

2nd IAEA Technical Meeting on the Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasma of Fusion Devices

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Book of Abstracts

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Tungsten density and influx evaluations based on the latest atomic data in EAST tokamak plasma

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Upper and lower graphite divertors in EAST tokamak were replaced by tungsten divertors in 2014 and 2021, respectively, to improve plasma performance in long pulse discharges and accumulate knowledges on the tungsten divertor operation. Studies on the tungsten behavior in edge and core plasmas are then crucially important for improving the plasma performance. For the purpose four fast-time-response [1-2] and four space-resolved [3-4] extreme ultraviolet (EUV) spectrometers have been installed on EAST to observe line emissions from tungsten ions and their radial intensity profiles in wide wavelength range of 5-520Å.

Photon emission coefficient (PEC) data for W43+ at 61.334 and 126.29Å and W45+ at 62.336 and 126.998Å have been used to estimate the density profile of W43+ and W45+ions in the core plasma [3,5]. Tungsten unresolved transition arrays (W-UTA) emitted in long wavelength ranges of 168-225Å, 225-268Å and 278-332Å are analyzed for the study of tungsten behaviors in the edge plasma. As a result, three lines of 186.28 Å, 190.48 Å and 192.02 Å with relatively strong intensities were identified as line emissions from W8+ ions by comparing the time behavior of line emissions from W6+ at 216.219 and 261.387 Å [6,7] and W7+ at 200.367 Å and 200.483 Å [8] [1-4], which are well known as the EUV line emission from low-ionized tungsten ions. The number of ionization events per photon (or inverse photon efficiency), S/XB, for line emissions from low-ionized ions are strongly required to evaluate the tungsten influx rate at plasma edge. A visible spectrometer aimed at spatial profile measurement covering the whole poloidal cross section has been newly installed on EAST tokamak for investigation of atomic tungsten and the M1 transition from tungsten ions, which are observed for W26+-W28+ ions in LHD [9] and W8+-W12+ ions in EBIT [10]. Analyses of full radial density profiles of highly ionized ions tungsten ions and influx rate of low-ionized tungsten ions are attempted based on the PEC and S/XB data.

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Extreme ultraviolet spectra and collisional-radiative model for mid-charged tungsten ions

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Tungsten used as a plasma-facing material for divertor in fusion devices is sputtered and transported into plasmas. The tungsten behaviors in divertor, edge, and core plasmas should be examined by spectroscopic methods, and the spectroscopic models and atomic data for a wide charge state range of tungsten ions are required to analyze tungsten spectra. Many studies have been done on tungsten ions experimentally and theoretically. Extreme ultraviolet (EUV) spectra of tungsten ions have been examined by comparison of measured spectra in fusion devices and electron beam ion traps (e.g. [1,2]) and calculated spectra by collisional-radiative (CR) models (e.g.[3,4]). Wide peaked spectral feature, so-called the unresolved transition array (UTA) at 4.5-7nm wavelength region is found in

plasma with electron temperature $\sim 1\text{keV}$ and is known as numerous overlapped 4d-4f and 4p-4d transitions of tungsten ions. Many little-wide peaks at 2-4 nm are produced mainly by 4g-5f and 4g-6f transitions of Wq^+ with $q=22-30$. These peaks are useful for estimating the charge state distribution and behaviors of these ions in plasmas [4,5]. For ions with $q<22$, no peaks are found in the 2-4 nm region, and we need to find some spectral peaks for ions with $q<22$.

We extend our study to EUV spectra at 10-30 nm where $n=5-5$ transitions of mid-charged tungsten ions are found. We have performed plasma experiments to measure tungsten spectra by pellet injection into Large Helical Device plasmas for this wavelength region. We also try to extend our CR model for tungsten ions down to $q=20$. Details of the comparison will be presented at the conference.

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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.

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Effects of surface roughness on W sputtering

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Kinetic sputtering of materials during bombardment with energetic particles is a well understood process for the case of perfectly flat surfaces. Both analytical models and numerical simulation codes have been established in the last decades showing good agreement for quantities accessible by experiments like the sputtering yield. Still, for many applications, e.g., plasma-facing materials in a fusion device, the assumption of a perfectly flat surface may fail to account for the important role of surface roughness.

