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Joint IAEA-FZJ Technical Meeting on the Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasmas of Fusion Devices

Summary Report

Virtual Meeting

29 March – 1 April 2021

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Contents

1. Introduction

Tungsten (W) shows useful features favoring it to be used as armour material in the first wall components of future fusion reactors such as ITER and DEMO. Its thermal conductivity as well as ability to withstand high heats and particle loads from the plasma makes it a promising material candidate for reactor regions with harsh conditions, such as the divertor target plates. However, severe off-normal plasma events like disruptions and transients induce energetic plasma particles (hydrogen, helium, intrinsic plasma impurities or impurities eroded from the main chamber) to interact with the W components making W atoms being emitted from the surfaces by sputtering and erosion. Once left the surface, ionization of W particles can take place through charge-exchange processes with electrons and plasma particles. W ions may traverse along the magnetic field lines and get redeposited locally (prompt deposition), proceed to longer distances in the edge region or even end up in the plasma core. In the latter event, much of the plasma energy is lost through radiation, which may lead to rapid termination of the plasma.

This technical meeting was held as a virtual online meeting from 29 March – 1 April 2021 due to the travel and meeting restrictions caused by the global COVID-19 pandemic. The event focuses to the concept of fundamental data needed for simulations and experiments studying the collisional processes of W atoms and ions with the plasma particles. Information gained from these collisional-radiative (CR) processes is crucial for the extrapolations of results from the present fusion devices to future fusion reactors. As importantly, quantification and reducing the uncertainties of the CR and atomic and molecular (A+M) input data is mandatory for the reliability of these extrapolations and other predictions.

Scientific organization of the meeting was a joint collaboration by the Atomic and Molecular Data (AMD) Unit of International Atomic Energy Agency (IAEA) and the Forschungszentrum Jülich, Germany. Session presentations are made publicly available on the event's web page hosted by the AMD Unit. The present meeting represented a unique gathering of experimentalists utilizing fusion devices and linear plasma devices as well as researchers performing edge plasma simulations, fundamental calculations of A+M processes and CR modelling. As an outcome, various data needs, gaps in the data and unknown processes were identified and assessed and future collaboration activities, such as benchmark experiments, were established. In the concluding remarks the session chairs together with the Scientific Committee recommended this meeting to be expanded to a biennial meeting series due to its topical nature. 41 experts representing fifteen IAEA Member States (Australia, Belgium, China, Finland, France, Germany, Hungary, India, Italy, Japan, Poland, Russia, The Netherlands, United Kingdom, United States) and one international organization (ITER Organization) presented their reports on recent data needs, experimental findings and computational results relevant for W and hydrogen procesess in fusion edge plasma conditions.

2. Topics and session summaries

There were in total 24 oral presentations in five sessions:

A. Experiments: Tokamaks, Linear Plasmas, Stellarators
B. Modelling: Tokamaks, Linear Plasmas, Stellarators
C. Experiments: Atomic and Molecular Data, Cross-sections, Processes
D. Modelling: Atomic and Molecular Data Calculations
E. Collisional-Radiative Models.

The scientific contributions were selected by the Scientific Committee with members from the IAEA (Kalle Heinola, Christian Hill), Forschungszentrum Jülich, Germany (Sebastijan Brezinsek) and Max-Planck-Institute Garching, Germany (Ursel Fantz). Brief summaries of the session contributions are given in the following sections.

2.1 Data requirements in experiments with fusion and linear plasma devices and modelling activities in fusion and linear plasma devices

S. Brezinsek (Forschungszentrum Jülich, Germany) chaired this session on edge plasma experiments with tokamaks, stellarators and linear plasma devices.

The session comprised of six oral presentations discussing hydrogen recycling and W sources and concentrations at PSI-2 and JET, spectroscopic studies and diagnostics of W and hydrogen at LHD and at ASDEX Upgrade, neutral particles in Magnum-PSI and applications of optical spectroscopic techniques on magnetized hydrogen plasmas.

The session on modelling activities in tokamaks, stellarators and linear plasma devices was chaired by Sven Wiesen (Forschungszentrum Jülich, Germany).

Seven presentations reviewed data needs in modelling of edge plasma interactions in fusion devices, such as DEMO, ITER, JET and DIII-D.

Xavier Bonnin (IO) gave a brief presentation on the W atomic data needs for ITER. For an improved assessment of W source and validation of transport models in ITER (e.g. SOLPS-ITER), an improved dataset of W S/XB ratios (ionization events per photon excitation) is required. The quantification of S/XB accuracies is critical to climb back from photon emission rates to W plasma concentrations. Especially, the lower-to-mid range of ionization stages W0 to at least W^{64+} is needed. In addition, w.r.t. the interpretation of W emission data, a refinement of the particle reflection data at low energies on W surfaces is needed, including dependencies on the W surface state (surface morphology, dynamic material properties, surface temperature), the incident angles and corresponding hydrogen isotope. Additionally, detailed sputtering yield models as function of local temperature, surface roughness and present impurities are needed. Fast and reliable prompt re-deposition models for W and an overall improved level of accuracy of rate coefficients for atomic processes, i.e. ionization, recombination, radiation and charge-exchange (CX), should be developed. All this will help to deduce a reliable charge distribution model for W migration towards the upstream and penetration into the core for ITER.

Jerome Guterl (GA/DIII-D) presented the status on the theoretical analysis and experimental validation of tungsten erosion and re-deposition in tokamaks based on recent experiments in DIII-D. It was observed that the W prompt re-deposition process in divertor is mainly governed by the ratio of the ionization mean-free path of the sputtered W particle over the sheath width at the target plate. This led to a new scaling law for W prompt re-deposition based on an analytical formulation. For the validation of this model and the in-situ monitoring of W net erosion requires the measurement of photon emission lines associated with the W ionization in charge states $Z > 2$, i.e. typically W-III, W-IV and W-V lines for ITER. It is realized that the governing parameter of W prompt re-deposition has similar values for the divertor plasma conditions in DIII-D experiments and in the ITER-far-SOL. Consequently, experiments that were conducted at DIII-D helped to validate the predictive modelling of W net-erosion for ITER divertor conditions. This was established my measurements of both, the sheath width from erosion of carbon micro-spheres, and the direct measurement of W prompt re-deposition. HPC simulation tools for W/Be PMI modelling have been also developed and are available through the PSI2-SciDAC project.

A similar presentation on W atomic data needs with the focus on validation of W erosion, migration and deposition models (e.g. employing detailed kinetic codes like ERO2.0) was given by Andreas Kirschner (Forschungszentrum Jülich GmbH). In addition, here, an update on the atomic data, i.e. rate coefficients for ionisation, recombination and excitation processes are required, including uncertainties/accuracies. Various sets of atomic data is already available for W, but comes partly with a large scattering w.r.t accuracy in particular for the excitation rates. Recent improvements with respect to metastable states have been developed, however the initial population of the excited states of sputtered W is not very clear (but has a strong influence seen by sensitivity studies). There is also the question of the role of light reflection in the assessment of W data. Overall, assuming that the main plasma is provided by external codes like SOLPS-ITER or EDGE2D-EIRENE (or similar) to the kinetic codes like ERO2.0, there is also a finite uncertainty on this background plasma. Especially plasma transport or surface/atomic data are input to the (fluid) plasma transport codes and the relevant processes are challenging to disentangle. With other words: the quality of the underlying plasma background physics model must be adequate and therefore the required validation process is significant (see below). Additionally, there are non-Maxwellian (i.e. kinetic) effects that are usually not included in codes like SOLPS-ITER (or are implemented only in a very crude way, e.g. by introducing flux-limit factors, etc.), that imposes another uncertainty.

Consequently, a short intervention on the kinetic modelling of fusion plasma had been presented by David Tskhakaya (IPP/CAS Prague). The presentation was split into two parts, i.e. the assessment of a stationary scrape-off layer (SOL) and a dynamic one (e.g. with ELMs). It was reported that electron impact collisions provide no significant deviations with respect to rate coefficients from Maxwell-averaged values, except for the W ionization rates right in the sheath. For ion impact collisions however, deviations were observed especially for CX collisions with impurity atoms and H_2 molecules. A (simple) reduced model for the deviation has been provided by substituting the expression of the temperature dependent rate coefficient $R(T) \rightarrow R(T + 2/3\ E_{\|})$ with the parallel kinetic energy $E_{\|}=mv_{\|}^2/2$. For the kinetic treatment of ELMs, rate coefficients seem to be even more sensitive on time constants and also distribution in space compared to the maxwellian averaged rate coefficient. With respect to data needs, cross-sections of the CX process of W with hydrogen isotopes (e.g. $W + D^+ \rightarrow W^+ + D$) for low impact energies is missing, ideally with high accuracy.

A large fraction of the modelling sessions was reserved also for the ongoing effort on the assessment of hydrogenic atomic and molecular emissions important for the validation process of edge codes. For the JET-ILW, Mathias Groth (Aalto University, Finland) highlighted the aspect of ion-molecular interactions in high density divertors. Fluid codes (like EDGE2D-EIRENE) do predict the onset of detachment but deep detachment has remained elusive. Whereas the variation of the upstream density and power into the SOL is according to the experiment, the predicted fraction of hydrogen recycled as molecules of the W target is between 30-40%, i.e. significant. Of course the mismatch is due to numerous factors, like unknowns in the surface model (i.e. TRIM), the estimated location of the separatrix location (from equilibrium reconstruction), numerical artefacts that stem from fixed boundary conditions in the code (power crossing separatrix). However, additional physics model parameters should help to improve the comparison, i.e. the inclusion of vibrationally resolved molecules (already proposed in 2001 by Fantz et al. but rarely used in the validation process) as well as the reduction of the divertor density (i.e. saturation current/particle flux at target) due to the inclusion of Ly-α opacity in the model. Kinetic transport of molecular ions is also not included in nowadays "standard" models and should be addressed. As next steps, Groth proposes for the validation process not only to infer the profiles from Te and ne (e.g. from improved diagnostics like divertor Thomson scattering systems at DIII-D and recently also at AUG) but also an improvement of the database of molecular data, especially to infer the molecular influx from Fulcher-α bands and the comparison of corresponding EIRENE predictions (e.g. for attached conditions to start with). Lyman-Werner bands are also of interest but unresolved thus far. Three-body recombination lines (i.e. high-n Balmer lines) could be taken into account. Interesting would be also to integrate the Fulcher band analysis into the EIRENE model of vibrationally resolved molecular states (e.g. up to v=14) and comparison with measured spectra. The database for isotopes and molecular isotopomers should be revised and validated. Up to date, only very rarely hetero-nuclear diatomic species (H-D, D-T) were introduced into edge-fluid modelling (even though the capabilities do exist in codes like EDGE2D-EIRENE or SOLPS-ITER since long).

