for the deployment of fusion as a viable energy source.

The international cooperation and access to worldwide facilities, as well as integral planning of how a particular facility is fitting in a structured programme to obtain results that allow to make optimum choices is of paramount importance to have a real progress in Fusion deployment.

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Future ITER fusion A&M data needs and applications

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The ITER Organization (IO) has recently proposed a new baseline to meet the challenges of timely construction of the machine and achievements of the project ' s objectives. One of the main changes the new baseline brings is the switchover of the first wall armour material from Beryllium to Tungsten. This of course increases the importance of diagnostic measurements and control systems aimed at keeping the core plasma tungsten concentration at a low enough level that will not hinder plasma performance. In this talk, the new baseline rationale and schedule will be presented, including the consequence of the changeover to tungsten. In particular, the IO is considering the need to install a boronization system as a risk mitigation measure to condition the tungsten wall surfaces and help with plasma stability and control. This would bring its own new set of A&M data requirements, replacing the need for Beryllium data, to monitor the Boron content in the plasma, model the Boron deposition and transport in the device, to deduce the lifetime and thickness of the boron layers on the first wall.

This talk then reviews the planned diagnostics systems, with emphasis on those relying on A&M data for their interpretation. These include the X-Ray Crystal Spectrometer and Charge eXchange Resonance Spectroscopy systems for core temperature and impurity content, the Divertor Impurity Monitor, and VUV spectrometers, both in the divertor and in the main chamber.

A separate set of data needs comes from the simulation side, for firming up the physics basis of the revised ITER Research Plan. Of particular importance is how to make sure that a consistent set of data from reliable sources is used when making calculations and measures being considered to guarantee the traceability and reproducibility of the results with the best accuracy available. At ITER, we rely on the Integrated Modelling and Analysis Suite of tools, in particular the AMNS (Atomic, Molecular, Nuclear and Surface) data service library. A preferred source for the needed data is envisioned to be the IAEA CollisionDB database, once technical solutions can be agreed upon for easy runtime code access.

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Atomic data and collisional-radiative models of tungsten ions for fusion plasma

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Tungsten is an impurity material in fusion plasmas since it is a plasma-facing material for divertor in fusion devices and is sputtered and transported into plasmas. Because of its large atomic number, tungsten is partially ionized even in core plasmas and could lose energy due to high radiation power. To understand tungsten behaviors, a spectroscopic method is useful, and a reliable spectroscopic model is required. Many experimental and theoretical studies have been done on tungsten spectra and we have compiled much knowledge on tungsten ions, but still some data are missing.

Wide continuous two-peak spectral profile, so-called unresolved transition array (UTA) is found at 4.5-7nm wavelength region for plasma with electron temperature ˜1keV [1], produced by overlapped numerous 4d-4f and 4p-4d transitions. Many little-wide peaks at 2-4nm, produced by 4g-5f and 4g-6f transitions, are useful to estimate ion abundance for Wq+ ions with q=22-30 [2,3]. Collisional-radiative (CR) models for tungsten ions have been constructed and examined by comparing calculated spectra with experiments (e.g. [3-5]). Atomic data necessary for the CR models are generally obtained by theoretical calculations. There are several atomic codes used and calculated results by CR models give different results. It is not easy to judge which one is reliable since atomic data are huge and cannot be compared one by one. The structure of CR models is different from each other. The UTA profile at 4.5-7nm is not yet fully explained by the CR models. Much effort to improve atomic data and CR models is necessary.

Other UTA profiles are found at around 20nm, produced by n=5-5 transitions of Wq+ ions maybe with q=23-18 [6, 7]. It is necessary to construct CR models for lower-charged tungsten ions to understand tungsten behaviors in peripheral plasma and divertor regions.

If the electron temperature is higher than 3 keV, the UTA profiles almost disappear and distinct lines from higher-charged tungsten ions appear. The CR models for such ions are also examined by several groups (e.g. [8]) and are useful for plasma diagnostics from peripheral to core plasmas.

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Recent progress of collisional radiative modelling of H2 with Yacora and steps needed for D2

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Collisional-radiative (CR) models for atomic and molecular hydrogen are essential for quantitative interpretation of atomic and molecular emission in low temperature plasmas such as the divertor plasma of fusion devices or negative hydrogen ion sources for the neutral beam injection systems for ITER. Moreover, CR models provide effective rate coefficients for neutral models, like the EIRENE code, to identify the role of hydrogen opacity in the analysis of Balmer line radiation and the role of molecules contributing to the high-recycling regime. In particular, the transition from ionising to recombining plasmas involves a complex interaction of molecular and atomic species. Using the Yacora solver [Wünderlich et al., J. Quant. Rad. Transfer 110 (2009) 62], several CR models are constructed based on a unique database compiled for this purpose. (i) Yacora-H: atomic hydrogen, which is coupled to molecular species, (ii) Yacora-H_2: molecular hydrogen with the electronic states resolved, (iii) Yacora-H_2(X1,v): molecular hydrogen for predicting the vibrational population of the ground state, (iv) Yacora-H_2(v): vibrationally resolved model for molecular hydrogen, and (v) Yacora-H_2(v,N)-Fulcher: ro-vibrational corona model for the Fulcher band. The contribution highlights the enormous progress achieved since the last IAEA Decennial Meeting in 2014, gives application examples together with a discussion on the steps needed for the deuterium molecule.

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Configuration-Average Collisional-Radiative calculations, Ionization and Emission of low-density tungsten plasmas in the temperature range [800-5000] eV

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After a discussion concerning differences between "high-density" plasmas (e.g. laser-produced plasmas) and "low-density" plasmas (e.g. tokamak core plasmas) in term of collisional-radiative modeling (CRM) for high-Z elements, we present specific configuration-average CRM calculations of tungsten plasmas at low electron density Ne = 5 10^{13} cm^{-3} for electron temperatures in the range 0.8 to 5 keV. These conditions are relevant to current tokamaks. In this temperature range, the modeling of the ionization balance and of the spectra is a long-standing problem.

We discuss here the problem of ensuring completeness of the list of configurations included in the calculations. We also present comparisons of experimental measurements in the EUV range performed at tokamak WEST, with calculated spectra based on the use of the unresolved transition array (UTA) and of the spin-orbit split array (SOSA) formalisms, those formalisms having been developed rather in a "high-density" plasma context. They are particularly adapted to the study of broadband spectral features (quasi-continuum structures).

A conclusion is that standard calculation methods (e.g. the distorted-wave method for collision cross sections) used for the evaluation of the configuration-average collisional and radiative rates, are fine provided that a correct list of configurations is used in the calculations.

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R-matrix electron-impact excitation/ionization calculations for near-neutral ion stages of Tungsten

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Tungsten remains the element of choice for plasma facing components (PFCs) in the divertor region of ITER [1] and other past and present tokamak experiments [2, 3]. The impurity influx of tungsten from PFCs into the plasma while undesirable, as highlighted by Pütterich et al. [4], needs to be accurately quantified if we are to model tungsten erosion and redeposition. Previous work of Isler [5] and Murakami et al. [6] state that the presence of as little as 0.1% of this high-Z element, within the plasma may be sufficient to quench the reaction, confirmed by Pütterich et al. [4] but at even smaller quantities.

One accepted method to provide a prediction of the expected impurity influx of Tungsten from the divertor region of a tokamak is the SXB ratio [7]. The SXB ratio for a given line has the effective ionisation rate in the numerator; with the denominator representing the population of the upper level times the Einstein A-coefficient for a given transition.

The Dirac Atomic R-matrix Codes (DARC) have been quite successful in providing sufficiently accurate atomic structure and electron-impact collision strengths that underpin the determination of the upper level population [8,9,10]. The effective ionisation rates have a higher degree of uncertainty attached to them. Perturbative methods such as the distorted wave method have been employed but have shown to overestimate ground and meta-stable ionisation cross sections for near-neutral lighter systems. New RMPS ionisation cross sections shall be shown for W^{2+} and compared with available experimental data. Future work will consider the electron-impact excitation and ionisation of W and W^{+}.

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Machine learning applications to line spectra emitted by magnetic fusion plasmas

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Artificial intelligence is spreading across all science fields, including plasma science and plasma spectroscopy [1]. Various applications have shown promising results in combining diagnostic measures with machine learning techniques, particularly in tomographic reconstruction from sparse bolometric measures and early disruption detection [2,3]. In this communication, we present ongoing work on applying different machine learning algorithms to tungsten spectroscopy and Balmer lines of hydrogenic species (Hα/Dα and Dα/Tα).

For tungsten spectroscopy, we use the measurements of a W quasi-continuum emitted in the extreme UV (EUV) range, namely 45-65 Å. The measurements are performed with a grazing incidence spectrometer [4] with a mobile line of sight. We aim to establish an approximate mapping between the measured brightness spectrum of the tungsten quasi-continuum and the maximum electron temperature viewed by the line of sight during its scan. We present an end-to-end framework from the preprocessing of the emissivity lines to the maximum electron temperatures, explaining and comparing preprocessing and machine learning algorithms to achieve this goal. This study uses data from different discharges performed in the WEST Tokamak. It is found that when the investigation is focused on a series of very similar discharges, the spectrum shape is well correlated with the electron temperature in such a way that the temperature can be inferred from a measured spectrum and vice-versa with an uncertainty of about 150 eV over a broad temperature range. On the contrary, when the training set comprises plasma discharges in a variety of scenarios, the correlation is substantially weaker, an indication that « latent » parameters such as the specific heating scenario, the tokamak wall conditions and MHD also play a role. The first step to check this explanation will be to include in our analysis the electron density and temperature profiles along the line of sight.