A range of effects can be introduced by the geometry of a rough surface, e.g., redeposition of sputtered particles, shadowing, or the influence of locally tilted surface segments on the incidence angle of incoming projectiles. Thus, the assessment of sputtering yields for rough surfaces remains a difficult task.

During the last years, the effect of roughness on W sputtering has been comprehensively investigated at TU Wien by conducting laboratory experiments with a quasi-non-invasive low-flux ion source and a high precision quartz crystal microbalance. Furthermore, the development of a binary collision approximation - based raytracing code called SPRAY allowed for quick calculation of sputtering yield data, where large-scale AFM images of rough W surfaces could be considered as input. It was possible to identify the mean inclination angle δm as a scale-independent roughness parameter that allows consistent prediction of sputtering yields for rough W surfaces [1,2].

Furthermore, oriented and periodically patterned topographies like nano-columnar W structures have also been investigated. In comparison to flat W surfaces, nano-columnar W shows a substantial reduction in the sputtering yield, which appears interesting for applications in nuclear fusion [3,4,5].

In this invited talk, an overview and explanation of roughness effects on W sputtering will be presented, including results for conventionally rough and nano-columnar W surfaces.

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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 $\approx 2\text{-}3.5 \times 10^{22}$ 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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Computational study of tungsten surface sputtering under various conditions

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Molecular Dynamics simulations is a powerful tool in investigating the effects on surfaces under various conditions. It is especially effective for studying the interaction between energetic particles and surfaces. Due to relevancy to fusion, tungsten surfaces have been studied under various conditions. Both pristine surfaces and atomistically rough surfaces have been studied under irradiation by various ion species and energies [1,2]. Simulations have in the last years revealed a plethora of insight into how different surface features will affect the sputtering and evolve under continuous irradiation [3,4]. It has been shown that the sputtering at high energies is directly related to the channeling in a certain direction of the incoming ion, which renders some of the simulation tools assuming amorphous materials questionable [5].

Another important factor under fusion conditions is the effect of hydrogen or its isotopes that are impacting the surface, causing sputtering, or get implantated into the surface layers. We have found that the sputtering by light elements, like hydrogen or its isotopes, is more complicated than previously thought. We found that the sputtering can happen due to several different mechanisms, which are not seen for heavier elements. We have also studied the effect of having the surface saturated with deuterium on the sputtering by both light and heavy ions. Again, we see that having a saturated surface versus a pristine one will affect the results.

All obtained results can be used as input in higher scale models in order to further predict their impact on material lifetimes and plasma properties.

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Challenges in the analysis of the spectra of tritium-containing molecules

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Fulcher Bands of the hydrogenic molecular spectra are complex triplet bands in the visible region (590-630 nm). The electronic transition is identified as $d(3p^3\Pi_u)$ at approximately 14 eV level energy to a $(2s^3\Sigma_g^+)$ at 12 eV, but this is not the sole electronic transition in this region, as the $g \rightarrow c$ ($3d^3\Sigma_g^+ \rightarrow 2p^3\Pi_u$) transition is present in this wavelength region as well. Lines from both of those bands have been identified e. g. in the experimental measurements from divertor regions of the JET tokamak. The $d \rightarrow a$ transition is widely used to learn about molecular behavior in the divertor plasma, but the spectral analysis of such a complex spectrum is challenging. There are large catalogues of experimentally verified wavelength of the rotationally resolved wavelengths of the electronic-vibrational-rotational transitions in the homonuclear H_2 [1] and D_2 [2] molecular spectra (also some for the heteronuclear HD). They include also those of the $g \rightarrow c$ interfering band. Unfortunately, experimental data even for main FB transition are sparse for tritium-containing molecules, and most of the diatomic constants are either calculated using isotope effect or from relatively restricted and old research published by Dieke and Tomkins in 1950. Even for homonuclear tritium the data are restricted to first several (at most ten) rotational transitions for each vibrational transition. In the TEXTOR [3] and JET-C deuterium [4] and tritium/DT [5] experiments the higher rotational transitions were not observed, but in JET-ILW we see a change of ro-vibrational population depending on local injection and recycling at the target places which was not seen in previous experiments. Those conditions result in a rotational overpopulation of the first main-diagonal band, where in the case of high molecular density the observed rotational temperature can even reach the electron temperature. In such cases lines up to $J=17$ can be easily observed (e.g. [6] in D_2 , [7] in H_2), which adds to the complexity of the analysis, both because the wavelengths for such lines may not be following low-order diatomic expansion values, and because the spectra from different vibrational contributions do overlap. For heteronuclear molecules the analysis even more challenging, as in this case there is an overlap between spectra from at least one homonuclear molecule and a heteronuclear one (see e.g. [8]).