A short report on the current status on Monte-Carlo methods for photon transport (and opacity) in dense divertors was given by Sven Wiesen (Forschungszentrum Jülich GmbH). Such a model exists already in EIRENE for two decades and has been successfully exploited for the ITER divertor design points. However, only recently with the transition towards metallic wall materials, the actual measurement of photon opacity effects (e.g. from Lyman lines) and response of the plasma has become more apparent. Hence, inclusion of photo transport has become again of interest and there seems to be evidence in large and/or dense divertors that Lyman line opacity plays a significant role in the ionisation-recombination balance in the SOL. Early attempts to simplify the problem were to allow collisional-radiative (CR) models to have (semi-) opaque lines just by setting the corresponding rate coefficient for line emission to zero. But depending on the line transition, and especially when transport becomes important, such a simple approach is not sufficient, and photon transport must be done self-consistently with the plasma-neutral transport inside edge codes. For the model needs, and in view of improving the model basis for ITER and DEMO reactors, the isotope effect in the broadening mechanism should be included, as well as collisional broadening that becomes a significant effect in very high density divertors (e.g. DEMO). Wall reflection models for photons are essentially missing, for example on W/Be surfaces or on deposited layers or on surfaces with finite roughness. Since EIRENE is a complex tool, there could be an advantage rom compare the implemented photon transport model and a re-verification for real 3D geometries (with reflections included), e.g. a benchmark with CHERAB could be foreseen. Hybrid transport models, i.e. to allow a split of the opaque (fluid-like) regime of photons from the photonic (kinetic-like) regime could be an option to speed up the photon transport and is part of the TSVV-5 activities in EUROfusion.

A more detailed experimental analysis on the impact of the plasma-molecule interaction on particle losses, atomic line emission and resulting power losses required for divertor plasma detachment has been given by Kevin Verhaegh (UKAEA). Even though the role of molecules in the transition into detachment has been raised by author authors earlier (e.g. on molecular active processes MAR or MAI), details on the actual processes involved have become available only recently with improved diagnostic capabilities. Especially the medium-n Balmer-lines seem to have a non-negligible impact on the ionisation-recombination balance. For the first time, at TCV, the full transition of attached conditions, crossing a detachment onset (with increase of Greenwald fraction for the density) and transition into full detachment could be quantified w.r.t the underlying A&M processes. Verhaegh presented how differences in the simulation vs experiment (e.g. no roll-over into detachment) could be removed by post-processing the data by allowing a dependence on vibrationally excited states in the molecular CX process leading to a much better match as function of density (including the a raising of Balmer-α radiation and roll-over of target-ion flux). Even though the presented results from TCV seem to be consistent with results from DIII-D as well as from JET, they have to be reconfirmed, with specific question arising, e.g. to what extent the isotope effect plays a significant role in the molecular physics for the detachment

onset and to what extent this can be identified/measured in the experiment and modelled, e.g. for JET with a metal wall environment.

2.2 Experiments for atomic and molecular data

Session on experimental research on atomic and molecular processes was chaired by S. Brezinsek (Forschungszentrum Jülich, Germany).

Recent spectroscopic investigations of sputtered W atom species presented by Stephan Ertmer (Forschungszentrum Jülich, Germany) focused on two main topics: 1) line shape measurements of sputtered W atoms to model the energy and angle distribution of sputtered W species (line intensity measurements with Imaging Spectrometer), and 2) measurements of atomic level population of W during sputtering (W emitted light measured with High Resolution Spectrometer (HRS)). Experiments were performed at PSI-2 facility using an Ar plasma (T_e=3 eV, n_e=10^{12} cm^{-3}, T=300 K) on polished W with impacting energies from 70 to 150 eV. Thompson energy distribution and Cosine angular distribution models were applied in a Doppler-shifted emission model and adjusted, when needed, for determining the energy and angular distribution of sputtered W, respectively. The Doppler-shifted emission model assumes a point source light emission and light reflection at the surface and was expanded to incorporate the Zeemann effect and instrument-induced broadening of the spectrometer. The Doppler-shifted model provided good agreement with the experimental results, but varying the Ar^+ impact energy was found to deform the line shape. In the model, the Cosine angular distribution was kept at b=1 and the Thompson energy distribution (literature value n=2.04) was varied. The model provided good agreement with the experiments when using n=2.17, …, 1.99 with corresponding impact energies 70, …, 150 eV. The SDTrimSP simulations showed good agreement with experiments only when an over-Cosine (b>1) fitting value was applied. Future work comprises of expanding the Doppler-shifted emission model to a 2D source, benchmarking the angular distribution with spatial intensity development and investigating the effect of surface morphologies on energy and angular distribution. The atomic level population of sputtered W concerns mainly the five ground states $^5D_{0,1,2,3,4}$ and the metastable state $^7S_3$. In the sputtering experiments with PSI-2 the Corona equilibrium approximation is valid and only spontaneous emission and electron impact excitation from strongly populated lower levels are needed to take into account. Other contributions, such as radiation excitation and electron impact emission as well as cascade contributions from higher states can be neglected in the current PSI-2 experiment. The emitted light was collected with HRS (resolution 50 μm/pixel) as a function of distance d to the target. As the Corona equilibrium was reached due to strongly populated states, the position of the maximum line intensity, i.e. the distance d, is proportional to the velocity v of W atoms leaving the surface and reciprocal to the Einstein coefficient $A_{i,j}$ between atomic levels i and j. However, the light intensity is affected by W ionization and by the geometrical losses by the small W target. The effect of angular distribution needs to be taken into account, which reduces the distance d by a factor of ½. The obtained results show, that the W atoms are sputtered with v=2100 m/s and the W are mainly in the ground state $^5D_0$ whereas the excited states $^5D_{x>0}$ as well as the metastable $^7S_3$ were not found to be populated: $^5D_{x>0}$ and $^7S_3$ are populated in the Ar plasma as their emission intensity peak. Was found to be in equilibrium far too late (resulting in unrealistically high v values). Further work is needed in using different W lines and W target temperatures, plasma source gases and plasma parameters. Also, direct measurements of the population of sputtered W by Laser-Induced Fluoresence LIF) are planned.

Baoren Wei (Fudan University, China) presented the experimental 150 kV Highly Charged Ions (HCI) Research Platform at Fudan University consisting of an Electron Cyclotron Resonance Ion Source and a Cold Target Recoil Ion Momentum (COLTRIM) system. Obtained experimental results for absolute electron capture (EC) cross sections for single and double charge exchange processes were shown for O^{6+} + CO_2, CH4, H_2 and N_2. The obtained EC cross sections were measured in the impact energy range from 7 keV•q to 52 keV•q (2.63 keV/u to 19.5 keV/u) and were compared to the existing values found in the literature. The results showed good agreement with previous works, and in the case of O^{6+} + H_2 process the cross section energy range covered significantly higher values than previously measured. Computational work comprised of charge-transfer cross section calculations for the Ne^{2+} + He collision process obtained with quantum mechanical molecular dynamics (MD) using time-dependent density functional theory calculations (TD-DFT). The theoretical result covered impact energies from less than 10 eV to 3 keV and was found to agree with the previous experimental works. Experiments with COLTRIM comprised of HCI collision studies of 120 keV impact of Ar^{8+} to CH_4 molecule. The resulted dynamics and intensities of CH_4 break-up channels to CH_3^+, CH_2^+ CH^+, C^+ C^{2+} and H^+, H_2^+, H_3^+ were measured with a Coincidence Time-of-Flight (TOF) setup. In addition, report on theoretical studies on the fragmentation of doubly charged hydrocarbon molecules (e.g. CH_4 and C_2H_4) to H_3^+ was given. Reaction paths

and corresponding transition states for the molecular break-up and transitions were calculated with DFT-MD using Atom-Centered Density Matrix Propagation (ADMP) method.

2.3 Fundamental data for atomic and molecular processes

This session was chaired by M. O'Mullane (University of Strathclyde, United Kingdom) and comprised of five presentations on fundamental data production and needs for atomic and molecular processes in fusion plasmas.

The session split into distinct considerations of atomic and molecular data. The commonality linking hydrogen and tungsten is the edge plasma of magnetic confined fusion plasmas. Here there is a great range of conditions with strong gradients in electron temperature and density and in the profiles of neutral species. For hydrogen, a proper description of its evolution from its H_2, or isotopologues D_2 and T_2, molecular form to the atomic forms of H^0 and H^+ requires good fundamental data for the different molecular break-up processes and for the atomic interactions of the neutral and ion. It was pointed out that finite density effects are evident by 10^{15} m^{-3} and shift the cross-over point of the H^0 to H^+ abundance by 0.08 eV at 10^{20} m^{-3}, which is of the same order as the shift due to opacity. This range of densities is easily achievable in the divertors of current and future tokamaks. Collisional-radiative models were addressed in other sessions of the meeting but high-quality data, preferably with an assessed uncertainty estimation, are needed as input. The improvements in close-coupling, and R-matrix, electron-impact excitation data for neutral hydrogen as a function of principal quantum number are due to advances in code and computational capacity. For atomic hydrogen, the dominant or primary processes are well characterized, and any changes in calculated or measured data will be incremental and will not change the interpretation of models based on these data. However, to quantify the results, and disambiguate effects such as opacity and finite density, better fundamental data for the secondary process are needed.

Density also affects the time evolution of metastables, and which levels should be considered as metastable. Modelling of molecular H_2 allows for many metastables but the lower ionized stages of tungsten also exhibit pronounced metastability. The outer n-shell in neutral to a few times ionized tungsten is typically n=5 but the 6s level can be energetically lower. Calculating a high-quality atomic structure, which is essential for the accuracy of any excitation or ionization cross sections built upon it, is non-trivial. Neutral tungsten has a ^7S level in the middle of the ground ^5D quintet of levels. An added, practical, complication is that the most used spectral line in tokamaks for influx measurements, originates from this ^7S metastable. To date the pragmatic and practical approach has been to deduce an influx by measuring an ionizations per photon coefficient (S/XB) in liner machines and apply this to tokamaks since the fundamental atomic data for the excitation and ionization rates was not of sufficient quality. Recent work has produced high quality R-matrix excitation data with confirming spectral measurements of ground, and metastable, originating lines. However, data for the ionization cross section is identified as the major missing fundamental process. For such a long-studied element, there are almost no experimental measurements. The estimations of the direct ionization cross section vary widely and it is estimated that the direct process may only be 50 % of the total. The improvements in the atomic structure calculations should aid in improving calculations of the large excitation-autoionization component.

Remaining in the atomic domain, processes driven by ions such as charge transfer, ionization and excitation are important for modelling abundance, power balance and diagnostic interpretation. However, there is no universal theoretical approach which covers all collision energies ranging from the thermal regime of low eV to fast particles with interaction energies of keV/amu to MeV/amu. Alain Dubois (Sorbonne Université) outlined recent progress on their approach to the faster collisions where the relative motion between target and projectile is classical, but the electron dynamics are described by a non-perturbative solution of the time-dependent Schrödinger equation (TDSE). Up to 4 active electrons, their couplings, and the total and/or target and projectile spins are taken into account with the scattering wavefunction expanded over asymptotic atomic or molecular states. Cross sections for excitation, single and double electron capture of the 3-electron, $H^+ + Li(1s^2\ 2s)$, system are in excellent agreement with experiment. Valence-shell contribution to the single capture, and inner-shell contributions to the single capture and excitation cross sections, show that the 3-electron model predicts the low energy structure missed by independent single electron potentials. Improved numerics also indicate that the oscillations reported for the neutralization cross section of $H^+ + H^-$ arise from coherence effects between double electron capture and other two-electron inelastic channels and are not due to quantum interference between the even and odd orbitals of the transient molecule. A final illustration of the capabilities of the model reported on n-resolved cross sections for $H^+ + H(nlm) - H(n'l'm') + H^+$ which then formed the basis of a combined scaling law over a wide range of energies.