On the other hand, we identified and dedicated 1D convolutional neural networks (CNNs) to predict the isotopic ratios of hydrogenic species from synthetic Hα/Dα and Dα/Tα), generated according to a theoretical model [5,6]. We show that the CNNs learn to predict the correct ratios from various lines and corresponding parameters While the training set is composed of synthetic lines corresponding to measurements parallel to the magnetic field, the CNNs can generalize their predictions to lines corresponding to various angles of measurements (from 0 to 90 degrees).

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Vibrational excitation of hydrogen molecules formed by atom recombination on tungsten

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The production of vibrationally excited hydrogen molecules by recombination processes on a tungsten surface exposed to hydrogen is relevant to the understanding and development of hydrogen negative ion sources (e.g. [1, 2]) and to a lesser extent to the modelling the edge plasma in tokamaks (e.g. [3, 4]).

Here we present an overview of our studies of the vibrational distributions in H2 and D2 molecules produced by atom recombination on tungsten [5]. In our experiments, we exposed a tungsten surface to a steady flow of atomic hydrogen and measured the vibrational distribution of desorbed molecules. Vibrational distributions were determined by specific spectrometers utilising the properties of dissociative electron attachment in hydrogen. We performed measurements in a few different experimental arrangements [6, 7, 8]. Measured populations of vibrational states roughly follow Boltzmann distribution corresponding to vibrational temperature between 2800 K and 3800 K [6, 7]. Observed vibrational temperature is lower for D2 than for the H2 [7]. Measurements in H2 [6] also clearly reveal that the rotational temperature is significantly lower than vibrational one. Some measurements also indicate a possible departure of the Boltzmannian state distributions [8]. We will discuss our experimental results by addressing recent theoretical studies of hydrogen-tungsten interaction (e.g. [9] and references therein).

We also provide some general discussion on our spectroscopic method, which is well suited for studies of vibrationally excited hydrogen isotopologues in order to promote its future use as well as to suggest possible further applications.

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Active spectroscopy on Magnum-PSI to characterize atomic and molecular hydrogen in detached conditions

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Divertor detachment is the leading candidate for solving the heat exhaust problem in future fusion reactors. Key to understanding detachment is the interaction of the plasma with a background of neutral particles in the divertor region. Collisions of the plasma with these neutral background particles result in a rich range of physical and chemical processes, causing the plasma to dissipate its energy and momentum, and finally to recombine, preventing damage to the wall. Whereas charged particles are routinely diagnosed, information on neutral particles is often missing. The properties of neutral particles can be measured using active spectroscopy. At Magnum-PSI, a linear plasma generator that can simulate the high heat and particle flux conditions of future fusion reactors, three types of active spectroscopy are being installed: TALIF, CARS and VUV-LIF. With this combination of diagnostics one can measure the (ground-state) densities of both atomic and molecular Hydrogen, as well as the ro-vibrational state distribution of H2 and its isotopologues. The ground state densities are important parameters in many of the detachment processes, and are also needed as input for scrape-off layer modelling. The ro-vibrational state distribution is important as it determines the reaction rate of MAR (Molecular Assisted Recombination), one of the dominant recombination processes in divertor plasmas.
Apart from the design and status of all three diagnostics, first TALIF and CARS data taken on the UPP linear device will be presented.

TALIF: Two photon Absorption Laser Induced Fluorescence
At high enough laser intensity, TALIF can be used to measure the density of H atoms in the electronic ground state. The needed laser wavelength of 205.14 nm is in the UV range. The resultant fluorescent Balmer alpha emission (in the visible range) is a measure for the density of the ground state Hydrogen atoms.

CARS: Coherent Anti-Stokes Raman spectroscopy
CARS is a four wave mixing process in which the plasma is simultaneously illuminated by two laser frequencies in the visible range, tuned to be resonant with the various ro-vibrational state transitions of H2 molecules. The resulting emitted CARS signal is a measure for the density of the resonant ro-vibrational states, including the H2 ground state density.

VUV-LIF: Vacuum Ultraviolet Laser Induced Fluorescence
For higher vibrational states the sensitivity of CARS is too low. The higher ro-vibrational states will hence be measured with VUV-LIF. The beamlines for both the laser and the fluorescence signal (detected using a VUV monochromator) need to be in vacuum.

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Review on plasma-particle processes in fusion devices and corresponding data needs (tentative title)

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SOLPS modelling of the edge plasma

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The SOLPS-ITER code uses atomic, molecular and surface data to model the edge plasmas of tokamaks and linear devices. This data is needed over a relatively wide range of plasma temperatures (0.1 eV or lower to approximately 5 keV for the pedestal of ITER) and plasma densities ($10^{17}\ m^{-3}$ to $10^{22}\ m^{-3}$) for the atomic data, and a somewhat smaller temperature range for the molecular data. For the surface data, sputtering and reflection data is needed for all considered plasma species hitting all considered surface species, in the possible presence of mixed materials, including the possible preferential sputtering of light atoms deposited on heavier atoms. For molecular data, a full data set of reactions involving molecules and molecular ions, including mixtures of isotopes, is desired. In this context, a reflection model capable of dealing with mixed isotopes is desired.

An important consideration for all data is that they should be **robust** over the range that they are used – by this is meant that the data should not blow-up even if used beyond their formal domain of applicability, and provide physically sensible results (reflections coefficients should not exceed 1, cross-sections should be positive).

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The EMC3-EIRENE kinetic trace ion transport module

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Impurity seeding in the scrape off layer plasma as well as controlling the contamination of the core plasma by high Z impurities are essential for ITER baseline scenarios. Predictions for the ITER baseline scenarios are often based on fluid descriptions of the impurity transport. However, especially lower ionization stages of high Z impurities (e.g. Ar, W) do not have the time to equilibrate to a Maxwellian velocity distribution and a kinetic treatment might be more appropriate than a fluid description for these short-lived ionization stages.

To simulate kinetic effects of impurities, the EMC3-EIRENE code package was extended by a kinetic ion transport module in guiding centre approximation. The kinetic ion transport module is part of the kinetic neutral Monte Carlo code EIRENE and currently contains grad-B and curvature drifts including mirror-force effects, anomalous cross-field diffusion and a model for Coulomb collisions. The kinetic ion transport itself is solved in EIRENE by a Monte-Carlo scheme in real space. The original implementation of the kinetic ion transport was thoroughly checked and some severe numerical problems including non-conservation of magnetic moment and severe numerical diffusion were identified. These shortcomings could be resolved by a complete redesign of the transport module.

In a first application for Nitrogen seeding in a medium density (attached) ITER L-mode scenario, it turned out that the original Coulomb collision model of EIRENE was oversimplified and did not include scattering of the kinetic ions. This resulted in an excessive trapping of the kinetic ions in the magnetic mirrors at the outer midplane and at the high field side of the X-point due to the missing scattering of the kinetic ions into the loss cone of the magnetic mirrors. The implementation of an improved Coulomb collision model which takes the scattering of the kinetic ions into account could resolve this issue. This new Coulomb collision model is treated by an operator splitting and solved locally by a Monte-Carlo scheme in velocity space. It is crucial to choose a small enough time-step for the Coulomb collision kernel, which led to the implementation of an adaptive time-step control with error estimates to optimize the runtime of the new and improved Coulomb collision module.

To check all the new implementations for the kinetic ion transport module of EMC3-EIRENE, it was benchmarked in a first comparison to the well-established ERO2.0 code. To focus first only on transport characteristics of both codes and avoid any influence from differences in the wall interaction models, we simulated a well-defined artificial and non-recycling beryllium source. The comparison showed good overall agreement. Only towards the inner core boundary an about 60% higher beryllium density could be observed in the EMC3-EIRENE kinetic ion transport module, which we think originates from small differences of the implementation of the reflecting core boundary condition in both codes. This density increase will be checked and analyzed further in the future to understand its origin.

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Overview of the NIST research program on atomic data and modeling for fusion

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Development of critically evaluated data sets for atomic parameters has long been a major part of the research program at the National Institute of Standards and Technology (NIST). Over the last decade NIST researchers and their collaborators created recommended sets of data for a number of fusion-related elements including, e.g., Be, Ar, Fe, Mo, and W. As a result, for example, the number of spectral lines in the most comprehensive of NIST atomic databases, the Atomic Spectra Database (ASD), increased by about 20%. The NIST Electron Beam Ion Trap (EBIT) is routinely used to accurately determine spectral characteristics of highly charged ions of mid- and high-Z elements. Also, extensive sets of recommended cross sections for electron-impact excitation and ionization (for, e.g., Be I and Be II) as well as for charge exchange (CX) between energetic neutral beams and highly-charged ions of tungsten were reported. Furthermore, the spectra of multiply-charged W due to CX interactions in the ITER core plasma were determined using large-scale collisional-radiative models.

In this presentation we will describe the major directions and components of the NIST research program on critical evaluation of spectroscopic data for fusion, measurement and analysis of extreme ultraviolet and x-ray spectra from heavy multiply charged ions, and collisional-radiative modeling of relevance to fusion.