In this presentation will be shown experimental spectra from JET tokamak divertor measurements, containing T_2 , HT and DT molecular contributions. The existing molecular data and resulting line identifications and estimations of energy distribution functions will be discussed and compared with available results from other isotope spectra.

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Validating Collision-Radiation-Predissociation Dataset for Molecular Hydrogen with Visible Emission Spectra

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The need for quantitative spectroscopy of molecular hydrogen has experienced substantial demand, leading to the accumulation of diverse elementary-processes data encompassing radiative transitions, electron-impact transitions, and predissociations. In this study, we attempt an experimental validation of this dataset by comparing the vibronic populations across multiple molecular hydrogen levels: EF1Σ⁺g, H1Σ⁺g, D1Π[±]u, GK1Σ⁺g, I1Π[±]g, J1Δ[±]g, h3Σ⁺g, e3Σ⁺u, d3Π[±]u, g3Σ⁺g, i3Π[±]g, and j3Δ[±]g, measured from thousands of emission lines observed with a custom-made Echelle spectrometer. Our analysis incorporates a collisional-radiative model (CRM) that relies on the most up-to-date dataset and on spectrally observed populations from Large Helical Device (LHD) plasmas. Remarkably, we find that predissociation, which is the spontaneous dissociation process of excited molecules, is crucial for accurately replicating the observed outcomes, although many of the previously-reported CRM for molecular hydrogen have neglected this effect. We also demonstrate the possibility of a new divertor diagnostic technique utilizing the measured molecular spectrum interpreted through the CRM with predissociation included. This research also highlights that incorporation of predissociation data for hydrogen molecular isotopologues (H₂, D₂, T₂, HD, HT, DT) is essential for the interpretation of future burning-fusion plasma spectroscopic diagnostics.

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Inclusion of opacity in collisional-radiative models of hydrogen-like He and D to explain discrepancies with line intensity measurements in the JET tokamak

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An understanding of the description of the discharge fuel, either D or He, is essential in order to model processes in the plasma edge and divertor, these processes including transport simulations of the plasma exhaust and the determination of plasma-facing surface erosion. The emission from the fuel species is described by collisional-radiative models. However, discrepancies have been found

between the models and observations made in the JET tokamak. Lawson et al. (2022 and 2023a) give detailed measurements of He II (He+) Lyman series line intensities and their ratios and also make comparisons with He II Balmer and Paschen series members. A collisional-radiative model involving routinely occurring opacity is developed in order to explain the observations. Attention is given both to the equilibrium discharge phase when constant line intensity ratios indicate very similar temperatures for the plasma regions emitting the hydrogen-like radiation and exceptional phases in which the line intensity ratios deviate from these near-constant values. In particular, the variation of the electron temperature throughout discharges is illustrated. Increases in temperature during the non-equilibrium, exceptional phases are understood in terms of transient effects of recycling particles. Pulses in which additional opacity beyond that routinely occurring are investigated. Both the routinely occurring opacity and the limited temperature range of the emitting plasmas are expected to have implications for the interpretation of various analyses.

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Lawson K D et al., 2023a, Report 'He II VUV and visible line intensity measurements in the JET tokamak'

*See author list of 'Overview of JET results for optimizing ITER operation' by J Mailloux et al., 2022, Nucl. Fusion, 62, 042026

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Electron collisions with molecular hydrogen and its isotopologues

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Electron-molecule cross sections resolved in the rovibrational levels of the target are required for determining the properties and dynamics of many low-temperature plasmas. We have applied the Molecular Convergent Close-Coupling (MCCC) method to produce a comprehensive set of vibrationally-resolved cross sections for electron collisions with molecular hydrogen and its isotopologues comprised of more than 60,000 entries. This complete collision data set is available to the research community via the dedicated MCCC database (mccc-db.org). For H₂ the data set includes transitions from all bound vibrational levels of the ground electronic state to all vibrational levels of 18 excited electronic states (all states in the $n = 2, 3$ shells) with similar datasets for each of the isotopologues. We are working on producing a vibrationally resolved set of cross sections for scattering on the electronically excited $c^3\Pi_u$, $a^3\Sigma_g^+$, $B^1\Sigma_u^+$, $C^1\Pi_u$, and $EF^1\Sigma_g^+$ states of all H₂ isotopologues with first results (not vibrationally-resolved) already available. Recent calculations have also been performed for vibrationally-resolved ionisation of the $n = 1-2$ states, as well as fully rovibrationally-resolved transitions within the ground state and between the ground and $n = 2$ states. An overview of the available MCCC dataset will be presented, and examples of its utilisation in fusion and astrophysical plasma modelling will be given.