The remainder of the session addressed calculations of fundamental atomic data for different electron driven processes of neutral and charged Z=1 molecules. The reality of fusion plasmas, with a mixture of H_2, D_2, T_2, H_2^+, D_2^+, HD^+ etc., was highlighted in all presentations because the hydrogenic molecular system is sensitive to the isotopic composition. Dmitry Fursa (Curtin University) described their molecular convergent close-coupling (MCCC) calculations for electrons scattering on molecular hydrogen and its isotopologues. Cross sections for excitation of all bound vibrational levels and dissociative excitation of singlet and triplet electronic states from all v_i=0-14 bound vibrational levels of the ground electronic ($X\ ^1\Sigma_g^+$) state are made widely available via the LXCat, AMDIS and the group's MCCC-DB databases. The energy range is from threshold to 500 eV and the comprehensive set of data comprises of more than 60,000 cross sections and is designed for use in collisional-radiative models. As part of the work a major discrepancy in the isotopic and vibrational-level dependence of H_2 dissociation was identified and resolved.

Vincenzo Laporta (CNR, Bari) reported on complementary calculations of vibrational excitation and dissociation of deuterium molecules by electron impact. A local complex potential (LCP) model is applied for the first time to calculate vibrationally-electronically-excited collisions which enables resonant scattering processes to be calculated. Through the capture of the electron into an intermediate D_2^- resonance state, the method is used to calculate vibrational excitation, dissociative attachment and dissociative excitation cross sections from the spectrum of competing final states. The results compare well with other approaches and are good at intermediate energies where non-resonant (high energy) and nuclear spin (low energy) contributions become important. The LCP theoretical approach requires input from electronic scattering calculations for resonance energies and widths but has the advantage of being a completely ab initio calculation for state-resolved electron-molecule collisions in which nuclear vibrations and rotations are correctly accounted.

The final presentation of the session by Ioan Schneider (Université Le Havre) addressed the excited H_2^+, HD^+ and D_2^+ molecule with extensive comparisons to experiment. The behaviour of the dissociative recombination cross section at different energies was outlined and how combining measurements from the TSR, CRYRING and ASTRID storage rings improved understanding. The multichannel quantum defect (MQDT) theoretical framework uses detailed potential curves and resolves resonances and isotopic effects for the rotational transitions building a full set of rovibrational transitions for the isotopologues of H_2^+. The versatile MQDT techniques has also been applied at higher energies where rotational effects can be neglected and above dissociation threshold cross sections for HD+ were shown. Brief highlights of similar work on beryllium and nitrogen hydrides were presented.

2.4 Collisional-radiative models for W and hydrogen

The session was chaired by U. Fantz (IPP Garching, Germany) and by D. Wünderlich (IPP Garching, Germany) comprising four contributions spanning the field from data producers to data users.

The status of CR models for atomic and molecular hydrogen based on the Yacora solver was summarized (D. Wünderlich, IPP Garching, Germany), highlighting the role of molecules in the divertor via the dissociative recombination and thus contributing to the transition from an ionizing to a recombing plasma. The isotope effect is of high relevance for molecules, resulting in particular data needs for deuterium, preferentially ro-vibrationally resolved. For H_2, available data sets of electron collision excitation cross sections show large discrepancies and the data sets are rarely consistent. The most recent and consistent data set is based on the Molecular Convergent Close-Coupling (MCCC) method and was established by the group of D. Fursa (Curtin University, Perth, Australia). In collaboration within the GNAMPP network, an experimental benchmark for these MCCC cross sections was successfully carried out. Vibrationally resolved ionization cross section for all isotopes became available as well, based on a semi-classical modification of the classical Gryzinski method. The Yacora models for atomic and molecular hydrogen have been made accessible to everyone via the “Yacora on the Web” web mask. Further improvements for molecular hydrogen and a CR model for molecular deuterium are the next steps as well as its (re)use for interpretation of molecular data in divertor plasmas.

A state-state kinetic modelling using the GPKin code was presented by A. Laricchiuta (CNR ISTP Bari, Italy), including the ground state vibrational kinetics. Again, the availability and accuracy of the input data used by the models is crucial. The available data are summarized, applying also a procedure for smoothing some of the included cross sections close to their threshold energy. The comparison of vibrationally resolved data calculated by the impact parameter method with data from the MCCC method shows good agreement. The GPKin code couples self-consistently a set of master equations describing the time evolution of the chemical species (atomic and molecular) densities and their internal (electronic and vibrational) distributions and the Boltzmann equation for the electron energy distribution function. Simulations were carried out for nanosecond repetitively pulsed discharges in pure hydrogen and for H_2/N_2 plasmas applied for ammonia formation. For both

cases, the relevance of coupling the vibrational states of the molecular ground state to the electronically excited states is highlighted. A model for H_2/ He is available as well, being of interest for analysing entry conditions in giant planets as well.

Direct R-matrix calculations for providing the atomic structure of tungsten and its ions as well as reaction rates of electron-impact excitation and ionisation were presented by C. Ballance (Queens University Belfast, UK). The existence of hundreds of Hamiltonians requiring diagonalization implicates the usage of GPU accelerated High Performance Computing. Focus is on application of the data for plasma diagnostics, namely the determination of the plasma temperature and density. The data set for W I is benchmarked by comparing calculated emission spectra with measured data, identifying also 30 new tungsten lines. The data set is used for temperature diagnostic from the line ratio of W I 255 nm/265 nm and compared to Langmuir probe data. Calculations for W II are new and currently tested against measured spectra. In general, the role of ionized tungsten for diagnostic interpretation was pointed out, as well still existing gaps in the data base: while W III needs to be done, for W IV an ADAS data file from 2013 is available. Both electron impact excitation and ionisation rates are used to produce temperature and density dependent Generalised Collisional Radiative (GCR) coefficients. Spectral lines together with the calculated number of ionization per photons (S/XB) yields the erosion impurity influx and the new calculation help to reduce the uncertainties for S/XB.

K. Lawson (UKAEA, JET Culham) pointed out that He II is well suited as proxy for D I because the atomic physics is similar but heavy particle collision rates can be more easily calculated. From the experimental side, He II data is much simpler to interpret compared to D I because the coupling to a respective molecular species is absent. A new atomic database for He II, the Culham He Model (CHEM) database has been established using the most recent atomic data with particular attention paid to low plasma temperature data. A Collisional-Radiative model derived from the CHEM data is applied to EDGE2D-EIRENE edge transport calculations for the JET geometry. Compared to the application of ADAS data to the low temperature, high density edge plasma, a shortfall in the simulated divertor radiated power is observed, emphasizing the importance of atomic physics in this plasma region. Comparisons with measurements are planned as a next step. Preliminary analysis of measured (JET) and theoretical line ratios give no agreement, as the simulated temperature dependence is not reflected in measurements. The dependence of measured VUV spectra and line ratios of He II and H I on the plasma parameters cannot be theoretically explained up to now but already point out the relevance of opacity.

3. Conclusions

In summary session of the meeting, the Scientific Committee, session chairs and the participants presented and discussed summaries of the sessions and main outcomes were reviewed.

Experimental research utilizing fusion devices requires information and data for the W source and plasma influx determination. In addition to W erosion data, such as sputtering rates, the complex ground states as well as metastable states of the eroded W species are needed, where low ionization states of W^{q+}; q = 0, 1, 2, 3, etc. relevant for the divertor plasma conditions are covered. It is recommended to have dedicated experiments with new and improved diagnostics to upgrade information on the ground state population of emitted W from the target. Formation and emission of WD molecules from the target as well as production of D_2 should be continued to be studied with Molecular Dynamics simulations and with spectra simulations. For the latter, the release of vibrationally excited D_2 should be included in these studies. In general, new data should be applied and tested in linear devices and tokamak machines. Further, the prompt redeposition of emitted W should be studied with dedicated experiments and modelling taking into account the effect of surface roughness. It is of crucial importance to understand the range of prompt redeposition and the travel distance of emitted W particles (nm or μm range or more). Also, it is recommended to consider dedicated experiments combining diagnostics and modelling with an aim for improving information on the W lines from W V to W IX. This is to establish a full W history from the W target source to upstream W influx up to pedestal and further to the plasma core. These lines have been identified and utilized in JET and their interpretation and benchmarking should be with the latest W CR modelling. Gained information can be transferred to other fusion devices and to plasma background modelling. Information on higher ionized states of W can be used in quantification of W in the confined plasma region, i.e. the plasma core. For the hydrogenic plasmas it is desirable to understand the role of hydrogenic molecules in the plasma detachment process. There is a need for more vibrationally resolved data as well as for rotationally and isotopically resolved data. In addition to H_2, HD, D_2 data there is an increasing need to have T_2, HT, DT data available. In general, there is new data and improved CR models available with vibrational resolution. However, consistent CR model need to be validated in experiments utilizing new

techniques and diagnostics. For this, it is proposed for IAEA to seek a possibility of a framework for joint experiments with linear plasma devices or high flux plasma experiments.

Discussion session on edge plasma modelling raised the question of uncertainties in the data for hydrogen reflection from W targets and the W sputtering and erosion data, which all are used as input data for simulating edga plasma. Typically the reflection, sputtering and erosion data are calculated with codes utilizing binary collision approximation, such as TRIM. These calculations are typically done using static surfaces, but more advanced methodologies applied to realistic surfaces should be implemented. It was proposed to create reflection and sputtering data using new version of SDTrimSP and with Molecular Dynamics simulations, which include target surface features and their evolution during the sputtering process with all hydrogen isotopes including very low T_e energies and shallow angles. This advanced reflection and sputtering data should be used as input in transport codes, such as DIVIMP, EIRENE and SOLPS-ITER.

The importance of opacity modelling was acknowledged now that increased computing power allows more sophisticated models to be taken into account. This includes utilization of revised CR models with opaque and semi-opaque lines and validation of various opacity models taking into account e.g. isotopologies and collisional broadening in high density plasmas relevant for JET DT experiment as well as ITER and DEMO plasma scenarios. In addition, the wall reflection models should be tested, which take into account the surface roughness of W and Be components and the surface modification due to deposition processes.

The currently used data for atomic and molecular hydrogen isotopes applied in modelling of processes in fusion plasmas, such as molecular assisted recombination, ionization and dissociation, should be evaluated for consistency where possible. For example, accurate hydrogen molecule Fulcher bands play a critical role in modelling of high-density plasmas or detached plasmas, which may be affected by the ro-vibrational states of hydrogen at high plasma pressures. For this, it was proposed IAEA to seek for a possibility to launch a benchmarking research activity performed with partners from the linear plasma device community to disentangle the fusion-relevant processes used in plasma modelling. It is worth to mention, that these activities highly rely on the availability of appropriate diagnostics.