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Main evolutions of ADAS (tentative title)

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Collisional processes of B and BH in fusion plasmas

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Wall conditioning is essential for controlling hydrogen recycling and the amount of intrinsic impurities to achieve high-performance plasmas in magnetically confined fusion devices. A technique for wall conditioning, boronization, is coating the chamber walls with boron. To examine the effectiveness of boronization, it is essential to investigate where and how much boron is deposited onto the plasma-facing materials (PFM).

BH spectral emission is a good diagnostic of boron deposition onto PFM. BH (or boron deuteride, BD) molecular bands have been confirmed in discharges after fresh boronization. Kawate et al. (2022 NucFu) performed impurity powder-dropping experiments (Nagy et al. 2018 RScI) with boron powders in the Large Helical Device toward real-time wall conditioning. Our spatially-resolved spectroscopic measurements of BH molecular bands suggest deposition and desorption of boron on the divertor plates.

In this study, we numerically investigate electronic excitation and ionization cross sections for the $e^{\hat{}}$ – BH and $e^{\hat{}}$ – $BH^{\hat{+}}$ collision processes and the rate coefficients. In addition, we derive S/XB and compare it to the preceding study, aiming for an application to plasma diagnostics and modeling near PFM in fusion devices.

The calculations were performed by the R-matrix and Binary Encounter Bethe methods utilized by Quantemol-EC software. To examine the uncertainty due to the calculation conditions, we compared the results by different basis sets and internuclear distances of the target model.

In the presentation, we introduce our experimental results by molecular spectroscopy and numerical results on electron collision processes of BH. In addition, we discuss the formation processes of BH molecules near PFM.

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Atomic collisional data for neutral beams and injected impurities in fusion plasmas

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Impurity seeding will be required for future reactors such as ITER and DEMO for radiative cooling, plasma control and diagnostics. Fusion plasmas are expected to contain impurities such as carbon, nitrogen, oxygen, argon, and tungsten ions. Some of these impurities are formed through ion seeding, others by erosion of plasma-facing components of the reactor. In the case of DEMO, due to the higher heating power required, highly charged impurities will be required to maintain the temperatures in the diverter region. Charge-exchange recombination spectroscopy (CXRS) is a diagnostic technique for measuring the impurity ion density, ion temperature, and plasma rotation within fusion plasmas [1]. The technique requires accurate state-resolved charge-exchange cross sections for collisions between seeded impurity ions and the neutral hydrogen beam injected during diagnostics and heating [2].

The wave-packet convergent close-coupling (WP-CCC) method can provide benchmark data on the total and state-selective cross sections for various processes taking place when fully stripped ions collide with atomic and molecular targets, see [3,4] and references therein. The approach is based on the expansion of the total scattering wave function using a two-centre pseudostate basis. This allows one to account for all underlying processes, namely, direct scattering and ionisation, and electron transfer into bound and continuum states of the projectile. The wave packets, constructed from the Coulomb waves, are used to discretise the continuum of the target and projectile atoms.

The WP-CCC approach has recently been extended to dressed-ion collisions with atomic hydrogen [5]. The method has been applied to calculate the total ionisation and state-resolved electron-transfer and target-excitation cross sections in C^{2+} and C^{3+} collisions with atomic hydrogen. The total electron-capture cross sections, calculated in a broad projectile energy range from 1 keV/u to 1 MeV/u, agree with available experimental and previous theoretical data. However, the results for ionisation overestimate the experimental data at the peak of the cross section supporting previous calculations.

Charge exchange in collisions of Ar^{16+} ions with hydrogen has also been investigated [6]. CXRS measurements performed at the ASDEX Upgrade [1] are based primarily on these impurities. For this projectile, capture into states with n=14–17, where n is the final-state principal quantum number, are found to be the most important. This is because the Lyman transitions from these states of Ar^{15+} are in the visible spectrum, which is well-suited for CXRS diagnostics. Experimental measurements are not available. Two different groups applied the classical trajectory Monte Carlo (CTMC) method for this system leading to very different results. We have calculated the state-resolved charge-exchange cross sections for n=6–19. For capture into the n=14–17 states a significant difference is observed between the present and previously published CTMC data. The cross sections differ by an order of magnitude within the most important energy range of 10–60 keV/u.

The WP-CCC method has also been applied to calculate various differential cross sections for ionisation in ion collisions with He [7] and H_2 [8]. Excellent agreement between the obtained results and the experimental data is found resolving longstanding discrepancies between theory and experiment. We review recent data relevant to fusion plasmas, obtained using the WP-CCC method.

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Hydrogen isotope dependence in dissociative electron attachment

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In my talk, I will present a theoretical investigation on electron-D_2 resonant collisions, via the low-lying and the Rydberg states of D_2^-. I will focus, in particular, on low-energy cross section calculations, vibrationally resolved, for the dissociative attachment process in the ground state, and two electronic excited states of D_2. Isotopologue effect for H_2 and D_2 will be shown and transitions between electronic excited states will be considered.

The electronic structures of deuterium are obtained by using ab-initio quantum chemistry approaches implemented in computer codes like MOLPRO and UK–R-Matrix whereas the nuclear dynamics is studied within the theoretical models of Bardsley ' s local-complex-potential model.

Comparisons with cross sections present in the literature, where applicable, will be presented.

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Electron and positron collisions with atoms and molecules

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Accurate electron and positron-impact excitation cross sections for collisions with atoms and molecules are important for modelling various plasmas with applications ranging from medical sciences and plasma processing to astrophysics and fusion. This talk will review recent progress at the Curtin University research group in developing collision codes and their use in modelling collision processes. To study positron collisions with atoms, a general atomic structure code has been developed and combined with the positron scattering formulation of the convergent close-coupling method. A comprehensive set of positron impact cross sections has been obtained for the range of light atoms (C, O, F, Ne, Ar, $\cdots$) [1] . With the use of the independent atom model, the cross sections for various reaction processes have been estimated for a large selection of molecules (O_2, CO, CO_2, F_2, $\cdots$) [2]. For electron collisions, the emphasis has been on providing a detailed set of rovibrationally resolved cross sections for molecular hydrogen and its isotopologues. These cross sections have been reported in four papers in Atomic Data and Nuclear Data Tables [3] and are available from the HCDB database hosted by the International Atomic Energy Agency and from the dedicated database mcccdb.org. The codes for collisions with molecules have been extended to more complex molecules such as HeH^+, LiH, and H_3^+. A cross section dataset was produced for HeH^+ molecular ions [4]. New data will be presented for LiH and H_3^+ molecules.

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Poster session / 26

Abstract for Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology in Cambodia

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Fusion science and technology present interesting answers as Cambodia looks to diversify its energy sources and move toward sustainable ones. This abstract examines how important it is to advance fusion research in Cambodia by using data on atomic, molecular, and plasma-material interactions. The process of fusion, which uses the energy of atomic nuclei, has enormous potential for producing large amounts of clean energy. But the success of fusion technology depends on a deep comprehension of the intricate interactions that take place at the atomic and molecular levels in plasma settings and in the materials that make up fusion reactors.

In Cambodia, where energy demand is rapidly increasing, embracing fusion technology could significantly contribute to achieving energy security and mitigating environmental impacts. However, realizing the potential of fusion requires a multidisciplinary approach, integrating expertise in physics, materials science, and engineering. Atomic and molecular data play a pivotal role in modeling fusion reactions, understanding plasma behavior, and predicting material responses under extreme conditions.

Obstacles specific to the Cambodian setting, like inadequate infrastructure and human resources for fusion research, highlight the significance of global cooperation and information sharing. For Cambodia to actively engage in the international fusion research community, it becomes imperative that it utilize the databases, experimental facilities, and computational tools already in place. Moreover, customized research programs emphasizing localized material characteristics and plasma diagnostics are required to tackle particular issues and prospects in the energy sector of Cambodia.

With the right investments in atomic, molecular, and plasma-material interaction data development, Cambodia can establish itself as a major participant in the fusion energy industry. In order to promote creativity and information sharing, this abstract supports strategic alliances between academic institutions, business, and governmental organizations. Additionally, outreach and education initiatives can develop a trained labor force and increase public knowledge of the role that fusion technology may play in determining Cambodia energy landscape.

In conclusion, the foundation of fusion science and technology is based on data on atomic, molecular, and plasma-material interactions, which presents revolutionary opportunities for Cambodia's sustainable energy production. Cambodia can use the power of fusion to promote economic growth, lessen the effects of climate change, and guarantee a prosperous future for its people by working together and making wise investments.

Poster session / 53

Space-resolved radiation spectrum in the 15-300 Å domain in keV plasmas of the WEST tokamak

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In magnetic fusion devices equipped with Tungsten (W) plasma-facing components (PFCs), dilution and radiation studies have become an essential feature of the experimental developments. Among several methods used to diagnose W transport and radiation in fusion plasmas, spectroscopy is one of the most powerful because it allows us to distinguish between the numerous ionisation stages of W. For example, in the visible range, it allows to assess the W sources on various PFCs and its transport in the scrape-off layer. In the VUV, it provides invaluable information on the confined plasma by resolving the mid- to high-charge ionisation stages of W [1]. However, W emission is so rich and complex that we are far from an exhaustive understanding of the measured spectra.