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Contributions of metastable states and non-Maxwellian EEDF to electron-impact ionization of tungsten ions

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Tungsten is being considered as a plasma-facing material in magnetically confined fusion devices, such as ITER. Electron collision ionization is a dominant atomic process in fusion plasma which determines the ionization balance of the non-local thermal equilibrium plasmas. Despite great effort have been paid the experimental measurements and theoretical calculations, however, the effect of long-lived excited states in low charged ionic stages need to be investigated[1]. Moreover, reliable EISI data are not available for many tungsten ions[2]. Last but not least, suprathermal electron influence and non-Maxwellian rate coefficients of high charged W ions remain unclear.

Therefore, we investigate the contributions of metastable states and non-Maxwellian EEDF to electron-impact ionization of tungsten ions, and aim to provide accurate electron-impact ionization rate coefficients of tungsten ions. Comparison between the previous experimental measurement results and present calculation show a prominent contribution of metastable states in low charged states such as W7+-W10+ ions[3-4]. Moreover, we performed calculations of detailed electron-impact single ionization cross sections for tungsten ions, spanning charge states W38+-W45+[5]. We demonstrate the influence of non-Maxwellian distribution on the rate coefficient of the W46+-W55+[6]. The data obtained are expected to be useful for modelling plasmas for fusion applications.

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Energy, angular and atomic level distribution functions of sputtered tungsten based on spectroscopic investigations

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Sputtering is one of the fundamental processes at plasma-facing components in fusion experiments as the lifetime of the components strongly depends on the sputtering rates. Therefore, it is of paramount importance to understand the processes underlying the sputtering, including the energy, angular and atomic level distribution functions of the sputtered tungsten (W). These distribution functions are further essential input parameter for erosion codes.

One aspect of the presented research deals with the investigation of the initial atomic level distribution of sputtered W. This distribution needs to be taken into account for the interpretation of spectroscopic data and further the determination of the net erosion via so-called S/XB values in fusion devices [1]. However, this initial atomic level population within the fivefold ground term $^5D_{0-4}$ and the metastable 7S_3 level of sputtered W remains an open question. On the one hand, experiments in the tokamak TEXTOR suggest a nonphysical effective temperature to describe the atomic level population distribution via a Boltzmann distribution [2]. This results in a strong population also of other levels and not only of the ground state. On the other hand, ion beam experiments for different materials show a strong population of the ground state only [3]. Using a new approach, we studied this open question in the low density and temperature plasma of the linear plasma device PSI-2. Via an imaging spectrometer with a high spatial resolution (50 $\mu\text{m}/\text{pixel}$) the temporal line intensity development as a function of distance to the target was studied for different transitions

of W I. In the experiments, the W atoms were sputtered by mono-energetic Ar^+ ions at 80 eV. The target was cooled using water-cooling and different target temperatures were investigated. A second aspect of the presented research deals with investigating the energy and angular distribution functions. These strongly influence the transport into the plasma and, moreover, the re-deposition of sputtered material on the inner vessel. Via ion beam experiments, these distribution functions are well accessible for high impact energies and can be described by a cosine angular distribution and the so-called Thompson energy distribution [4]. However, for the impact energies relevant in fusion research, of up to several hundred electron volts, the data is only rare and deviations from the distribution functions are reported [2]. To investigate these deviations and close the remaining gap of information, we carried out experiments and subsequently modeled the line shape emitted by sputtered W atoms via a Doppler-shifted emission model. The experiments were carried out in the linear plasma device PSI-2, where W samples were exposed to low density ($n_e \approx 2 \times 10^{12} \text{ cm}^{-3}$) and temperature ($T_e \approx 3 \text{ eV}$) argon plasmas. The ions hitting the sample were accelerated due to biasing the sample to mono-energetic impact energies in the order of 100 eV. The light emitted by the sputtered atoms was detected via a high-resolution spectrometer with a resolving power of $\lambda/\Delta\lambda \approx 7 \times 10^5$. Until now, the finite size of the targets has not been taken into account in the analysis of the observed spectral lines during sputtering. The standard emission model used so far, which assumes an infinite target or point source, fails for observations with two lines of sight. This gap could be removed due to the new finite-size model.