The non-linear kinetic modelling activities require huge data sets for describing numerous processes taking place in the plasma edge which includes the target surfaces. Bundling and compressing of data e.g. for ionized states is doable, but the computational cost is still too expensive for non-linear kinetic modelling. The Particle-in-Cell (PIC) method requires also plasma process cross-sections and can take into account non-maxwellian particle and energy distributions, which are relevant for plasma transients or for other events with strong time-dependencies. Model for the ionization events per photon (*S/XB*) is needed for the experimental spectroscopic line evaluations, e.g. for W sputtering events, but equally, or more relevant is the understanding of the W^0 ionization rates and the W population states after sputtering.

Edge plasma modelling needs recommended and evaluated data as well as data availability and adequacy. Effect of uncertainties in W transport modelling should be discriminated and assessed: uncertainties and unknown parameters related to transport modelling itself as well as data used in other models related to transport, such as atomic data, surface data, reflections, plasma backgrounds, etc. Therefore, reducing the number ad hoc calibration factors with results from experiments or with alternative computational methodologies should be an ongoing coordinated activity.

Summary and discussion session on the atomic and molecular data concluded in general that significant progress had been made in the measurements, analysis, fundamental calculations and collisional-radiative models for hydrogen and W in fusion edge environments. There is new excitation data for atomic hydrogen but the focus is on opacity modelling using realistic reactor wall geometries. Number of comprehensive data sets of electron collisions with molecular hydrogen and hydrogenic molecules is increasing with an inclusion of hydrogen isotopologues (H, D, T). Activities on data validation with experiments and testing of consequences for revised data on molecular CR codes are ongoing. New set of CR data for W^{q+}; q = 0 – 13 is available for testing with edge plasma transport codes and experimental observations of W^{6+} provide a strong motive to model the transition region from the influx site to the confined plasma region, where the quasi-continuum W spectral features dominate.

It is recommended to reconcile and evaluate the existing different data sets being used for the W^0 modelling. Further, possible modelling of low charge states W^{q+}; q = 2 – 13 using the 2D edge plasma codes should be explored to assess new recombination data with the goal of reporting and recommending data needed for wider studies. Concern was raised on the adequacy and sufficiency on the presently available data charge transfer W^0+H^+ and other CX pairs in the divertor plasma conditions and other far edge plasma environments.

Different collisional radiative models for atomic hydrogen, molecular hydrogen, and neutral and singly ionized tungsten are available. As a proxy for D I, a He II CR model was built with emphasis on low

temperature data. Within the context of establishing and benchmarking these models, new reaction data have been generated or identified and comparisons of different data sets have been carried out which allowed to highlight shortages and discrepancies. In general, all data comparisons also included a suggestion for input data sets to be preferred. Key is to benchmark CR data with experimental data and the application of data for diagnostic purposes; both has been nicely demonstrated for all contributions.

Huge steps forward have been made regarding the input data used within CR models for molecular hydrogen but still some open points exist. The available data sets for W made progress but are not complete yet. The CHEM data base adds a data set for singly ionized helium. In the future, simplified methods, e.g. the classical Gryzinski method, can be applied for closing gaps in the atomic database, one possible example being the ionization of W.

For investigations of the role of hydrogen molecules in the divertor region and for interpretation of recorded spectra, the relevance of CR modelling became evident and the need for vibrational (or even rotational) resolution is stressed. The interplay of CR models with more complex (transport) codes is seen as a very much relevant point because 0D CR models cannot self-consistently treat 3D effects like optical thickness (these needs to be approximated) while transport codes can follow a limited number of states or species only. Cross-code benchmarks together with sensitivity studies to reduce the number of levels in the transport codes can result in coupled codes well suited for interpretation of diagnostic results. Additionally, the move towards a model for molecular deuterium is regarded as high priority.

In a lively discussion, a lot of interest in data and application was expressed, also desirable comparisons mentioned and future collaboration identified. The need and wish of centralized CR models, and centralized data in a uniform data format was expressed. The latter is in particular required for ro-vibrational data bases with hundreds of thousands of cross sections, whereby the point of making total or differential cross sections available was touched. The question was formulated if all these mentioned points can be an IAEA activity acting as umbrella or if this is (partly) performed within already collaboration activities and made available.

In a follow-up meeting in May 2021, the Scientific Committee together with the session chairs reviewed meeting outcome, proposed collaboration activities and outlined a framework for the organization of future meetings on the topic of W and hydrogen in edge plasmas. As a major outcome it was proposed to form Working Groups (WGs) with an aim to coordinate and steer various topics and activities raised at the meeting and its summary session, such as encouraging collaboration between experimentalists (data providers and data users), plasma modellers (data users) and theorists (data providers) in the form of benchmarking experiments and calculations as well as exchange of information and data requirements. The WGs to be established were categorized as follows:

- WG 1: Atomic and Molecular Data Recommendation and Validation for W and Hydrogen in Edge Plasmas
- WG 2: Plasma Experiments and Comparison Activities with CR Models
    - 2.A: W and Hydrogen Experiments with Fusion Devices and Linear Plasma Devices
    - 2.B: Photon Opacity Models of Hydrogenic Atomic and Molecular Species
- WG 3: Plasma-Surface Process Properties, Trends and Underlying Effects.

The above-mentioned WGs each would have a committee with 4-6 members to steer the WG activities and WG membership would require active contribution to the corresponding activities. Each WG should collect data, benchmarking and other scientific requirements from the corresponding fusion research communities and further coordinate any activities as considered necessary for the WG. High importance concerning ITER-specific issues such as specifications, definitions and terminology was acknowledged and increased communication with ITER should take place e.g. through WG meetings. The first monitoring meeting for WG 1 and WG 2 took place from 6 – 10 December 2021 in connection of the IAEA's 2nd Meeting of the Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP-2). The WGs will have a joint review meeting biennially, the second joint meeting scheduled to take place in Autumn 2023.

Appendix I: List of Participants

Presenters

BALLANCE Connor, Queen's University Belfast (QUB), UK

BONNIN Xavier, ITER, France

BREZINSEK Sebastijan, FZJ, Germany

CLASSEN Ivo, DIFFER Eindhoven, The Netherlands

DING Xiaobin, Northwest Normal University (NWNU), China

DUBOIS Alain Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR), Sorbonne Université France

ENGELN Richard, Eindhoven University of Technology (TUE), The Netherlands

ERTMER Stephan, FZJ, Germany

FANTZ Ursel, University Augsburg, Germany

FURSA Dmitry, Curtin University, Australia

GOTO Motoshi, NIFS, Japan

GROTH Mathias, Aalto University, Finland

GUTERL Jerome, General Atomics, USA

KIRSCHNER Andreas, FZJ, Germany

LAPORTA Vincenzo, Bari Politecnico, Italy

LARICCHIUTA Annarita, Bari Politecnico, Italy

LAWSON Kerry, CCFE, UK

NEU Rudolf, IPP Garching, Germany

O'MULLANE Martin, University of Strathclyde, UK

PAWELEC Ewa, University of Opole, Poland

TSKHAKAYA David, IPP.CR, Czech

VERHAEGH Kevin, CCFE, UK

WEI Baoren, Fudan University, China

WIESEN Sven, FZJ, Germany

WÜNDERLICH Dirk IPP, Garching, Germany

Attendees

ALI Musharaf, Bhabha Atomic Research Centre Mumbai, India

BORODIN Dmitry, FZJ, Germany

COLGAN James, Los Alamos National Laboratory, USA

GUIRLET Remy, CEA-IRFM, France

HARTING Derek, FZJ, Germany

KREMEYER Thierry, IPP Garching, Germany

LI Bowen, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, China

MOHAN Man, University of Delhi, India

REITER Detlev, University Düsseldorf, Germany

SCARLETT Liam, Curtin University, Australia

SCHNEIDER Ioan, University of Le Havre, France

SINGH Narendra, University of Delhi, India

TENNYSON Jonathan, University College of London, UK

VAN DER MEIDEN Hennie, DIFFER, The Netherlands

WU Yong, Institute of Applied Physics and Computational Mathematics, China

ZSOLT Mezei, Institute for Nuclear Research (ATOMKI), Debrecen, Hungary

IAEA

DENECKE Melissa, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, AUSTRIA.

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

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

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

Appendix II: Meeting Agenda

Monday, 29 March 2021

Welcome - Virtual meeting (09:00 - 09:30)

time	title	presenter
09:00	Welcome to Joint IAEA-FZJ Technical Meeting	DENECKE, Melissa (IAEA) KONING, Arjan (IAEA) HEINOLA, Kalle (IAEA) HILL, Christian (IAEA)

EXP/1 fusion devices - Virtual meeting (09:30 - 10:30)

Experiments 1: tokamaks, linear plasmas, stellarators

-Conveners: Sebastijan Brezinsek

time	title	presenter
09:30	Hydrogen recycling and Tungsten sources in fusion-relevant edge plasmas: spectroscopy in PSI-2 and JET	BREZINSEK, Sebastijan (Forschungszentrum Jülich, Germany)
10:00	Spectroscopic studies for tungsten and hydrogen in LHD	GOTO, Motoshi (National Institute for Fusion Science)

virtual coffee (10:30 - 10:45)

MOD/1 fusion devices - Virtual meeting (10:45 - 11:45)

Modelling 1: tokamaks, linear plasmas, stellarators

-Conveners: Sven Wiesen

time	title	presenter
10:45	Tungsten atomic data needs for ITER	BONNIN, Xavier (ITER Organization)
11:15	Application of Monte-Carlo methods for photon transport in divertors	WIESEN, Sven (Forschungszentrum Jülich, Germany)

Discussion - Virtual meeting (11:45 - 12:15)

break (12:15 - 12:45)

EXP/1 fusion devices - Virtual meeting (12:45 - 13:45)

Experiments 1: tokamaks, linear plasmas, stellarators

-Conveners: Sebastijan Brezinsek

time	title	presenter
12:45	Investigating the role of neutral particles in the linear device Magnum-PSI	CLASSEN, Ivo (DIFFER, Dutch Institute for Fundamental Energy Research)
13:15	Reaction dynamics in a magnetized hydrogen plasma unraveled by optical spectroscopic techniques	ENGELN, Richard (Eindhoven University of Technology, The Netherlands)

virtual coffee (13:45 - 14:00)

MOD/1 fusion devices - Virtual meeting (14:00 - 15:00)

Modelling 1: tokamaks, linear plasmas, stellarators

-Conveners: Sven Wiesen

time	title	presenter
14:00	Hydrogenic atomic and molecular emission measurements in JET-ILW for assessing the role ion-molecular interaction in divertor detachment	GROTH, Mathias (Aalto University)
14:30	An experimental analysis of the impact of plasma-molecule interactions on particle losses, atomic line emission and resulting power losses	VERHAEGH, Kevin (Culham Centre for Fusion Energy, United Kingdom)

Discussion - Virtual meeting (15:00 - 16:00)

Tuesday, 30 March 2021

EXP/1 fusion devices - Virtual meeting (09:00 - 10:00)

Experiments 1: tokamaks, linear plasmas, stellarators

-Conveners: Sebastijan Brezinsek

time	title	presenter
09:00	Measurements of the W concentration in the low- and mid-temperature range	PAWELEC, Ewa (Institute of Physics, University of Opole)
09:30	Spectroscopic Diagnostic of Tungsten at ASDEX Upgrade	NEU, Rudolf (MPI for Plasma Physics)

virtual group photo and coffee (10:00 - 10:15)