The WEST tokamak is equipped with a grazing incidence VUV spectrometer which has *i)* two detectors, each with an adjustable wavelength range in the 15-300 Å domain and *ii)* a line of sight which can scan the lower plasma half several times during each single plasma discharge. The wavelength interval width of each detector is relatively narrow. It varies from 23 Å to 60 Å from the short to the long wavelength end of the spectrometer domain. Therefore each pulse provides only a small window in the whole VUV emission spectrum of W. Nevertheless, it is possible to reconstruct broad spectra provided two instrumental features are taken into account: the brightness calibration and the non-uniform detector response.
The absolute brightness calibration of the spectrometer has been already performed [2]. It shows that the spectrometer sensitivity is rather flat in the 80-130 Å interval while it drops very steeply on both sides of that interval. what we focus on here is the method and results obtained about the detector response.

We have performed series of identical pulses during which the whole spectrometer domain was explored by changing the detector wavelength interval pulse after pulse. The setting of the detector position is chosen such that an overlap exists between adjacent spectra. By combining the measurements with the absolute calibration, we thus obtain the non-uniformity of the detector response. By combining it with the strongly varying brightness calibration coefficient, broad VUV spectra were obtained for each possible line of sight of the spectrometer.

Such a global spectrum can be used to better identify the numerous spectral lines observed in WEST by using time correlations between them, line brightness ratios, and line brightness dependence on electron temperature. It is also very useful to evidence the quasi-continuous features characteristic of W in WEST plasmas and compare them with theoretical computations [3].

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WEST impurity spectra variation through ohmic reference pulses during C9 campaign in the 225-302 Å range

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Since December 2022 WEST has tested actively cooled solid W monoblock plasma facing units mounted on a flat crown forming the lower divertor. These tests aim at long plasma discharges, with thermal loads of the same order of magnitude as those expected for the ITER vertical part of the lower divertor (10 MW/m^2). Deuterium plasma durations of more than 360 seconds have been obtained in a stable L-mode X-point configuration. The plasma impurity content must be as low as possible to minimise main ion dilution and radiation cooling, both deleterious for performances of a future burning plasma.

Two VUV spectrometers are used to characterise plasma contamination due to impurities coming from plasma facing components. One is equipped with two mobile detectors and dedicated to physics studies, the other one is equipped with a single fixed detector dedicated to monitoring impurities along a campaign and from campaign to campaign. Here the focus will be put on this latter spectrometer which spectral range is 225-302 Å and acquisition time is 11 ms. Its fixed line of sight crosses the plasma centre almost in the midplane.

A thorough line identification of the VUV spectra has been performed since 2018 in various configurations: ohmic, with LHCD heating, with ICRH heating, with both heating. These lines are identified mainly from the Kelly tables [1] and the NIST database [2] and with the HULLAC code [3] for validation. We present here our line identification work for Ne. It was injected in the X-point region for X-Point Radiator studies [4] during the previous (C8) campaign.

During the last experimental campaign C9 (January-April 2024), we performed monthly an identical ohmic pulse scenario ("reference pulse") in lower X-point configuration at the start of a session. Here we compare the spectra observed during the stationary phases of the February, March and April reference pulses.

First, the brightnesses deduced from the spectra decreases from month to month both for lines and for the background. The strongest contribution to the latter is a W quasi-continuum. Although the radiated fraction during ohmic pulses remains stable [5], we see Cl and O lines diminishing along the campaign and boronisations. This brightness decrease is confirmed by the Zeff and the total radiated power decrease from pulse to pulse. There are also qualitative differences: for example the March spectra do not show Copper and Nitrogen lines while these latter largely dominate the April spectra.
The detailed study of the "reference pulses" show that differences exist in plasma parameters: over the three months, the central temperature decreases from 1.4 keV to 1.1 keV and the distance from the plasma separatrix to the closest LH antenna changes from a few millimeters to several tens of millimeters. When the central plasma temperature is lower than 1.5 keV then radiation increases with temperature. Here the background level changes by a factor 2.5 and 4.5 which shows that other parameters play a role. The comparison with the visible spectra measured on the lower divertor shows clearly that the lower divertor is not the main source of impurities. More probably the main contributor is the closest LH antenna where Copper elements face directly the plasma.

Second, the April spectra show clearly the legacy of the previous session: X point radiator with N_2 gas injection. To conclude, the impurity line identification helps on the one hand to determine the

impurity production processes and consequently to adapt the plasma's magnetic equilibrium; on the other hand it helps to assess the plasma conditioning state and performance.

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Poster session / 37

Molecular dynamics simulations of the defect evolution in tungsten on successive collision cascades

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Molecular dynamics (MD) simulations of successive collision cascades within the same simulation domain and further defect evolution were performed using two different inter-atomic potentials (IAP) in tungsten, one EAM based and the other a 'quantum accurate' machine learning potential, SNAP. The micro-structural changes are analyzed as a function of displacements per atom (dpa) up-to irradiation dose of 3 dpa. Five simulations are carried out at primary knock-on atom (PKA) energies of 20 keV and 50 keV with 3000 PKAs each, for observing stochastic differences in the evolution of damage. The simulation output was analysed after each PKA. The annealing simulations at different temperatures of damage accumulated at different dpa are also analysed using Machine Learning and deterministic methods for defect analysis. Results for the variation of the number of defects, number of defect clusters, their size and morphology distribution are compared for the two energies and two IAPs.

It is seen that for a given IAP, the number density of defect clusters as a function of dpa does not depend on the energy of the PKA used in the simulations implying that, like dpa, it could be a good measure of material property changes in irradiated materials. In contrast, the defect sizes depend strongly on the energy of the PKA. It is also seen that the micro-structure resulting from the EAM potential was mostly composed of <111> and <100> dislocations, while that from the SNAP potential was mostly composed of small, sessile, C15 ring like structures with a smattering of smaller <111> dislocations and very few <100> dislocations. The rings formed in SNAP potential remain stable and sessile for 10 ns simulations even at 2000K, resulting in significantly different microstructure from the EAM based potential. The results from the two IAPs with regard to defect morphology are validated against the experimental results of dislocation types, density and size distributions.

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The effect of an atomic hydrogen on the kink formation in a <111>{110} screw dislocation in bcc tungsten: atomistic study

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During D-T nuclear fusion reaction, plasma-facing materials, e.g. Tungsten (W) in ITER, are exposed to a hydrogen-rich environment. Hydrogen is easily absorbed into W and alter the material behavior. Conventionally, hydrogen is well known to cause hardening behavior of materials. Solute hardening is a typical phenomenon associated with hydrogen-induced hardening and it is traditionally understood by dragging or pinning effect as hydrogen atoms impede dislocation motion. On the other hand, enhanced dislocation activity by hydrogen, either by easy kink nucleation or migration, was recently reported, and this observation claims hydrogen-induced softening behavior. In this presentation, we try to reveal the effect of hydrogen on dislocation motion in W, by investigating how the kink nucleation energy barrier changes with the applied shear stress when an atomic hydrogen is around a screw dislocation in W using the chain-of-states method.

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Spectroscopic analysis of wall conditioning and ECR-heated pre-ionization phases in MT-I spherical tokamak

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The optical actinometric technique is used to investigate the addition of impurities in the argon and helium microwave discharges during the wall conditioning process of the MT-I spherical tokamak. This technique normalizes the change occurring in the electron energy distribution function with changing plasma conditions through the emission intensity of the selected Ar/He lines. Any change in relative spectral intensities correlates with the group of electrons involved in the electron impact excitation and the concentration of the plasma species involved in the optical emission. The study investigates the impurity level and the change that occurred in the electron temperature and electron density by using relative intensities, Boltzmann plots, and stark broadening of the selected Ar/He lines. Optimization of the pre-ionization phase is also necessary to step forward to the main tokamak operation. The spectroscopic characterization is performed in terms of plasma parameters, with the sequential imaging of the electron cyclotron resonance (ECR)- heated plasma zones displaying their growth and progression. At lower fill pressure, plasma imaging illustrates the two distinct ECR-heated plasma zones corresponding to the first and second harmonics. The studies provide insights into the physics of preferential plasma heating in space and time-varying magnetic fields producing ECRH zones.

Keywords: MT-I Spherical Tokamak, Microwave resonance heating, Optical actinometry, Impurity level, ECR-heated plasma zones, Sequential plasma imaging

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Development of a Numerical Solver for Partially Ionized Plasma for Fusion Using an MHD Scheme

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It appears that a partially ionized plasma is formed around any protruded interface of different material phases in a fusion plasma. Such interface potentially and intrinsically releases neutral gas from outgassing, sputtering and evaporation, and ablated vapor from solid, for examples dust, sublimated plasma facing components (PFC), and liquid, for examples molten droplets, liquid PFCs, materials. This is induced by ambient pressure, heat deposition and mechanical structural stress of the interface in contact with a hot fusion plasma. In addition, neutral gas can be fed from external sources for several objectives, for example heat load mitigation during Type-I ELMs and disruption [1], probing [2], pellet ablation [3]. Even the fuel plasma particles can be neutrally recombined at PFCs, so that neutral particles are produced [4]. Such neutral gas mixes with plasma, and consequently, atomic processes, mainly via collisions, render such a mixture to be a partially ionized plasma. Certainly, some atomic processes can be ensured via visible light emission from fusion devices [5].

For multiple-element plasma, a full set of kinetic equations, as equation of motions, of all species are numerically solved with the coupling terms describing all possible atomic processes. These are associated with an excitation, a de-excitation, an ionization, a neutral recombination, and so on, among dissimilar species [6-8]. These include the source and sink rate, the momentum transfer rate and the energy loss and gain rate via collisions. However, computational power is strongly required to achieve such heavy calculation.