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Overview of Thailand's Tokamak 1 Experimental Studies

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Thailand is one of the countries that recognizes the importance of fusion technology and has a national plan for its implementation. The Thailand Institute of Nuclear Technology (TINT) has been engaged in the development of a tokamak device known as Thailand Tokamak-1 (TT-1) since 2015. This device is derived from the HT-6M, a previous tokamak device developed by the Chinese Academy of Science (ASIPP) in China. The TT-1 tokamak is scheduled to be the inaugural fusion device to be installed at the Thailand Institute of Nuclear Technology (TINT), located at the Ongkharak location in Nakhonnayok province. The objective of the TT-1 is to provide researchers from Thailand and surrounding areas an opportunity to access a facility that facilitates scientific investigation of fusion technology and design. Additionally, it provides a platform for human resource training in plasma control, experimental planning, tokamak operation, and the conduct of fusion-related research. The TT-1 exhibits a compact form, characterized by a major radius (R) of 0.65 m and a minor radius (a) of 0.20 m. The plasma current (I_p), and the toroidal magnetic field strength (B_t) have the potential to be enhanced to values of 150 kA and 1.52 T, respectively. The main parts of the device were assembled at ASIPP before being shipped and installed at Thailand Institute of Nuclear Technology (TINT). In terms of hydrogen plasma discharge, it will be initiated with ohmic heating in the first phase of plasma operation, which is expected to start in 2024. In the next operating phase, the TT-1 will be equipped with the neutral beam injection (NBI) system in order to generate plasmas characterized by high temperatures and density. Based on the on-site discussion of the device design, the diagnostics that will be developed and installed as planned for the first phase are introduced in this paper. In addition, a schematic overview of the sites for installing the diagnostics is reported.

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ITER Spectroscopic Diagnostics and Atomic Data Needs

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Studies of H₂ molecules in the plasma boundary of Wendelstein 7-X

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Charge-exchange deuterium flux to the main chamber wall and its induced material erosion in EAST

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Erosion of the ITER main chamber first wall (FW) beryllium (Be) armour is expected to affect the lifetime of FW panel, dust formation, and release of Be impurities potentially leading to enhanced sputtering of the W divertor and tritium retention due to co-deposition. The ITER FW panels are shaped to protect leading edges and misalignments, which leads to magnetically shadowed regions, where impurity re-deposition and fuel co-deposition can occur. In addition to plasma ions, charge exchange (CX) neutrals in ITER and future reactors will play an important role on the first wall erosion and overall fuel retention, but the extent to which they contribute is still unknown.

A low-energy neutral particle analyzer (LENPA) based on the time-of-flight method has been developed on EAST to measure the flux and energy of neutral particles to the first wall. The LENPA works in the pulse-counting mode and the energy distribution of neutrals is obtained based on the flight-time of particles. A 220 mm diameter chopper disc with 32 equally spaced slots has a maximum rotating speed of 300 Hz, resulting in a LENPA detecting period of 104 μ s and a slit half-open time of 1.07 μ s. After freely streaming 4170 mm, the chopped neutral particles reach the detector located at the end of LENPA. In the LENPA detection range, more than 85 % of neutral particles are in the energy range of 20–1000 eV. The integrated neutral flux in the energy range of 20–1000 eV increases with line-averaged density in ohmic discharges due to the increased CX reaction rates in a higher density plasma. Compare to the discharges fuelled with SMBI, the discharges without

SMBI have more lower energy neutrals at the similar line-averaged density due to higher edge neutral density and proximity of fuelling. Due to the deeper penetration depth by SMBI fuelling, the neutral particles are generated closer to the core plasma and have higher energy. It was found that the neutral flux increases with heating power in all energy range. The mean energy of neutral particles increases significantly compared to the ohmic discharges. The higher ion temperature and edge density in auxiliary heated discharges result in higher neutral flux in all the energy range.