CR - Virtual meeting (10:15 - 11:15)

Special session for Collisional Radiative Models (CR models)

-Conveners: Ursel Fantz

time	title	presenter
10:15	Collisional radiative models for atomic and molecular hydrogen in the edge plasma of fusion devices	WÜNDERLICH, Dirk (Max Planck Institute for Plasma Physics, Garching, Germany)
10:45	State-to-state self-consistent kinetic modelling of hydrogen plasmas	LARICCHIUTA, Annarita (CNR ISTP Bari)

Discussion - Virtual meeting (11:15 - 11:45)

break (11:45 - 12:15)

CR - Virtual meeting (12:15 - 13:15)

Special session for Collisional Radiative Models (CR models)

-Conveners: Dirk Wünderlich

time	title	presenter
12:15	Electron-impact excitation and ionisation R-matrix calculations in support of Tungsten tokamak diagnostics.	BALLANCE, Connor (Queen's University of Belfast)
12:45	He II as a proxy for D I	LAWSON, Kerry (Culham Centre for Fusion Energy, United Kingdom)

virtual coffee (13:15 - 13:30)

MOD/2 A+M Data - Virtual meeting (13:30 - 14:30)

Modelling 2: A+M data, cross-sections, processes

-Conveners: Martin O'Mullane

time	title	presenter
13:30	Fundamental atomic data for tungsten and hydrogen and the effect of the finite density edge plasma	O'MULLANE, Martin (University of Strathclyde, United Kingdom)
14:00	Production of cross sections for atomic collisions with Asymptotic Orbital Semiclassical Coupled Channel calculations	DUBOIS, Alain (Sorbonne Universite)

virtual coffee - Virtual meeting (14:30 - 14:45)

Discussion - Virtual meeting (14:45 - 15:45)

Wednesday, 31 March 2021

MOD/2 A+M Data - Virtual meeting (09:00 - 10:30)

Modelling 2: A+M data, cross-sections, processes

-Conveners: Martin O'Mullane

time	title	presenter
09:00	Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues	FURSA, Dmitry (Curtin University)
09:30	Vibrational excitation and dissociation of deuterium molecule by electron impact	LAPORTA, Vincenzo (CNR, Bari)
10:00	Electron collisions with H2+, HD+ and D2+: computation of cross sections and rate coefficients, and comparison with storage ring measurements	SCHNEIDER, Ioan (Université Le Havre Normandie, LOMC-UMR-6294)

virtual coffee break - Virtual meeting (10:30 - 10:45)

EXP/2 A+M data - Virtual meeting (10:45 - 11:45)

Experiments 2: A+M data, cross-sections, processes

-Conveners: Sebastijan Brezinsek

time	title	presenter
10:45	Charge Exchange Cross Section Measurement in Fudan University	WEI, Baoren (Fudan University)
11:15	Spectroscopic investigations on energy, angular and atomic level distribution functions of sputtered tungsten	ERTMER, Stephan (Forschungszentrum Jülich)

Discussion - Virtual meeting (11:45 - 12:15)

break (12:15 - 12:45)

MOD/1 fusion devices - Virtual meeting (12:45 - 14:15)

Modelling 1: tokamaks, linear plasmas, stellarators

-Conveners: Sven Wiesen

time	title	presenter
12:45	Needs of atomic data for kinetic modelling of fusion plasma edge	TSKHAKAYA, David (Institute of Plasma Physics of the Czech Academy of Sciences)
13:15	Theoretical analysis and experimental validation in DIII-D of predictive modeling for tungsten erosion and redeposition in tokamak divertors	GUTERL, Jerome (General Atomics, USA)
13:45	Atomic data needs for tungsten erosion, migration and deposition modelling in fusion devices	KIRSCHNER, Andreas (Forschungszentrum Juelich GmbH)

virtual coffee (14:15 - 14:30)

Discussion: Special session for MOD/1 fusion devices - Virtual meeting (14:30 - 15:30)

Discussion - Virtual meeting (15:30 - 16:30)

Thursday, 1 April 2021

EXP/1 fusion devices: Summary - Virtual meeting (09:00 - 09:30)

Experiments 1: tokamaks, linear plasmas, stellarators

-Conveners: Sebastijan Brezinsek

MOD/1 fusion devices: Summary - Virtual meeting (09:30 - 10:00)

Modelling 1: tokamaks, linear plasmas, stellarators

-Conveners: Sven Wiesen

EXP/2 A+M data: Summary - Virtual meeting (10:00 - 10:30)

Experiments 2: A+M data, cross-sections, processes

-Conveners:

Sebastijan Brezinsek

virtual coffee

(10:30 - 10:45)

MOD/2 A+M Data: Summary - Virtual meeting (10:45 - 11:15)

Modelling 2: A+M data, cross-sections, processes

-Conveners: Martin O'Mullane

CR: Summary - Virtual meeting (11:15 - 11:45)

Special session for Collisional Radiative Models (CR models)

-Conveners: Dirk Wünderlich; Ursel Fantz

Discussion - Virtual meeting (11:45 - 12:45)

Appendix III: Book of Abstracts

Welcome

Welcome to Joint IAEA-FZJ Technical Meeting

Authors: Melissa Denecke[1]; Arjan Koning[1]; Kalle Heinola[1]; Christian Hill[1] [1] *IAEA*
Corresponding Author: k.heinola@iaea.org

Opening words

Introduction

Adoption of agenda

EXP/1 fusion devices

Hydrogen recycling and Tungsten sources in fusion-relevant edge plasmas: spectroscopy in PSI-2 and JET

Author: Sebastijan Brezinsek[1]

[1] *Forschungszentrum Jülich, Germany*

EXP/1 fusion devices

Spectroscopic studies for tungsten and hydrogen in LHD

Author: Motoshi Goto[1]

Co-authors: Nilam Ramaiya [2]; Tetsutarou Oishi [1]; Daiji Kato [1]; Izumi Murakami [1]; Yasuko Kawamoto [1]; Tomoko Kawate [1]; Hiroyuki Sakaue [1]; Shigeru Morita [1]

[1] *National Institute for Fusion Science*

[2] *Institute for Plasma Research*
Corresponding Author: goto.motoshi@nifs.ac.jp

The pellet injection is a standard method for the impurity-relating studies in the Large Helical Device (LHD). We have accumulated experiences and established a technique for providing the plasma with tungsten ions adequate for spectroscopic measurements without causing a radiation collapse. A number of emission lines of tungsten ions in the wavelength range from visible to EUV have been successfully observed to date and are being used for the impurity transport study and for the atomic data evaluation study.

Recently, we have identified visible M1 lines of W^{+26} ion (335.7 nm and 333.7 nm) and W^{+27} ion (337.7 nm) [1], and the radial density structures of these ions are derived with the help of a collisional-radiative model. Under the assumption of ionization equilibrium, the total tungsten ion density is estimated to be approximately 0.5% of the electron density in the core region. In addition to that, in the VUV wavelength range measurement, other M1 lines of W^{37+} ion (64.67 nm) and W^{38+} ion (53.29 nm and 55.91 nm) have been also clearly identified [2]. The temporal development of intensities of these M1 lines and of some E1 lines of higher charge state ions, i.e., W^{45+} (12.70 nm) and W^{41+} (13.12 nm), shows clear correlation with the central electron temperature, and it is confirmed that these line intensities take their maximum in the temperature range where the fractional abundance of the corresponding charge state ion becomes the largest.

As for the hydrogen atom line emissions, the study of anisotropy in the electron velocity distribution function has found a use for the Lyman-α line in combination with the polarization spectroscopy. We have succeeded to detect the polarization degree of several percent for the Lyman-α line [3] with an innovative technique originally developed for the solar radiation observation [4]. An analysis with an atomic model which deals with the alignment as well as the population for the excited level indicates that the electron temperature in the direction perpendicular to the magnetic field is higher than the parallel temperature [5]. This result qualitatively agrees with our understanding of the particle confinement characteristics in the edge open-field region of LHD.

References

[1] D. Kato, et al., 26th IAEA FEC (17-22 Oct., 2016, Kyoto, Japan), EX/P8-14.

[2] T. Oishi, et al., Nucl. Mater. Energy 26, 100932 (2021).

[3] N. Ramaiya, et al., J. Quant. Spectrosc. Radiat. Transf. 260, 107430 (2020).

[4] R. Kano, et al., Astrophys. J. Lett. 839, L10 (2017).

[5] M. Goto and N. Ramaiya, Symmetry 13, 297 (2021).

MOD/1 fusion devices

Tungsten atomic data needs for ITER

Author: Xavier Bonnin[1] [1] *ITER Organization*
Corresponding Author: xavier.bonnin@iter.org

This talk will present an overview of the spectroscopic diagnostics and modelling needs for tungsten atomic data for operation of the ITER tokamak. The goals are to be able to predict and measure the W influx into the ITER plasma and the W core concentration during operation. The spectroscopic lines of main interest will be provided, as well as the current state-of-art A&M data on which the modelling relies. Opportunities from improvement of the data or the quality of the simulations will be highlighted.

MOD/1 fusion devices

Application of Monte-Carlo methods for photon transport in di- vertors

Author: Sven Wiesen[1]
[1] *Forschungszentrum Jülich, Germany*

15 years ago the EIRENE Monte-Carlo code was developed to solve the radiation transport equation by acknowledging an analogy to the kinetic Boltzmann equation. At that time the relevance of pho- tonic reabsorption of strong (Lyman) lines in divertors was proven, leading into a revision of the SOLPS4.3 model used for the ITER divertor design to include Lyman line opacity effects. Although the accessible operational window of the ITER divertor was not strongly affected (e.g. in terms of target heat-flux as a function of divertor neutral pressure) a change in the ionisation-recombination balance was predicted with an impact on the eroding particle fluxes. Recently, Lyman-line opac- ity in divertors has gained a larger attention due to its significant impact on the interpretation of visible/VUV spectra for the purpose of edge code validation.

A review on the numerical treatment of photon transport in fusion plasma using the EIRENE Monte- Carlo methods is given. The required ingredients of divers broadening mechanisms are summarised, including effects that will become more important in high-density DT fusion experiments in a metal- lic environment (JET-DT, ITER or DEMO), i.e. isotope effects and

Zeeman splitting. A large uncer- tainty exists in the description of surface reflections on (deposited) metal surfaces (W or Be). The relevance of revised collisional radiative models with Lyman opacity including various line broad- ening mechanisms is discussed with supporting examples. The status of a continued development of the radiation transport EIRENE module is summarised.

EXP/1 fusion devices

Investigating the role of neutral particles in the linear device Magnum- PSI

Authors: Ivo Classen[1]; Hennie van der Meiden[1]; Gijs Akkermans[1]; Renato Perillo[2]; Jonathan van den Berg[1]; Richard Engeln[3]

[1] *DIFFER, Dutch Institute for Fundamental Energy Research*

[2] *University of California San Diego*

[3] *Eindhoven University of Technology*

In the linear plasma device Magnum-PSI up to 5eV hydrogen plasmas can generate reactor-relevant heat and particle fluxes. Due to the simplified geometry, stable plasma conditions and excellent diagnostic accessibility, Magnum-PSI is an attractive device to study the basic physical and chemical processes in recombining and detaching SOL plasmas. During pulsed operation, high density ELM- like bursts with temperatures up to 15eV can also recreate ionizing plasma conditions. In this talk a number of studies involving plasma-neutral interactions will be reviewed.