The aim of the presentation is to illustrate the overview of the numerical solver of a partially ionized plasma under a magnetic field using a magnetohydrodynamic (MHD) formulation [7-9] in our project. Apart from a thin sheath next to the interface, beyond the sheath edge, that is from a presheath region, the quasi-neutrality is approximately held for transient events driven by MHD. This means that the MHD effect provided to a fusion plasma within the timescale larger than the electron collision time but less than the MHD time should be well approximated by the MHD scheme. This inspires the development of such numerical code to investigate the impurity transport in a partially ionized fusion plasma affecting the MHD transport, which includes the MHD stability induced by impurities, the triggering of MARFE and disruption, the radiative mantle in a mitigation process. The presentation also aims to provide the potential applications of the MHD scheme for a partially ionized plasma, for example the modeling of the impurity transport in a low power fusion device and the investigation of liquid metal PFC.

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Poster session / 27

Energy levels, transition rates, lifetimes of transmutation of tungsten atoms He-like-(Hf, Ta, Re and Os) deduced from relativistic multiconfiguration Dirac–Hartree–Fock and many body perturbation theory calculations

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The present study has determined excitation energy of the 127 states of the transmutation of tungsten atoms He-like-(Hf, Ta, Re and Os). In this work, we use the ab initio MCDHF and MBPT methods implemented in GRASP2018 and FAC codes, respectively. We extend the calculation for n = 8 to improve the precision of the atomic data used in line identification, plasma modeling and diagnostics of astrophysical plasmas. The BI + QED effect has been included in the calculations to improve the generated wave functions. Wavelengths, weighted oscillator strengths and transition probabilities for E1, E2, M1, and M2 transitions among these levels are also given. A comparison is made between our two sets of results obtained from GRASP2018 and FAC codes, as well as with the available theoretical ones, although there are only a few levels. A satisfactory agreement is found between them. In fact, while comparing the lifetimes calculated with both MCDHF and MBPT methods we find a good agreement around 3 % for helium like isoelectronic sequence Z = 72–76. The present set of complete results for radiative and excitation rates for all transitions of He-like-ions will be highly useful for the modeling of a variety of plasmas such as those investigated in controlled thermonuclear fusion, laser and plasma physics as well as astrophysics.

Poster session / 44

Unveiling Surface Chemistry and Hardening Mechanisms in Fusion and Nuclear Materials

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This work presents a combined theoretical and experimental approach to understand the complex surface phenomena occurring in fusion and nuclear materials.
Fusion Materials: We investigate the interaction of low-Z (lithium and boron) coatings with carbon under extreme fusion plasma conditions. A multi-scale approach using computational modeling, real-time plasma diagnostics, and ex-vessel in-situ experiments unravels the evolving characteristics of these surfaces. We explore the effects of these coatings on deuterium retention and chemical sputtering, with a focus on the critical role of oxygen in driving the surface chemistry during hydrogen irradiation. These findings can hold significant implications for fusion plasma confinement behavior. Additionally, computational studies expand beyond limitations of empirical methods, paving the way for a strategic approach integrating advanced modeling tools with in-vessel and ex-vessel diagnostics.

Nuclear Materials: We analyze the hardening behavior of irradiated and pristine BCC and FCC alloys for nuclear applications. Nanoindentation testing reveals significant hardening effects by both experiments and computational modelling. The observed qualitative agreement between experimental load-displacement data and MD simulations suggests sluggish dislocation diffusion, reduced defect sizes, and tetrahedral stacking fault nucleation as key strengthening factors. Notably, experimental observations point towards the nucleation of interstitial-type prismatic dislocation loops during loading, shedding light on the material's hardening mechanisms. In FCC materials specifically, these loops interact to form pyramidal stacking faults, primarily driven by ⅓⟨100⟩ Hirth dislocation lines. The co-existence of both defect types observed in the plastic deformation zone further supports the combined experimental and computational approach. Reported mechanical data, experimental and numerical, are validated by microstructural SEM and TEM investigations. Finally, we discuss the advantages and limitations of conventional interatomic potentials and machine-learned models in simulating nanoindentation tests.

This work provides valuable insights into surface chemistry and hardening mechanisms in both fusion and nuclear materials, paving the way for advancements in material design and optimization for extreme environments.

Poster session / 38

Multiscale Modelling of Hydrogen Retention in High Dose Irradiated Microstructures

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Component-scale predictive models for how hydrogen isotopes interact with, and are retained by, irradiation-induced defects are required to inform design decisions in materials for fusion power. This is a multiscale materials modelling challenge, with a conceptual gap between electronic structure calculations on one hand, which provide high accuracy estimations of idealised elemental defect structures and binding, and partial differential equations on the other, which provide the long timescale evolution behaviour. This gap is due to the complexity of realistic irradiation microstructures.

We have developed and validated an interatomic potential suitable for large-scale molecular dynamics simulations in tungsten with hydrogen isotopes present[1], and used it to explore how defects respond to decoration by deuterium and tritium. In parallel, we have refined and simplified the mathematical formalism required to model generic gas-retention by complex defects, and developed a library of code providing a simple, flexible framework for modelling tritium retention in complex microstructures integrated into MOOSE.

In this talk I will describe recent work at UKAEA generating hydrogen isotope-decorated high-dose microstructures in tungsten[2,3], and validating atomistic and finite element simulations[4] against laboratory-scale experiments.

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Poster session / 50

Refinement of Edge Plasma Density Measurement Using Bayesian Inference, Gaussian Process Methods, and CR Model Utilizing Hydrogen Atomic Data in the KSTAR BES System

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In this study, we present an approach for the precise determination of edge plasma density profiles in the KSTAR tokamak, leveraging Bayesian inference and Gaussian process regression techniques in conjunction with atomic data. The methodology relies on a collisional radiative model that captures the interactions between neutral deuterium beam atoms and plasma constituents. This model, built upon atomic cross-sections and rate coefficients, enables the representation of D-alpha line intensities as functions of plasma density. The hydrogen beam emission spectroscopy (H-BES) diagnostic, with its 16 radial and 4 poloidal channels offering ˜1 cm spatial resolution, provides high-resolution measurements of Doppler-shifted D-alpha emissions. The incorporation of poloidal measurement channels and the assimilation of equilibrium data significantly enhance the precision of radial density profile estimations. Gaussian process priors are employed to model the density profiles, and the posterior distribution is investigated using Markov Chain Monte Carlo (MCMC) methods. The integration of H-BES measurements with data from two-color interferometry and Thomson scattering enables the simultaneous estimation of edge plasma density profiles and the calculation of an absolute calibration factor. The successful application of Bayesian inference and Gaussian process density profile prior, coupled with the utilization of atomic data in the collisional radiative model, represents a significant advancement in plasma diagnostic capabilities. This development enables more accurate and reliable edge plasma density profile estimations, which are crucial for understanding edge plasma physics in KSTAR tokamak.

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Exploring Line Shapes in Fusion Plasmas under the Influence of Periodic Electric Fields

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The impact of varying periodic electric fields on the emission line shapes in fusion plasmas, is a subject of significant interest. Tokamak devices, universally employing radio frequency (rf) waves, aim to heat, control, or diagnose plasma through effective coupling. This research focuses on developing a spectroscopic diagnostic tool to analyze the periodic electric field's propagation within the plasma, essential for understanding rf wave-plasma interactions. Additionally, it explores diagnostics for periodic fields generated by nonthermal effects and instabilities, such as those induced by runaway electrons, which influence wave generation in a tokamak. An early detection mechanism for runaway electrons, crucial for the ITER project, is proposed through spectroscopic diagnostics. This study intends to simulate the oscillating electric field's impact on emission line shapes, incorporating the dynamics of charged particles, the oscillating field, and a constant magnetic field. We will present hydrogen line shapes under various fusion plasma conditions, as observed in several experimental fusion devices.

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Study of Electron impact single ionization tungsten ions W64+-W71+

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The cross-sections and Maxwellian rate coefficients of electron impact single ionization is theoretically investigated for tungsten ions (W^{68+} to W^{71+}) for fine structure levels of configurations containing n = 2 orbitals. Maxwellian rate coefficients for ground state are evaluated at the temperature range 20keV to 300keV. Detailed comparison between results from different approximations, binary encounter dipole (BED), distorted wave (DW) and coulomb born exchange (CBE) is presented graphically. The present study of tungsten ions may be useful in fusion plasma modelling and in future comparison.

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Plasma and Neutral Beam Injector Guard Wall interaction using MCNP6 and GEANT4

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The choice of elements in structural materials such as stainless-steel can reduce radiation levels due to particle activation. The dose rate to workers and electrical components is managed by the material used for radiation shielding. This work analyses candidate materials used in the ITER neutral beam duct. Quantitative analysis of radiation effects in the Neutral Beam Injection (NBI) section closest to the ITER plasma region was carried out using GEANT4 and MCNP6 simulation.