A quartz crystal microbalance (QMB) was installed together with the LENPA system on the equatorial port of EAST [2]. The neutral-induced material erosion rates and the neutral energy spectrum were measured simultaneously by the two real-time and in-situ diagnostics. The neutral-induced Al erosion rates for the 11 long-pulse full discharges are given by experimental measurement from the QMB and the theoretical calculations according to the neutral energy spectrum from the LENPA, which are consistent with each other. It is proved that higher density and heating power can increase the flux and energy of neutral particles, which results in stronger neutral-induced material erosion. The real-time Li powder injection during discharges can reduce the erosion rate due to the lower recycling and the resulting lower neutral flux.

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Detailed charge exchange neutral distribution modelling for the ITER main wall

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A summary on the numerical assessment of detailed distribution of neutral particles impinging specific diagnostic surfaces in ITER (i.e. mirrors on upper-outer limiter or midplane) was given. Demonstrated are the EIRENE post-processing of ITER SOLPS4.3 simulations including an extension of plasma on an artificial grids up to first wall (c.f. based on previous simulations by A. Khan NME 2019). Some modifications in EIRENE were required to also have both energy and angular distributions were implemented (for the poloidal angle α on a given surface). As a main result it was found that detailed distributions give 2 – 3 larger D-on-W physical sputter yields ($\propto \cos(\alpha)$) compared to standard estimates ($\propto 1$). The actual factor depends on far-SOL assumptions used for the extension of the grid to the wall, as well on H/L-mode. The $\cos(\alpha)$ -dependence gives a factor 2. In H-mode the main contribution comes from the tail of the energy distribution (physical sputtering is suppressed for particle below the threshold 200 eV).

As a next step Ne-on-W calculation should be pursued and compared w.r.t its relevance to D-on-W. Also, refined SOLPS-ITER with wide-grid option should provide a better picture. So far only uncorrelated energy and angular distributions collected and an extension to multi-variate distribution functions possible $\propto (\cos(\alpha))$ should be pursued (requiring longer EIRENE run-times for improved statistics and requires large memory). Data compression through MaxEnt regularization techniques are proposed, also to find a better figure-of-merit when mixed (i.e. multi-component) energy and angular distributions are saturated.

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Impact of H, D, T and D-T Hydrogenic Isotopes on Detachment in JET ITER-like Wall Low-Confinement Mode Plasmas

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Measurements in JET ITER-like Wall low-confinement mode plasmas showed that the scrape-off layer at the low-field side midplane was 30% broader and the low-field side divertor plasma a factor of 2 – 3 more strongly detached in pure-tritium than in pure-protium plasmas for otherwise similar core plasma conditions. The conditions in pure-deuterium and in a 40% – 60% deuterium-tritium plasmas were found to be between those in protium and tritium plasmas. These results are statistically significant and consistent with the lower triton than proton velocities and shorter ionisation mean free path for tritium than for protium atoms, as predicted by the EDGE2D-EIRENE code. For all four isotope species and mixes, the onset of detachment was observed within 10% of the same electron density at the edge of the core plasma. The formation of detachment with increasing edge density is identical between the isotope species and mixes: the electron temperature at and adjacent to the low-field side target plate decreased from 20 eV to 1 eV in non-linear fashion over a narrow edge density range, and the onset of detachment was achieved when the electron temperature at the low-field side plate reached 2 eV. The high electron density (pressure) region, formed at the low-field side plate in the near-separatrix SOL when the electron temperature was 0.7 – 1.0 eV, was observed to transition non-linearly from the target plate to the low-field side X-point region. The formation of the high-density/pressure region in the low-field side divertor was independent of the molecular gas pressure in the sub-divertor, and thus the fuelling and pumping rates of the experimental setup. The density limit was 30% lower in tritium than in protium plasmas. The potential impact of hydrogenic collisional-radiative models including the isotope mass and Lyman-alpha opacity will be discussed.

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Modelling of Reflection and Sputtering properties from structured and crystalline surfaces: Old and new insights

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The reflection and sputtering properties of surfaces under energetic particle impact have been studied theoretically and experimentally since several decades and for many systems (especially planar, mono-elemental and amorphous target-systems) a comprehensive level of knowledge does exist. The situation is considerably less satisfying once the target system exhibits more complex features. Here we outline the present state of the modelling capabilities with a focus on SDTrimSP, their comparison and validation with experimental data and on some unexpected features of Fe-W-systems under irradiation.