First: Divertor detachment can be simulated in Magnum-PSI by varying the background neutral pressure. A detailed characterization of the plasma parameters, heat and particle loads and opti-cal plasma emission (Balmer series and Fulcher band) was performed, revealing a clear transition between regimes dominated by ionization, MAR, and electron ion recombination (EIR).

Second: During Nitrogen seeding experiments an increase in recombination was observed. A global plasma model has been set up to investigate the complete N2/H2 chemistry, revealing two new recombination reaction paths to be dominant: 1) the ion conversion of NH followed by dissociative recombination, and 2) proton transfer between H2+ and N2, producing N2H+. These two processes are referred to as N-MAR (nitrogen-molecular activated recombination). The main N2/H2 processes derived from the global model have been implemented into B2.5-Eunomia, confirming the significant contribution of N-MAR to the total recombination rate.

Third: TS and CTS measurements very close to the target were compared to the energy and particle fluxes measured at the target surface, revealing significant momentum and energy losses in the last 3 mm of plasma. Also, the expected pre-sheath acceleration due to the Bohm criterion was not observed in high density scenarios. In this regime (the ‘thermal pre-sheath’) ion acceleration is overruled by momentum and energy transfer to neutrals.

Finally: DIFFER is currently seeking funding to build an active spectroscopy diagnostic based on laser induced fluorescence (LIF) in the vacuum ultraviolet (VUV) wavelength range. This VUV-LIF diagnostic would accurately measure the ro-vibrational state distribution of Hydrogen molecules in divertor detachment conditions, elucidating the importance of the MAR process under various plasma conditions and wall materials. Together with the current set of diagnostics, this will result in a unique complete picture of the near surface plasma processes.

EXP/1 fusion devices

Reaction dynamics in a magnetized hydrogen plasma unraveled by optical spectroscopic techniques

Author: Richard Engeln[1]

[1] *Eindhoven University of Technology, The Netherlands*

The development of efficient sources of reactive hydrogen radicals is important in many research fields and applications. For instance, atomic hydrogen radicals serve as primary reactive particles for surface modification or thin film deposition. For fusion plasma heating, one of the main research challenges is to develop efficient negative ion sources. A promising route is via dissociative attach- ment of ro-vibrationally excited[2] hydrogen molecules Hr,v. The ro-vibrationally excited molecules are important precursors in volume reactions leading to excited hydrogen atoms. During my presen- tation I will discuss the importance of several molecular activated recombination (MAR) processes in an expanding thermal hydrogen plasma, and especially, the formation of excited atoms via the[2] mutual neutralization process of H− and H+.

When an expanding hydrogen plasma jet, produced from a cascaded arc source, is weakly magne- tized, the emission of the expanding plasma jet is dominated by the red Hα emission in the first centimeters from the exit of the source, but changes to blue at larger distances from the exit due to higher Balmer lines (n > 4) (see attached Figure 1). Since electron energies in the jet are too low (1 eV and less) to excite atomic hydrogen to the state n = 3, a possible formation route is via mutual recombination of atomic ions: $H^+ + H^- \rightarrow H + H(n = 2, 3)$. After 22 cm Hβ to Hδ light be- comes dominant (i.e. the reason for the blue appearance of the jet at larger z) and the corresponding weighted densities n/g become higher than the one for n = 3. The proposed formation mechanism for these highly excited hydrogen atoms is the mutual recombination reaction of positive molecular (H+) and negative atomic ions (H−). The molecular ions are produced in charge exchange reactions of Hr,v with H+, while the latter are formed by dissociative attachment of electrons with Hr,v. Both 2 2 processes depend strongly on the internal excitation (r, v) of the neutral molecule. In earlier studies we have shown the presence of large densities of these highly ro-vibrationally excited hydrogen molecules. During my presentation I will focus on the reaction dynamics and kinetics leading to excited molecular and atomic hydrogen.

MOD/1 fusion devices

Hydrogenic atomic and molecular emission measurements in JET- ILW for assessing the role ion-molecular interaction in divertor detachment

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Detailed comparisons of measured and predicted plasma conditions at the divertor plates, and atomic and molecular hydrogenic emission across have been carried out with the edge fluid codes EDGE2D- EIRENE and SOLPS-ITER for low-confinement mode plasmas in the JET ITER-like wall materials configuration with its tungsten divertor. In deuterium plasmas and low-recycling scrape-off layer plasma conditions, EDGE2D-EIRENE predicts the measured plasma conditions, the total radiated power and the deuterium Balmer line emission to within 20%, thus well within the uncertainties of the measurements. In plasma conditions representing the onset of divertor detachment, EDGE2D- EIRENE predicts that the reduction in the total ion current to the target plates is produced by an exponential increase in the predicted molecular density at the low-field side target plate, leading to plasma pressure losses predominately due to ion conversion to molecular ions adjacent to the plate when the electron temperature at the plate is of the order 2 eV. Volume recombination plays a negligible role on the onset of detachment, and is significant for temperature below 1 eV only. On the other hand, the simulations show a significantly less pronounced detachment onset, and weaker reduction of the ion currents to the target plates for electron temperatures below 1.5 eV, implying that the pressure losses should even be stronger than presently predicted.

The contribution describes the status of analyses of hydrogenic (hydrogen and deuterium) atomic line and molecular Fulcher-alpha band emission to characterize the atomic and molecular influxes for assessing the impact of ion-molecular interaction in edge fluid code predictions. These studies include the hydrogen isotopes hydrogen and deuterium, and future studies in tritium and deuterium- tritium plasmas will be discussed in the context of atomic and molecular fundamental data needed for including these isotopomers.

MOD/1 fusion devices

An experimental analysis of the impact of plasma-molecule in- teractions on particle losses, atomic line emission and resulting power losses

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Spectroscopic analysis techniques for the hydrogen Balmer series are presented 1 using Yacora-Online [2], where the quantitative role of processes leading to hydrogen emission are traced. These are used to estimate the contribution of both plasma-atom and molecule interactions to power/particle balance. Application of this to data from the divertor of the TCV tokamak results in a series of im- portant observations [3]:

Plasma-molecule interactions result in excited atoms which significantly impact the hydrogen atomic line emission and the resulting radiative losses.

Plasma-molecule interactions, involving D^+ resulting in MAR, enhance the Dα emission at the detachment onset.

Plasma-molecule interactions should be accounted for when low and medium-n hydrogen spectroscopy data ($n < 7$) is analysed.

The hydrogen emission enhancement from plasma-molecule interactions occurs near the tar- get (where the molecular density is the highest) while the Fulcher band emission detaches off the target. That may have implications for using Fulcher band emission measurements for MAR estimates.

Detailed comparisons of the inferred particle balance as well as the measured and atomic extrapolation of Dα against those obtained from SOLPS-ITER simulations [4] (which is vibrationally (D_2) unresolved) indicates that the impact of plasma-molecule interactions involving D^+ is underestimated. Agreement with SOLPS-ITER simulations is improved when the SOLPS-ITER simulations are post-processed using a $D_2 + D^+ \rightarrow D^+ + D$ rate specifically derived for deuterium [5].

This research has implications for analysing hydrogen spectroscopy measurements and the diagnosis of Molecular Activated Recombination (MAR). Its outcomes highlight the necessity of a more in-depth investigation on the importance of: 1) having isotope resolved rates for plasma-molecule in- teractions; 2) including vibrationally excited states individually in plasma-edge simulations.

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EXP/1 fusion devices

Measurements of the W concentration in the low- and mid-temperature range

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Tungsten is one of the most important impurities in the magnetic confinement fusion plasma. It is a deleterious impurity, because its radiation is a large part of the radiative loss from core and pedestal plasma, diminishing the plasma performance and destabilizing the pulse. In the core the main radiation of tungsten is in SXR region, whereas the more long-wavelength structures radiate in VUV from the external regions (or even from the core, during the low-power pulses). The SXR is used for tungsten concentration estimation in the high-temperature core plasma (see e.g. 1) but the concentration of tungsten in lower temperature regions are not so obtainable.

In both JET and ASDEX the XUV region around 5 nm, where the model spectrum has been calculated by Pütterich et al [2], makes possible an estimation of tungsten density in 1.5-2 keV temperature region. This means upper pedestal regions in high-power pulses or plasma cores in low intensity ones (e.g. the ones used to study L-H transitions in JET). There is another very well visible tungsten feature in VUV, roughly in 15-30 nm region, which could be used for estimating tungsten density in temperatures of 1 keV and below. The problem is, that it still cannot be reproduced using any kind of model spectra, at least not sufficiently to make any tungsten density estimations based on it. It is still one of the main tungsten signals (real time as well) used in JET, and is used to study tungsten behaviour (e.g. [3]). Due to the lack of atomic data, it cannot be used for more, and it's especially important in tritium/DT campaigns, when it is frequently the only tungsten signal apart from SXR obtainable, due to restrictions in spectroscope utilization.

Recently, also lower ionization stages of tungsten were observed in JET [4], – lines of W VI to W XIII, with the most visible being W VII lines of 21 and 26 nm. As more and more tungsten erosion studies show that the eroded tungsten, visible as W I radiation, is screened and redeposited, therefore not entering the deeper plasma at all, this W VII lines could be an estimation of SOL tungsten, the one that is more readily entering and exiting the fusion plasma core. Unfortunately, whereas the temperatures estimated using their intensities look realistic for where they are emitted from, the estimated densities are way too high. This suggests some problems with atomic parameters for those lines (ADAS database, [5]). Having better atomic parameters would greatly enhance utility of those signals for tungsten erosion and impurity source studies.

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EXP/1 fusion devices / 54

Spectroscopic Diagnostic of Tungsten at ASDEX Upgrade

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ASDEX Upgrade (AUG) is pursuing a program on W plasma facing components since the beginning of the ninetieth. After preparatory experiments on W components as well as first spectroscopic investigations for the diagnostics of W sources and transport, a divertor with W coated graphite PFCs was installed in 1995 and successfully run for one campaign until 1996. Besides important results on the W behaviour in a divertor tokamak, it became clear, that carbon erosion in the main chamber had a strong impact on the overall impurity content and the deposition in the divertor. Therefore, it was decided that on the way to all W PFCs to start converting the main chamber PFCs first and then successively implement W limiters and finally the W divertor. This transition started in 1999 and was completed in 2006/07.

From the first investigations to the routine operation of an all W device, spectroscopy was a key tool to characterize the source and the transport of W. In the early years of W operation information on atomic data, both on the ionisation equilibrium as well and the excited states and transition was scarce but over the years a lot of spectroscopic information has been accumulated in AUG and many investigations on dedicated devices were triggered which complemented excellently the spectroscopic data.