The materials analyzed includes ferritic martensitic (F-M) steels at different chromium composition (9-25wt %), bainitic (Fe-3Cr-3W), 316L ITER grade Stainless Steel, Nickel base alloy1 (Ni-25Cr-20Fe-12.5W, 0.05C), SS Nickel base alloy2 (Ni-23Cr-18W-0.2C), 316L ITER grade and 304B4 Stainless Steel. GEANT4 and MCNP6 input geometry was developed based on concentric finite cylinders along a common axis of the neutral beam duct. Included in the ITER geometry are the plasma region, outboard blanket and shield, a neutral beam injection (NBI) port with a stainless steel - water layered beam guard, mid-plane port walls, an adjacent toroidal field coil, cryostat and biological shield. GEANT4 and MCNP6 simulation were used to determine plasma interaction in the heating neutral beam duct closest to the ITER toroidal plasma region.

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The side effects of hydrogen ions on tungsten surface due to glow discharge cleaning procedure in DAMAVAND tokamak

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Hydrogen glow discharge cleaning (H-GDC) is a routine conditioning procedure for the present tokamaks and the future fusion machines, including the ITER. Due to the low energy of hydrogen ions in glow discharge plasmas, the probability of any considerable damage to the plasma facing components was mainly ignored among researchers in the field. In this work, Tungsten and Molybdenum, as the primary candidates for the plasma-facing materials in tokamaks, are considered for studies regarding effects of the H-GDC procedure on these materials during a routine vacuum vessel conditioning in Damavand tokamak. After performing routine H-GDC using pure hydrogen, the formation of loosely attached nano-structure bundles (NSBs) on the surface of the tungsten and molybdenum samples were observed. The presence of the NSBs, which can be a source of dust, would be significant due to their possible effects on the functionality of the future fusion plasma devices. The NSBs are observed on the tungsten and molybdenum samples with the surface temperature of <370 K after 2.5-4 hours of hydrogen ion bombardment having incident energy of ≈ 100 eV and fluence of ≈ 2-3.5×10^{22} m^2. The surface modifications of specimens exposed to H-GDC were examined using a material probe experiment and several surface analysis techniques such as SEM, EDX, and ERDA. Therefore, the formation of loose nanostructures on the wall of plasma confinement vessels, due to H-GDC draws attention to probable damaging effects of this phenomenon upon functionality and outcomes of tokamaks.

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Fuel retention and transport in fusion components

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Tritium (T) transport through the first wall into the coolant is a major concern in fusion reactor studies. When irradiated by plasmas, hydrogen permeation flux through in-vessel components would be significantly higher than that of gas-exposure cases. To support reactor design studies, low energy plasma-driven hydrogen isotope permeation through the first wall has been extensively investigated. This review will introduce our recent research progress in three relevant topics:
(1) Surface damage effects on hydrogen isotope permeation [1,2]. In-situ measurements of low energy deuterium (D) through helium pre-damaged tungsten (W) has been done. With the increases of helium (He) pre-irradiation fluence, the D permeation flux was found to reduce effectively.
(2) The role of W-structural materials interface [3]. The transport behavior of D in W-Cu joining sample was explored using gas driven permeation and thermal desorption spectroscopy. A large number of D atoms were found to be trapped by dislocations and impurities at the intermediate layer.
(3) Isotope effects [4,5]. The co-permeation experiments of H and D isotopes through~mm thickness materials. The H/D ratio of the steady state permeation fluxes was found to be close to the classical theoretical. Hydrogen isotope exchange is an effective method for T removal in fusion reactor materials.

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Fuel retention properties in first wall material: the influence of microstructure, displacement damage and helium

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In future thermonuclear devices such as DEMO displacement damage by 14 MeV fusion neutrons will be created in the plasma-facing materials while they are exposed to high fluxes of ions and neutrals of hydrogen isotopes (HIs) at elevated temperatures. It was shown in several studies in the past twenty years that HI retention and transport will be dominated by trapping at the defects created by the neutron irradiation [1]. Moreover, the synergism between displacement damage creation and presence of HIs needs to be taken into account for realistic predicting of fuel retention and transport in future fusion devices.

I will give an overview on the knowledge gained so far for tungsten (W), being the main plasma facing material in future fusion devices. As presently there is no existing 14 MeV neutron source, most studies were performed by using MeV heavy ions to create displacement damage in W. In order to be able to describe the interaction between HI and defects as well as the creation and evolution of defects and their dependence on temperature and HI flux one needs to isolate and understand the individual processes. An overview of the relevant set of experiments will be given where individual aspects were addressed. For instance, the creation and evolution of defects with temperature was studied where D retention and desorption kinetics were obtained by measuring D depth profiles and D thermal desorption spectra, showing that created defects act as traps for D and the defect densities increase with damage dose [2] and decrease with temperature [e.g. 3, 4]. The synergism between defects and HI was studied by simultaneously irradiating polycrystalline W MeV W ions and exposed to low-energy D at different temperatures ranging from 450 K to 1100 K [3,4], showing increased D retention when defects were created with the presence of deuterium. The effect of microstructure [5] and helium on the surface and in the bulk [6] on HI retention will be addressed and discussed. Recent attempts to study the location of trapped D in displacement-damaged W will be presented [7].

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Database for modelling of D transport and accumulation in W-based and Fe-based materials for ITER and DEMO

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To model hydrogen isotope migration and inventory in a metal under ion irradiation, rate equations are used. The diffusivity, solubility, surface barrier, reflection and sputtering coefficients, mean ion range, and binding energies of deuterium (D) with different types of defects are input parameters in the rate equations. Such parameters can be defined by ab initio calculations by DFT or MD or TRIM code and can be validated by comparison with experiment. TDS experiments are usually performed to derive de-trapping energies and recombination coefficient of D and permeation experiments to derive the diffusivity and solubility. D concentration in defects up to 10 microns can be measured by 3He nuclear reaction analysis, NRA. Defect characterization in materials is carried out by state-of-the-art experimental methods (STEM, PALS, EBSD, FIB-APT, etc.) before and after irradiation. In this contribution, the parameters of deuterium-defect interaction for W-based and Fe-based materials will be critically reviewed. The difference between speculative and reliable data and the interpretation of the experimental results will be shown.

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Tritium transport data for fusion (tentative title)

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Deuterium retention in self-ion irradiated tungsten: influence of irradiation temperature, damage dose, and alloying elements

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Tungsten (W) is considered as a promising plasma-facing material for future fusion reactors. W components will be subjected to an intense flux of 14 MeV neutrons. This will result in creation of radiation defects, production of H and He, and transmutation of W to Rhenium (Re). Radiation defects can trap tritium fuel, posing a stringent limitation to tritium self-sufficiency.

MeV self-ion irradiation is widely used for simulating the displacement damage created by 14 MeV neutrons because it induces dense collision cascades and does not alter the material composition. This approach is being used at IPP over a decade. Several aspects were addressed in the past, such as the evolution of trap sites with annealing temperature or the influence of the presence of hydrogen isotopes. Here we focus on the influence of irradiation temperature, damage dose, and alloying elements. In all cases the irradiated samples are exposed to a low-flux of low-energy deuterium (D) ions extracted from an ECR plasma at low temperature (370 K). This allows to decorate the irradiation-induced defects with D without introducing additional damage and deduce trap densities. Trapped D concentration profiles are measured using D(3He,p)4He nuclear reaction analysis. The D binding states in the defects are analysed using thermal desorption spectroscopy (TDS).

The dependence of the trapped D concentration on the damage dose (0.0001-2.3 dpa) and irradiation temperature (290, 800, 1350 K) was investigated. In the case of irradiation at 290 K, a linear increase of the D concentration with the damage dose is observed up to 0.001 dpa. At higher doses the D concentration starts to level off and eventually (> 0.1 dpa) reaches a saturation value of 1.8 at.%. The same trend is observed in the case of irradiation at 800 K, but the D concentrations are a factor of four lower, indicating a reduced defect density due to defect annealing. Irradiation at 1350 K exhibits a completely different behaviour. At damage doses below 0.1 dpa the D concentrations are lower than in the 800 K case, indicating further defect annealing. At higher dpa levels the D concentration exceeds the 800 K values and reaches 1.8 at.% at 2.3 dpa, showing no tendency for saturation yet. TDS indicates that the nature of D trapping sites is different for irradiation at 1350 K as compared with 290 K and 800 K. Transmission electron microscopy revealed the formation of nm-sized voids in the samples irradiated at 1350 K, which is not the case after irradiation at 290 K and 800 K.

To study the effect of Re transmutation products, W samples containing 0, 1, 3, and 5 % Re were irradiated to 0.5 dpa at 295 K and 1350 K. In the case of irradiation at 295 K, Re addition has little effect on trapped D concentration and the nature of trapping sites. In the case of irradiation at 1350 K, the trapped D concentration decreases compared with pure W: 5 times for W-1 % Re, 36 times for W-3 % Re, and 43 times for W-5 % Re. This can be attributed to the reduction of void growth caused by the presence of Re.

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On the damage threshold in an interstitial hydrogen-occupied tungsten lattice

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Hydrogen isotope (HI) retention in plasma-facing materials, especially of the radioactive tritium, presents severe concerns for the operation cost and safety of future fusion devices. For tungsten (W) with intrinsically low HI solubility, HI retention is dominated by trapping at irradiation-induced defects. To create irradiation defects (i.e., stable Frenkel pairs) in W, a minimum energy transfer of ~40 eV from the incident particle to the lattice atom is required; equivalent to incident HI ion energies of ~1840 eV for hydrogen (H), ~920 eV for deuterium (D) or ~600eV for tritium (T) [1, 2]. However, low-energy HI (415/215 eV for H/D) plasma exposure of W surfaces resulted in the formation of a few nm thin HI-supersaturated surface layer (HI-SSL), which retained an unusually large amount (~10 at.%) of HI [3-5], attributed to trapping at lattice damage during plasma exposure. Although a complete understanding of the sub-displacement-threshold defect production and the resulting SSL formation are still missing, the experimental observations posed an important question to the fusion community, namely: is it meaningful to extrapolate the displacement threshold determined via electron beam damaging [1] to the irradiation conditions in fusion reactors?