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(withdrawn) Update on electron-H₂ and -D₂ cross sections

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In this talk will be presented our last results on electron-H₂ and -D₂ collisions. We will focus in particular on the vibrational-excitation, dissociative-attachment, dissociative-recombination and dissociative-excitation processes rotationally and vibrationally resolved.

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Atomic data needs for studying of W sputtering in high density divertor plasmas

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W generation and transport study represents one of the hottest topics for next generation tokamaks with full metal plasma-facing components [1-4]. The existing W sputtering models are based on low density plasma sheath approximation [5-7], which might be not applicable for high density divertor plasmas expected in future machines, e.g. like ITER and DEMO.

In the given presentation we discuss results of recent full kinetic modelling of W sputtering and re-deposition in a high-density plasma sheath. The simulations indicate that

i) using atomic data based on the coronal approximation results at negligible prompt re-deposition of the W ions. This might have important consequences, as the corresponding net sputtering rates (i.e. gross sputtering rates minus prompts re-deposition) might become significant and cannot be neglected as it was assumed up to now.

ii) the coronal approximation is not sufficient for such study and multiple atomic transitions have to be included in the model. We identified the corresponding atomic processes which have to be included into the W sputtering models in a high density plasma.

Based on above-listed results, we present a list of W-relevant data necessary for realistic estimation of the W net sputtering rated in future fusion machines.

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Vibrationally and ro-vibrationally resolved collisional radiative modelling of molecular hydrogen: current status and outlook

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Collisional radiative (CR) models represent the most versatile type of population models used for determining plasma parameters or for predicting for known plasma parameters the plasma behavior. In plasmas used in fusion research the particle temperatures and densities can cover a wide range. Typically, the edge plasma of fusion devices is much cooler than the core plasma, resulting in the presence of atoms and molecules and thus a high complexity of the reaction kinetics. Together with the presence of strong density gradients, processes like Molecular Assisted Recombination or the transition from an ionizing to a recombining plasma regime can play a crucial role. The situation is similar in the negative hydrogen ion sources for neutral beam injection (NBI) at ITER. An ionizing plasma ($T_e > 10$ eV) in the driver region is cooled down by a magnetic filter field to a recombining plasma with $T_e \approx 1$ eV close to the extraction system. Consequently, CR models for atomic and molecular hydrogen are needed, being precise over a broad parameter range.

While the development of models for atomic hydrogen is mostly finished and well benchmarked models exist, the situation for molecular hydrogen is less definite. The reason is that due to the presence of vibrational and rotational sublevels a huge number of input parameters (reaction probabilities for collisional and radiative processes) are needed. Up to a few years ago mostly models resolving only the electronic states were applied due to the lack of appropriate reaction probabilities even for electron collision excitation. Even within the input used for these models large inconsistencies were present. Recently, some gaps in the available set of electronically and vibrationally resolved excitation cross sections for molecular hydrogen have been filled, shifting the main point of interest from electronically resolved models towards vibrationally or even ro-vibrationally resolved models. The presence of deuterium and tritium in fusion-relevant plasmas makes the development of molecular CR models desirable also for isotopomers of H_2 , further increasing the data needs.

Starting point for the present investigations are the well-known Yacora CR models for molecular hydrogen. A combined approach is followed, using three models with different levels of detail: an electronically resolved model for basic investigations on the kinetics of excitation and de-excitation of electronic molecular states, a vibrationally resolved model mainly for the reaction kinetics within the manifold of vibrational states within the electronic ground state X^1 and their impact on electronically excited states and a ro-vibrationally resolved Corona model for the Fulcher band transition ($d^3 \rightarrow a^3$). Final aim are well-benchmarked ro-vibrationally resolved models that can be applied to selected molecular optical emission bands over a broad range of plasma regimes. The current status of the models and the process of benchmarking them versus experimental data is introduced and current data needs are pointed out and discussed.