The investigations in AUG concentrated on the transitions which are accessibly by the available di- agnostic hardware. This means that the influx measurements were restricted to the visible range and here mainly concentrated on the 400.8 nm WI line. Whereas this excludes dedicated spectroscopic investigations on prompt redeposition, it allows a very high spatial coverage of all W sources in the main chamber as well as the in the divertor. Operating with high transmission spectrometers allows in parallel high temporal resolution as well as reliable identification of background contributions. Similar to the influx measurements, the emphasis of the measurements of the W content was also put on the routine applicability and best use of scarce diagnostic resources. This led to a focus on the monitoring of the 4.5-7 nm region in the VUV complemented by X-ray measurements in the range of 0.5 – 0.8 nm. This allowed sensitively measuring W concentrations in a broad temperature range (˜0.8 – 5 keV) thereby covering a large fraction of the plasma radius in most AUG discharges and providing a sensitive measure for the evolution of the W density profiles.

This contribution will give an overview on the spectroscopic investigations for the deduction of W influx and density and highlight their applications to AUG plasma discharges.

CR

Collisional radiative models for atomic and molecular hydrogen in the edge plasma of fusion devices

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Population models are an important tool for interpreting observed plasma parameters or for predicting for known plasma parameters the plasma behavior. The properties of the edge plasma in fusion devices as well as the processes taking place within this region are of great relevance for the overall behavior of a fusion plasma. Typically, the edge plasma is much cooler than the core plasma, resulting in the presence of atoms and molecules and thus a high complexity of the reaction kinet- ics. Together with the presence of strong gradients in particle temperatures and densities, processes like Molecular Assisted Recombination or the transition from an ionizing to a recombining plasma regime can play a crucial role. Consequently, population models for atoms as well as for molecules are needed, being precise over a broad parameter range.

Collisional radiative (CR) models represent the most versatile type of a population model. A huge number of input parameters (reaction probabilities) are needed, in particular in the case of molecules where vibrational or rotational sublevels are present. Due to the presence of deuterium and tritium in fusion plasmas, the development of molecular CR models also for isotopomeres of H_2 is desirable, further increasing the data needs. The present results are based on the well-benchmarked Yacora CR models for atomic and molecular hydrogen, both being accessible also online via the tool Yacora on the Web.

Large gaps exist in the available set of molecular excitation cross sections needed as input for CR models. Even for the hydrogen molecule, the simplest existing neutral molecule, no complete data set of cross sections exists that includes vibrational sublevels, excited state-excited state reactions and the isotope effect. Recently a set of electron collision excitation cross sections, calculated by using the Molecular Convergent Close-Coupling (MCCC) method at Curtin University, Perth, Aus- tralia became available. In a common effort, the non-vibrationally resolved MCCC cross sections for the triplet system of H_2 were implemented in Yacora for H_2 and a benchmark was successfully performed versus results from a planar ICP discharge. An extension to the singlet system, including singlet-triplet mixing is planned next.

An existing comprehensive set of dissociative and non-dissociative ionization cross sections for the ground state and electronically excited states of H_2, based on the semi-classical Gryzinski approach, is extended by data for D_2, T_2, HD, HT and DT. The total ionization cross sections for H_2 were successfully validated versus MCCC cross sections. The existence of cross sections for all isotopomeres opens the door towards the development of CR models for the isotopomeres of hydrogen.

The general availability of cross sections for the hydrogen atom is much better compared to the molecule. Open points are still present mainly regarding the connection of excited atomic states to the molecule or molecular ions. Nonteheless, the steady improvement and availability of data are important steps for increasing the reliability of model predictions for the edge plasma in fusion devices.

CR

State-to-state self-consistent kinetic modelling of hydrogen plasmas

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The kinetic scheme, build in the past for the investigation of the vibrational kinetics of the ground electronic state in low-pressure negative ion sources and in the radiative-coupled simulation of en- try conditions in the Jupiter atmosphere, has been improved including the H+, H− ion kinetics, and the detailed dynamics of the electron-impact excitation of singlet states of H2 molecule (B, B′ 1Σ+, C, D 1Πu) 1 resolved on both initial and final vibrational manifolds, together with the de-excitation channels, i.e. the radiative decay and the collisional quenching, and also accounting for the VT and VV collisional processes responsible for the redistribution of energy between vibrational and trans- lational degrees of freedom.

The state-to-state kinetic simulation has been carried out with the GPKin code that couples self-consistently a set of master equations describing the time evolution of the chemical species (atomic and molecular) densities and their internal (electronic and vibrational) distributions and the Boltz- mann equation for the electron energy distribution function, eedf, taking into account the external electric field.

The state-to-state self-consistent approach, implementing the detailed kinetic scheme, has been exploited for the simulation of non-equilibrium conditions in nanosecond repetitively pulsed discharges in pure hydrogen [2], in H2/N2 plasma [3], of interest for the investigation on nitrogen seeding experiments in tokamak divertor and in H2/He plasma [4], of interest for the interpretation of shock tube experiments for atmospheric entry of gaseous giant planets. The chemical model for H2/Li plasma is under construction, including the electron impact induced processes in LiH [5], for the interest in liquid metal divertors.

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CR

Electron-impact excitation and ionisation R-matrix calculations in support of Tungsten tokamak diagnostics.

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Dirac Atomic R-matrix calculations (DARC) for level-resolved electron-impact excitation of neutral and singly ionised tungsten have been carried out.These models include several hundred

levels in the close-coupling expansion of each scattering model. Where NIST experimental energy level iden- tifications are available for each ion stage, these have been adopted within the our models. For electron-impact ionisation we shall discuss a term-resolved RMPS (R-Matrix with Pseudo-States) model which may be statistically split to provide level-resolved ionisation. Impurity influx from tungsten plasma facing components may be associated with an SXB 'ionisations per photon' ratio. The atomic structure, electron-impact excitation and ionisation underpin the ratio of the effective ionisation to the photon emissivity coefficient. I will show that the electron-impact excitation cal- culations reproduce spectra from laboratory plasma devices such as the Compact Toroidal Hybrid (CTH), Auburn University, but the confidence in the effective ionisation rates, dependent on excited- state ionisation is not as high.

CR

He II as a proxy for D I

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The similarities between the atomic physics of hydrogen-like He, He II, and neutral D, D I, result in similar behaviours of these ions in tokamak plasmas. The study of He is important in its own right, but can also inform the study of D without the complication of molecular contributions to the radiated power. Another advantage of He is that the heavy particle collisions are more tractable involving collisions with ions rather than with neutrals as is the case for D. The Culham He Model (CHEM) database has been generated, in the first instance, for He II using the most recent atomic data with particular attention being paid to the lowest temperature data. A Collisional-Radiative model derived from the CHEM data is illustrated. This model has been used in EDGE2D-EIRENE edge transport simulations and shows that significant differences result from the use of different atomic data. At the highest densities lower simulated divertor temperatures are reached than with the more frequently used ADAS data. Differences between observations and theory of He II and D I spectral line intensity ratios are also described.

MOD/2 A+M Data

Fundamental atomic data for tungsten and hydrogen and the effect of the finite density edge plasma

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Both tungsten and hydrogen pose a set of challenges in assembling a set of data suitable for modelling emission from tokamak edge plasmas. Understanding the edge plasma of tokamaks is essential to controlling the fusion plasma and the environment demands that collisional-radiative models are required to make effective use of the fundamental atomic data. As a high Z element, a large volume of data is needed for tungsten little of which was available just 10 years ago. A multi-year, multi-team effort was needed to produce high quality data for the atomic structure and all processes (excitation, ionization, recombination and charge exchange). Although more work is still needed the situation is much improved. Hydrogen has the problem of familiarity but the precision needed to properly account for high-n influences, opacity and non-Maxwellian electrons also requires new approaches. This talk will outline the collection and processing of tungsten and hydrogen data from an ADAS perspective and indicate where there are still gaps to be filled.

MOD/2 A+M Data

Production of cross sections for atomic collisions with Asymptotic Orbital Semiclassical Coupled Channel calculations

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Cross sections for bound-bound (excitation, capture) and bound-free (ionisation) transitions occur- ring in ion-atom and ion-molecule collisions are required for diagnostic and modelling of plasmas. These collisions involve low-Z atoms naturally present in the plasmas but not only (impurities, el- ements from the vessels, …), all in various oxidation degrees but also in ground and excited states, prior to the collisions.

The present contribution will present our approach and code implementation to produce cross sec- tions for these processes and collisions, for impact energies ranging from below keV/u to MeV/u. It is based on the semiclassical approximation, with a classical description of the relative motion be- tween target and projectile, while the electron dynamics is described by solving non perturbatively the time-dependent Shrödinger equation (TDSE). This kind of treatment is required for the impact energy domain of interest but can be declined in different approaches. We use an approach where the TDSE is solve using a scattering wavefunction expanded on asymptotic atomic or molecular states, i.e. on states describing isolated target and projectile, and for which up to 4 active electrons are taken into account. All coupling are then taken into account, as well as the total spin state but also the individual target and projectile spin states, when required. In the presentation we shall illustrate the use of our approach and code for several collision systems of interest.

MOD/2 A+M Data

Complete collision data set for electrons scattering on molecular hydrogen and its isotopologues

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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 Con- vergent 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 57,000 entries 1. This complete collision data set is available to the research community via the LXCat database and the dedicated MCCC database (mccc-db.org). For H2 the data set in- cludes transitions from all 14 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 3Πu, a 3Σ+, B 1Σ+, C 1Πu, and EF 1Σ+ states of all H2 g u g isotopologues with first results already available [2] as well as producing a dataset of fully resolved rovibrational cross sections. An overview of

the available MCCC dataset will be presented and an example of modelling calculations based on the MCCC dataset will be given for collisional-radiative (CR) modelling [3].

The MCCC dataset allows for a detailed investigation of dissociation processes of H2 and its iso- topologues by electron impact. In low-temperature plasmas, electron-impact dissociation proceeds almost exclusively via excitation of the dissociative b $3\Sigma+$ state. The latest measurements for dis- sociation of the ground vibrational level of H2 are in excellent agreement with MCCC calculations [4]. However, in the absence of similar measurements for vibrationally-excited or isotopically sub- stituted H2, cross sections for dissociation of these species must be determined by theory alone. We have recently [5] identified large discrepancies (up to a factor of 3) between MCCC cross sections and the recommended and widely used R-matrix cross sections [6] for dissociation of vibrationally- excited H2, D2, T2, HD, HT, and DT, with disagreement in both the isotope effect and dependence on an initial vibrational level. The source of the discrepancies and the consequences for plasma models which have incorporated the previously recommended data will be discussed.

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MOD/2 A+M Data

Vibrational excitation and dissociation of deuterium molecule by electron impact

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In the talk, a theoretical investigation, in the framework of Local-Complex-Potential approach, on electron-deuterium molecule resonant collisions - via the low-lying and the Rydberg states of D2- anion - will be presented for vibrational excitation, dissociative electron attachment and dissociative excitation processes.

Full sets of vibrationally resolved cross sections (Fig. 1), involving the ground electronic state and the first two electronic excited states of the D2 molecule, are given for fusion plasma applications in their technologically relevant partially dissociated, detached divertor regimes. In particular, transitions between electronic excited states are also considered. Comparisons, where available, are made with cross sections present in the literature.