In the present work, we revisit the fundamental displacement process and focus on the threshold energy to produce lattice defects in W upon low-energy HI plasma exposure. When interstitial HI and defect sinks co-exist near the primary ion-W collision site, the threshold for lattice damage creation was demonstrated to be even lower than the theoretical formation energy of self-interstitial atoms (SIAs) in W (9.6 eV [2]). HI atom-ion synergy in the presence of a nearby defect sink is proposed to account for the lattice damage observed at the extremely low HI ion energy with respect to the conventionally considered values measured with MeV electron beam [1, 2]. Such a concerted defect production process under HI plasma exposure is expected to occur in PFMs of future fusion devices: under high-energy neutron irradiation, interstitial H/He atoms via diffusion- or transmutation-induced gas production will be present in the PFM lattice nearby defect sinks such as cracks, interfaces, GBs and phase boundaries. Under such conditions, the resulting saturation level of fuel retention may be enhanced significantly, and therefore, should be monitored carefully. Some possible solutions to suppress the described synergistic defect production in future fusion applications.

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Overview of Research Activities and Fusion Facilitites in Thailand

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The first Tokamak Facility (TT-1) is commissioned in Thailand since July 2023. Various research and development activities in connection TT-1 are taking shape, domestically, regionally and internationally. There is an ongoing collaboration work between Thai researchers, NIFS (Japan), and ASIPP (China) on fusion neutron detection and measurement. A facility of linear device for fusion-related materials is also available under the Center for Plasma and Nuclear Fusion, Thailand (CPaF). An overview and summary of these activities will be presented.

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Present status of modelling dynamically modifying rough and/or crystalline surfaces under energetic particle bombardment: Consequences for reflection and sputter yield distributions

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Key input quantities for the modelling of plasma-wall interactions are the energy and angular distributions of the particles impinging onto the wall as well as the corresponding distributions for the particles (re-)entering the plasma.

Traditionally the focus has been on the modifications of the wall induced by the incoming particle influx (i.e. sputtering) and extensive simulation efforts have provided a good understanding of the processes involved (preferential sputtering, recoil implantation etc.) and the main consequences of surface roughness, which typically reduces the effective sputter yield. Significantly less effort has been dedicated to the analysis of the effects of the resulting morphology changes on the distributions of reflected particles. Here we show that - in contrast to the case of sputter yields - changes of the reflected particle distributions are not only quantitative but also qualitative, ie. specular reflection is often strongly suppressed and the preferred direction of reflection is sometimes - and perhaps surprisingly - even shifting towards(!) the impact direction for non-perpendicular influx. BCA-based simulations for a number of cases relevant for fusion applications (e.g. Hydrogen on tungsten and on FeW-systems) using SDTrimSP-2D and molecular dynamics (MD) simulations are given and the involved mechanisms are clarified. As consequence an efficient representation of the reflection distributions is required. For the parametrization in terms of angles and energies an approach resting on a hemispherical orthogonal function system with Chebyshev-based regression coefficients appears beneficial in terms of storage and access efficiency. Consequences for PWI-experiments and simulations will be discussed.

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Global 3D Modelling of Plasma-Wall Interactions in Fusion Devices: Applications and Data Needs in View of ITER and DEMO

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Plasma-wall interactions (PWI) in fusion devices pose significant challenges, including erosion of plasma-facing components (PFC), fuel retention, and plasma contamination by impurities. Accurate modelling of these interactions is crucial for the design and operation of future fusion devices. This talk presents recent advancements in 3D modeling of PWI, highlighting the capabilities and applications of the Monte Carlo code ERO2.0, as well as specific data needs for ITER and DEMO.

ERO2.0 facilitates simulations of PWI with realistic PFC geometries and plasma backgrounds from codes such as SOLPS-ITER and EMC3-EIRENE. Its massive parallelization allows for comprehensive modeling of the entire plasma boundary, including wall material erosion, impurity transport and re-deposition. The code employs a kinetic approach to trace eroded impurities, incorporating atomic and molecular processes such as ionization, recombination, and collisions.
Recent developments in ERO2.0 include handling spatially inhomogeneous multi-species plasma backgrounds and implementing thermal force corrections. These enhancements are critical for simulating erosion and re-deposition. For ITER, ERO2.0 predictions have provided valuable insights into wall lifetime and impurity behavior [1]. The code ' s application to DEMO highlights the challenges of extrapolating plasma parameters to the first wall, as well as the role of charge-exchange neutrals (CXN) in first wall erosion [2].

The presentation will introduce the code, discuss validation efforts in contemporary devices, and present predictive studies for ITER and DEMO. In particular, it will detail the importance of energy- and angular-resolved CXN distributions in erosion simulations for DEMO. Finally, the role of ERO2.0 modelling in the integral approach to PWI in DEMO within EUROfusion activities will be outlined [3].

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In-situ enhanced erosion of re-deposits: conclusions from modelling of tracer injection experiments

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The erosion of redeposited layers is typically larger than the erosion of the corresponding bulk material. However, the modelling of impurity tracer injection experiments in various fusion devices indicates an additionally enhanced re-erosion of particles during the process of layer formation. This can be interpreted as an "in-situ erosion" of transient layers involving particles, which are not yet fully bonded to the surface.

A large number of impurity tracer experiments has been carried out at various devices including for instance TEXTOR, ASDEX-Upgrade, JET and most recently also W7-X. As impurity source originally silane (SiH_4) and ^{13}C containing molecules such as methane ($^{13}CH_4$) or ethene ($^{13}C_2H_4$) have been used, later on also WF_6 and MoF_6 to minimise the influence of chemical erosion. In all experiments a well known amount of these impurities is injected into the edge plasma under well defined and constant conditions. After retrieval of the samples, extensive post-mortem analysis covering NRA, SIMS or colorimetry provided detailed information of the (local) deposition of the impurities in the vicinity of the injection location. The experiments have been modelled with the 3D impurity transport and plasma-wall interaction code ERO. To reproduce the locally deposited amount of injected impurities, in all simulations an enhanced erosion (compared to bulk material) had to be assumed. The magnitude of the enhancement factor depends on various parameters such as impact energy and flux of depositing particles.

The present contribution summarises the main outcome of the available injection experiments and according modelling. Conclusions concerning possible adaptions of erosion yields under certain conditions will be drawn. Finally, a brief discussion about possible studies of enhanced erosion in lab experiments and MD-based modelling will be provided.

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A+M data for validation of tungsten erosion and transport simulations: status and prospects

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Predicting the erosion and deposition of tungsten (W) from plasma-facing components, and the resulting impact of W on the fusion performance, requires an appropriate description of plasma interaction with W ions, atoms, and surfaces. Accurate and validated data on these interactions, and the application of such data to simulations of experiments in existing devices, enables the benchmarking and improvement of crucial predictive capabilities for designing future devices.

Simulations of W erosion and transport in JET, combining the kinetic Monte Carlo code ERO2.0 [1] and the JINTRAC integrated suite of codes [2], successfully reproduce the observed W I emission in the divertor [3] as well as the W density in the core plasma [4] in both L-mode and H-mode scenarios with experimentally validated background plasma conditions. However, comparison of predicted and observed line emission from W ions in the edge plasma (approx. W II to W XX) is challenging, partly due to uncertainties in the calculated photon efficiencies of the W emission lines. Conclusively identifying and isolating individual W lines from the measured visible and UV spectra is another challenge.

The atomic data in W transport modelling include W ionisation, recombination, and photon emission rate coefficients from ADAS [5]. In addition, a multitude of atomic and molecular processes and databases are applied within the EIRENE code [6] in the JINTRAC background plasma simulations. Sputtering and reflection yields for plasma-surface interactions in ERO2.0, and the energy and angular distributions of the sputtered and reflected particles, are based on tabulated SDTrimSP [7] data. While current ERO2.0 simulations interpolate pure-material yields to approximate the mixing of deposited and bulk materials, development is currently ongoing to incorporate mixed-material SDTrimSP calculations with varying material concentrations into ERO2.0.

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Computer study of sputtering mechanisms of fusion relevant materials

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Sputtering of the wall materials of fusion reactors will both affect the plasma as well as the longevity of the wall itself. Even though sputtering as a phenomenon has been known for a long time, the intricate details are still not fully understood. Especially if the wall material is not a pure metal, but either an alloy or decorated by some other elements, the sputtering becomes more complex. At high energy the sputtering yield is dominated by the deposited energy in the surface region, and channeling is, therefore, affecting the sputtering and reflection dramatically. However, at lower energies, the mechanisms are different, as it gets more dependent on the exact configuration of surface atoms and impurities on the surface. We study, utilizing Molecular Dynamics simulations, the atomistic phenomenon of sputtering at low energies (up to around 1 keV). The table data gathered is sputtering and reflection yields, and outgoing angle and energy distributions. In addition to this data needed as input in larger scale models, we can also identify the exact mechanisms present during the sputtering event and identify them for different surface orientations. These mechanisms become even more complex when the surfaces are not pure, for instance decorated with deuterium, which is fusion relevant. We identified that deuterium decoration of the surface will affect the sputtering yield of the tungsten surface.