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Global tungsten erosion and impurity migration modeling for the DEMO with the ERO2.0 code

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Dedicated computer codes are used to address the physics of plasma-wall interaction and related issues of wall lifetime and long-term tritium retention in fusion devices. The Monte-Carlo code ERO2.0 is such an example, which allows numerical modeling of realistic three-dimensional device geometries based on its massive parallelization [1]. In addition to (net) erosion and re-deposition maps on plasma-facing components, the code yields volumetric information about impurity concentrations in the plasma. A fully kinetic approach is used to trace impurities throughout the background plasma, thereby also addressing atomic processes like ionization, recombination, and collisions along the particle trajectory. The code was validated against experimental data from the largest European fusion device JET in the past [2], and predictions were made regarding the wall lifetime for the next step international experimental fusion reactor ITER [3].

In the present contribution, recent code developments, such as the contribution of spatially inhomogeneous multi-species plasma backgrounds to gross erosion calculations will be presented. These developments will then be applied for the first time to modeling the full tungsten European demonstration reactor DEMO, which is currently in the design phase. The ERO2.0 simulations are based on the currently only available DEMO-specific plasma solution [4], which was generated on basis of the 2017 Baseline equilibrium. Due to gaps in the range of (15 - 80) cm between the last simulated plasma grid-point and the first wall, special emphasis will be put on extrapolation assumptions of plasma parameters to the wall and their impact on the transport of tungsten in the scrape-off-layer plasma. The simulations also reveal charge-exchange neutrals to be the driven source of main chamber erosion, while the divertor erosion is mainly driven by seeded Argon ions and tungsten self-sputtering. Beyond, the importance of energy- and angular-resolved charge-exchange spectral characteristics for main chamber erosion calculations will be discussed in detail.

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Ion irradiation of Tungsten metal target for the study of Pakistan Spherical Tokamak (PST) divertor

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The Pakistan Spherical Tokamak (PST) is a small-sized spherical tokamak currently in the design and development phase. A double null divertor configuration is being considered for the steady-state operation of the PST. Two different divertor materials concepts are under consideration for the PST and other devices in the future. The interaction between plasma and tungsten surfaces

leads to noticeable alterations in microstructure and material properties. Tungsten is considered as a divertor material in fusion devices, where it can withstand large heat loads. The interaction of high-energy ions and electrons leads to swelling, blistering, and the formation of nano-cracks, ionization, recombination, and voids in the material.

The aim of this research effort involves examining the impact of helium ions irradiation on tungsten material. Tungsten samples were irradiated with high flux (1×10^{14} , 1×10^{15} and 1×10^{16} ions/cm²) of helium ions to investigate structural changes and surface morphology. Changes in microstructure, residual strain, surface morphology, and hardness of the samples were then observed using XRD (X-ray diffraction), SEM (scanning electron microscopy), and Micro-Vicker hardness techniques. Ion depth profiling was also conducted using SRIM (Stopping and Range of Ions in Matter) simulation for 1 – 10 MeV energy. It was observed that the penetration depth directly increases with particle energy, and Displacement per Atom (DPA) decreases with an increase in energy.

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Redesign of EAEA Plasma Focus Device-1

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- Egyptian Atomic Energy Authority –Plasma Focus device 1 (EAEA-PF1) was successfully redesigned in terms of its electrode system material and dimensions, insulator shape and the energy storage bank to investigate the best plasma focus action.
- A simple-to-perform technique was applied to investigate the distribution of the azimuthal magnetic field induction and the induced magnetic force acting on the plasma current sheath.
- The redesigned device can be efficiently used in many important applications including Controlled Fusion and working as Neutron and X-ray Source.
- Plasma Focus (PF) devices are considered as one of the most effective sources of pulsed neutron emission which is relevant for controlled fusion.
- Using deuterium as the filling gas, fast neutrons with energy of around 2.5 MeV and energetic protons with the energy of around 3 MeV are produced from PF devices [1].
- A passive radioactive source of fast neutrons with similar energy emits continuously, causing inconveniences in handling and storing. In turn, PF generators do not have activation problems for storage and handling [2].
- PF devices have the advantage of the ability to operate with some other types of gases or gas mixtures which makes it a generator of a pure x-ray radiation (not accompanied by the neutrons) [3].
- Redesigning the device was the first step to be able to use it in these applications.
- X-ray and Neutron yield had to be improved to make the device applicable in these applications which couldn't be done without modifying the device.

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CollisionDB - an open IAEA database for collision processes in fusion plasmas

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Open issues in the new ITER baseline

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Introduction to open issues in the new ITER baseline with a W wall for $Q = 10$ operation that require experimental assessment.