By using the calculated reaction rate, relaxation time for the ground electronic state of deuterium molecule will be also presented (Fig. 2).

MOD/2 A+M Data

Electron collisions with H2+, HD+ and D2+: computation of cross sections and rate coefficients, and comparison with storage ring measurements

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Dissociative recombination, ro-vibrational excitation and dissociative excitation 1 strongly drive the electron and cation kinetics in the edge of the fusion plasma. They occur via super-excited molecular states of the neutral complex singly or doubly excited, embedded in the ionization continuum of the target ion. Quantum chemistry and R-matrix techniques are used to produce the relevant potential energy states and their mutual interactions. We use these molecular structure data in methods based on the Multichannel Quantum Defect Theory [2, 3] for computing accurate state-to-state cross sec- tions and rate coefficients, displaying a resonant character and a strong dependence on the target's initial state. I will illustrate our most relevant results for H+, HD+ and D+ in a broad energy range 2 2 - 0 − 12 eV - of the incident electron, and for numerous ro-vibrational levels of the ion.

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EXP/2 A+M data

Charge Exchange Cross Section Measurement in Fudan University

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Cross section, being amongst the most important parameter in describing atomic collision processes, can point towards the relevant reaction mechanisms and also have been used as key physical quanti- ties for checking many-body theories 1. On the other hand, cross sections for the interaction between ions and atoms play an important role in understanding astrophysical plasmas and fusion plasma diagnostics. However, due to the complicated collisional processes and high costs involved in exper- imental measurements, cross sections for highly charge ions interacting with atoms/molecules are still limited.

Recently, the absolute electron capture cross sections for single and double charge exchanges be- tween the highly charged ions O6+ and CO2, CH4, H2, N2, the dominant collision processes in the solar wind, have been measured in the energy from 7 keV•q (2.63 keV/u) to 52 keV•q (19.5 keV/u). These measurements were carried out in the new experimental instrument set up at Fudan Univer- sity, and the error of cross sections for single and double charge exchanges at the 1σ confidence level are about 11% and 16%, respectively 2.

At the same time, Base on time-dependent density functional theory non-adiabatically coupling with molecular dynamics, we investigated the ion-atom/molecule collision processes. Aiming at many-electron systems with large spacial scale, we proposed an approximate method to extract the electron capture cross sections, avoiding explicit dependence on the final scattering wave functions. To demonstrate the reliability of the method, we reconstructed the electron capture and ionization cross sections in the Ne2+ and He collision [3]. The results agree reasonably well with the experi- mental data and semi-empirical results in the keV energies.

In this report, I will first introduce the experimental facilities for highly charged ion colliding with atoms and molecules, then present some new results.

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EXP/2 A+M data

Spectroscopic investigations on energy, angular and atomic level distribution functions of sputtered tungsten

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The understanding of the ongoing processes during sputtering of plasma-facing components is of large importance in fusion research. For example, the angular and energy distribution of sputtered atoms strongly influence the transport into the plasma and, moreover, the redeposition of sputtered material on the inner vessel. Therefore, these distribution functions are also important input pa- rameter for simulations. For high impact energies, the angular and energy distributions of sputtered atoms are well known and can be described by a cosine angular distribution and the so-called Thomp- son energy distribution 1. However, the situation changes for low impact energies relevant in fusion research. Here, the data is only rare and deviations from the cosine angular and Thompson energy distribution are reported 2. To investigate these deviations and close the remaining gap of infor- mation we carried out experiments and subsequently modeled the line shape emitted by sputtered tungsten (W) atoms via a Doppler-shifted emission model. The experiments took place in the lin- ear plasma device PSI-2, where W samples were exposed to low density (ne 2 1012 cm−3) and temperature (Te 3 eV) argon plasmas. The ions hitting the sample were accelerated by 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 spectral resolution of λ/Δλ 7 105. In agreement with recent theoretical work [3], we found that the energy and angular distribution can be determined from the light emitted by sputtered atoms. The line shapes modeled by the usage of a cosine angular and a Thompson energy distribution show good agreement with the experimen- tally detected line shapes [4].

In addition to the energy and angular distribution of sputtered W the initial atomic level population within the fivefold ground term 5D and the metastable 7S level of sputtered W remains an open question. On the one hand, ion beam experiments for different materials show a strong popula- tion of the ground state only [5]. On the other hand, for experiments in the Tokamak TEXTOR a nonphysical effective temperature was introduced to describe the level population distribution via a Boltzmann distribution within the ground term and the metastable 7S3 level [6]. This resulted in a strong population also of other levels and not only of the ground state. The knowledge of the atomic level distribution is of importance for interpretation of spectroscopic data and further the determi- nation of the net erosion via so-called S/XB values in fusion devices [7]. 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 µm/pixel) the temporal line intensity development as a function of distance to the target was studied for of different transitions of W I. The W atoms were sputtered by mono-energetic Ar+ ions at 80 eV and due to water-cooling the target was kept at room temperature. The experiments show a strong population only for the ground term 5D0 of sputtered W atoms [8].

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MOD/1 fusion devices

Needs of atomic data for kinetic modelling of fusion plasma edge

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Presentation consist of two parts. First we discuss the effects of non-Maxwelian velocity distribu- tion functions (VDF) on effective plasma-neutral and plasma impurity (W, Ar) interaction rates. It will be shown, that in the stationary SOL the rates of electron-impact processes (e.g. W, W+ ioniza- tion) well agree with the Maxwell averaged values. The exception is plasma sheath where the cutoff in electron VDF introduces some deviations. Contrary to this, the rates of ion-neutral interactions might significantly deviate from the Maxwell averaged values. In the ELM-ing SOL the majority of plasma-impurity and plasma-neutral interaction rates differ from the Maxwell-averaged values.

In the second part of the presentation we discuss needs for atomic data for kinetic modelling and consider new technique, “dressed” cross sections, for kinetic treatment of multichannel atomic pro- cesses using collisional-radiative model.

MOD/1 fusion devices

Theoretical analysis and experimental validation in DIII-D of predictive modeling for tungsten erosion and redeposition in tokamak divertors

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Fundamental mechanisms governing the prompt redeposition of tungsten impurities sputtered in tokamak divertors have been identified and analyzed to enable quantitative estimations and in-situ monitoring of the net erosion and lifetime of tungsten divertor plasma-facing components (PFCs) in ITER. In tokamak divertors, the width of the electric sheath is of the order of the main ion Larmor radius, and a vast majority of sputtered tungsten impurities are ionized within the sheath region in high-density attached divertor plasma conditions. Tungsten prompt redeposition is then mainly governed by the ratio of the characteristic ionization mean-free path of neutral tungsten over the width of the sheath, and a new scaling law for tungsten prompt redeposition in tokamak divertor was derived. It is also shown that in-situ monitoring of the prompt redeposition of tungsten impurities in divertors requires the measurement of photon emissions associated with the ionization of tungsten impurities in charge states $Z > 2+$, typically, and for divertor plasma conditions expected in the far- SOL of the ITER divertor. Besides, S/XB coefficients (number of ionization events per photon) for tungsten impurities are significantly modified in high-density divertor plasma conditions because of the decrease of the electron density in the sheath region where sputtered tungsten impurities are ion- ized and because of the transient populations of

metastable states of tungsten atoms. Finally, various experiments conducted at DIII-D to benchmark predictive models of tungsten prompt redeposition and net erosion in divertors are presented.

MOD/1 fusion devices

Atomic data needs for tungsten erosion, migration and deposition modelling in fusion devices

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Tungsten is foreseen as plasma-facing material for future fusion devices like ITER and DEMO due to its high melting point and low sputtering. However, as high-Z material the tungsten concentration in the core plasma has to be limited to very low numbers to avoid plasma cooling and dilution. Thus, it is of extreme importance to minimise the tungsten net erosion sources as far as possible for which an extensive understanding of the involved physical processes is indispensable. Experiments in combination with modelling are required to achieve that aim.

The present contribution provides examples of ERO and ERO2.0 [1, 2] modelling of tungsten erosion, migration and resulting deposition for various fusion devices like TEXTOR, the linear device PSI- 2 and JET-ILW. The eroded tungsten is observed in-situ by means of spectroscopy in the plasma, which is compared with the modelling. For that purpose, the modelling has to make use of atomic data for ionisation and excitation. The gross erosion source is typically estimated from the emission of tungsten atoms, whereas the emission of ionised species can be used to draw conclusions about the net erosion, i.e. considering the re-deposition of eroded tungsten particles. On the basis of the various modelling examples, the use of different available ionisation and excitation data, the importance of physical processes like metastable states or the excitation state of eroded tungsten will be discussed. The possible lack of atomic data and further data needs will be addressed.

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EXP/1 fusion devices

Digital Atlas of Electronic Vibrational-Rotational Transitions in Deuterium and Protium Molecules (withdrawn)

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MOD/2 A+M Data

Vibrational excitation and dissociation of deuterium molecule by electron impact

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In the talk, a theoretical investigation, in the framework of Local-Complex-Potential approach, on electron-deuterium molecule resonant collisions - via the low-lying and the Rydberg states of D2- anion - will be presented for vibrational excitation, dissociative electron attachment and dissociative excitation processes.

Full sets of vibrationally resolved cross sections (Fig. 1), involving the ground electronic state and the first two electronic excited states of the D2 molecule, are given for fusion plasma applications in their technologically relevant partially dissociated, detached divertor regimes. In particular, transitions between electronic excited states are also considered. Comparisons, where available, are made with cross sections present in the literature.

By using the calculated reaction rate, relaxation time for the ground electronic state of deuterium molecule will be also presented (Fig. 2).

MOD/2 A+M Data

Highly Charged W Ions: Atomic Data and Collisonal Radiative Modeling (withdrawn)

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The atomic data and spectral properties of highly charged Tungsten (W) ions were urgently required by the development of the magnetic confinement fusion. The tungsten was chosen as the cover mate- rial of the divertor and the wall of the various reactor, such as ITER, ASDEX-upgrade, EAST, etc., due to its favorable physical, chemical, thermal and mechanical properties. Although the heavy highly charged impurity tungsten ions may cause serious radiation power loss, their emission line may still helpful for the diagnostics of the core and edge plasma of MCF. Therefore, accurate atomic data and plasma model of the line emission is indispensable for the diagnosis of the plasma parameters.

The relativistic, electron correlation and QED effects play important roles in the energy level and transition properties of the heavy highly charged W ions. The Multi-configuration Dirac-Fock method with the implementation of GRASP2K 1 is a widely used ab-initio method to investigate the complex ions which could take these important effects into account. The energy level and E1, M1, E2, M2 transition rates were calculated for the W26+, W27+, and W54+

ions2. The electron correlation contribution to the transition wavelength and rate from the same shell are emphasized to be essential.

In order to analyze the spectrum observed from EBIT and EAST, a collisional-radiative model was constructed with atomic data calculated by RCI and distorted wave method with the implementation of FAC code3. The calculated energy levels, transition energies, and rates are well agreed with the one calculated by MCDF methods and the experiments. The present model can be used to interpret and assign the observed spectrum from EBIT and EAST facilities4.

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