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Computational analysis of physical and chemically assisted physical sputtering in plasma-facing components

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Understanding plasma-wall interactions is crucial in the development of fusion reactors. These interactions could cause performance loss and contribute to tritium retention by eroding plasma-facing components (PFCs) through physical or chemically assisted physical sputtering (CAPS) [1]. This makes the investigation of sputtering pivotal in fusion reactors. Specifically, CAPS, and more generally the behavior of molecules released from PFCs, where a data gap is evident.

To address this gap, our study focuses on beryllium (Be), for which a large body of experimental data has been obtained from JET, and where the presence of CAPS is confirmed [2, 3]. Since there is a correlation between CAPS and plasma particle content in the surface, we investigate the erosion of Be structures with different surface concentrations (obtained by kinetic Monte Carlo technique [4]).

The Sputtering is modeled by molecular dynamics (MD) simulations, with an extra focus on CAPS. Additionally, binary collision approximation (BCA) calculations are performed for comparison, since BCA increases computational efficiency by neglecting many-body interactions. However, this superior efficiency is accompanied by lower accuracy.

We find that the balance between physical sputtering and CAPS is clearly impacted by changes in the plasma particles ' properties, including isotope type, impact energy, and incident angle. Moreover, we evaluate the effect of the plasma particle concentration in the surface layers, on the contribution of CAPS to the total sputtering yield and on the types of sputtered molecules. Finally, we compare the results of BCA and MD simulations to determine if and where BCA calculations are valid.

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Bulk, surfaces, and grain boundaries in the lifetime of cascades

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Neutron irradiation is an engine in a fusion reactor that generates power, but not all that controllable. The uncontrollable nature of neutron in a magnetic field still needs to be controlled to some extent in order to safely operate the fusion power plant, and one of the potential solutions is to use a tough plasma-facing material. W as a plasma-facing material unavoidably has grains, and the durability of W under neutron irradiation is affected by microstructural properties such as grain size distribution.

In this talk, we compare and contrast the differences in defect population, evolution, and annihilation in the damage cascades in various environments, i.e. periodic bulk, near surface, or near grain boundaries, from atomistic calculations. In particular, we try to identify the origin of the kinetic characteristics in each environment, and how we can further improve the damage predictions from atomistic calculations to make them compatible and quantitatively consistent with experimental measurements.

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Simulation of interaction between dislocations and hydrogen/helium in tungsten

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Tungsten is considered one of the most promising plasma materials for future fusion reactors. In the fusion reactor environment, the irradiation of high-energy neutrons leads to material collisions, generating vacancies and interstitial atoms, such as Frankel defects. These microscopic defects gradually evolve into larger-scale complex defects, such as dislocations and dislocation loops, through diffusion and aggregation. These linear defects often form simultaneously during material fabrication and irradiation, and they can absorb point defects, thereby influencing their processes of aggregation and annihilation. Furthermore, dislocation defects have the ability to capture hydrogen or helium atoms, affecting their penetration and retention behavior, thereby impacting the safe operation of fusion reactors.

Atomic-scale simulation methods, including molecular statics and molecular dynamics, are employed to systematically study the interactions between dislocations in tungsten and point defects, hydrogen, and helium atoms. This includes (1) the interaction and migration behavior of two types of point defects in tungsten: 1/2<111> screw dislocations and vacancies/self-interstitial atoms (SIAs) along the <111> direction; (2) the interaction and diffusion behavior of hydrogen/helium atoms with 1/2<111> screw dislocations and 1/2<111>{110} edge dislocations in tungsten; (3) the interaction and diffusion behavior of hydrogen/helium atoms with 1/2<111> interstitial dislocation loops in tungsten; (4) the synergistic effects of dislocations and helium clusters on hydrogen atoms.

These simulation results contribute to a deeper understanding of the mechanisms by which intrinsic dislocations in tungsten affect defect evolution and the penetration and retention behavior of hydrogen and helium atoms. Furthermore, they provide input parameters for larger-scale computational simulations and offer theoretical support for explaining experimental phenomena. These research findings provide crucial theoretical support for explaining experimental observations of the aggregation of defect clusters, hydrogen bubbles, and helium bubbles near dislocations.

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Time-Dependent Plasma Surface Interaction Modeling to Address Dynamic Recycling in a Tungsten Divertor

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Integrated modeling of plasma-surface interactions (PSI) provides a comprehensive and self-consistent description, moving the field closer to developing predictive and design capabilities for plasma facing components. This technique, using descriptions for the scrape-off-layer plasma provided by SOLPS, the sheath by hPIC, ion-surface interactions by F-TRIDYN and the sub-surface by Xolotl, has been successfully applied to interpret and predict steady-state PSI experiments in current and future tokamaks [1–4]. Here we describe further developments in our workflow to incorporate time-dependence and two-way information flow, to model transient scenarios (e.g., ELMs). We predict the evolution of W samples pre-damaged by He and exposed to ELMy H-mode plasmas in the DIII-D DiMES [5]. This presentation will describe two simulations to predict dynamic recycling. In the 1st, we explore the effect of ELM frequency. Our simulations show that the plasma solution bifurcates, as the solution converges towards the intra-ELM equilibrium for short ELM cycles, and towards the inter-ELM for long ELM cycles. The plasma temperature increases with the inter-ELM duration, which leads to increases in impact energy (E_{in}) with the inter-ELM duration. For long ELM cycles, high impact energies and shallow impact angles (A_{in}) lead to reflection rates $\sim$1, which dominate D recycling. The high D recycling (rather than ELM cycling) in turn directly impacts the D content accumulated in the W samples. In the 2nd, we explore code-coupling frequency, optimize the initial SOLPS solution and transport parameters, implement E_{in} and A_{in} values calculated by hPIC2, and improve the heat transfer description [6] in Xolotl. These simulations predict particle fluxes increase and heat fluxes decrease by 10-20% with the coupling time-step. A less shallow impact angle leads to smaller reflection rates and significant D implantation. The higher fraction of the implanted flux (and deeper), in particular during ELMs, increases the accumulated D content in the W near-surface region. Future expansion of the workflow includes coupling hPIC2 and GITR to ensure accurate prediction of Ein and Ain, and W impurity transport.

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FESTIM and HTM: leading Open-Source hydrogen transport modelling

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Hydrogen transport modelling is crucial for the development of fusion energy, where understanding tritium behaviour in materials is essential for both safety and component design, such as the breeding blanket and plasma-facing materials. Traditionally, this modelling has been dominated by closed-source tools like TMAP7 or in-house codes, leading to fragmented efforts and limited accessibility within the research community. This presentation aims to introduce and advocate for two pioneering open-source solutions: FESTIM and HTM, which address these challenges and exemplify the benefits of **open-source software**.

FESTIM is a Python-based tool built on the FEniCS finite element library simulating hydrogen transport in materials. It stands out with its extensive verification and validation, comprehensive documentation, and a growing user community spanning over 23 institutions worldwide. FESTIM facilitates simulations of tritium transport, offering transparency, flexibility, and ease of use.

HTM complements FESTIM by providing a dynamic and interactive Python library for hydrogen transport properties. Replacing outdated static paper reviews, HTM automates many manual processes, such as unit conversions and data fitting, and integrates seamlessly into research workflows. Its open-source nature allows for continuous updates and community contributions, ensuring accuracy and relevance.

Together, FESTIM and HTM represent a significant step forward in hydrogen transport modelling. They have been applied to a variety of scenarios, from retention studies in ITER to hydrogen embrittlement research. By fostering a collaborative environment, these tools not only enhance the accuracy and efficiency of hydrogen transport simulations but also democratise access to advanced modelling capabilities.

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Multi-scale modelling of H interactions on W surfaces and W/Cu interlayers

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In this contribution, we will provide an overview of the approach we have been developing over the last few years to model the interaction of hydrogen isotopes (HIs) with fusion-relevant materials. This approach now allows us to model the material from the plasma-exposed surface to the coolant boundary. Following a multiscale (MS) approach, our modeling relies upon electronic structure calculations based on density functional theory (DFT), classical molecular dynamics (MD), kinetic, and/or thermodynamic theory. DFT enables an accurate description of the material's structure at a scale of hundreds of atoms. MD allows us to simulate larger systems of hundreds of thousands of atoms, while kinetic and thermodynamic theories use atomic data as input and deliver macro-scale physical quantities as output. We applied this MS approach to tungsten and copper, considering perfect material structure, point defects, and extended 2D defects such as interfaces [1]. In tungsten, this led us to determine the macroscopic physical conditions that make the surface processes the rate-limiting step for HIs transport. Based on these findings, a kinetic model has been developed and further incorporated into the macroscopic code MHIMS [2]. These results will be briefly reviewed to illustrate the MS approach we developed. Then we will focus the presentation on our latest developments that extend to the coolant side of the divertor plasma-facing components. Two models of W/Cu interface are built to obtain the HIs solution and diffusion properties there. DFT models allow us to determine the stable interstitial sites where HIs could be placed. While thermodynamic and kinetic models were developed to study their solubility within and out of thermal equilibrium conditions. Finally, with MD, we investigated the impact of the mismatch on the copper structure near the W/Cu interface: it leads to the formation and propagation of defects like vacancies and dislocation lines.

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