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The Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)

Summary report of the Technical Meeting

IAEA Headquarters, Vienna, Austria

6-10 December 2021

Prepared by
Christian Hill
Kalle Heinola
Lidija Vrapcenjak
IAEA Nuclear Data Section

September 2024

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Table of Contents

Introduction

The meeting was opened by scientific secretary of the meeting, and participants were welcomed by the Section Head, Arjan Koning.

Two working groups (WGs) had been created previously within the Technical Meeting series on CR Properties of Tungsten and Hydrogen in Edge Plasmas [1]: WG1 on *Atomic and Molecular Data Recommendation and Validation with Collisional-Radiative Models*, chaired by Ursel Fantz and Dirk Wunderlich; WG2a on *Plasma Experiments and Comparison Activities with Collisional-Radiative Models: W and Hydrogen Experiments with Fusion Devices and Linear Plasma Devices*, chaired by Sebastijan Brezinsek; and WG2b on *Photon Opacity Models for Edge Plasmas* chaired by Sven Wiesen.

The presentations of the GNAMPP meeting participants were followed by discussion and planning sessions, as outlined below.

Session by WG1 on Atomic and Molecular Data Recommendation and Validation with Collisional-Radiative Models

Main points of discussion were about data providers and modellers with data needs and ideas concerning who can assist benchmarking validation and to foster collaborations possibly within the GNAMPP Network, and to identify a scope for cross-comparison of data and computational methods.

Data is available to benchmark and validate the fundamental cross sections against both experiments and collisional-radiative models.

The collaboration between the groups of Dmitry Borodin and Derek Harting at Forschungszentrum Jülich (FZJ), Germany could serve as template for future collaborations. The most fruitful collaboration is between the groups who can calculate data and the groups who can use data from different sources in a way that can then show the differences induced in its usage. It is important to know if and by how much calculations deviate from measurements and previously-accepted values. This in turn raises the question of how to justify using the new data values and what criteria to use in comparing data. It is understood that this is an ongoing topic which can only be addressed by doing validation against measurements and determining the boundaries within which the calculations fit.

Also to be considered is the fact that the experimentally obtained data should have uncertainties presented; the most reliable validation is accurate experiment: If we can stimulate more research groups to perform the same experiments that would be the best outcome of this meeting. In most cases there are no dedicated experiments (for example, involving beryllium) at present because these are very tricky, but there is calculated data. A comparison of data sets for the same process calculated using three or more different theoretical methods is another approach to validation in this case.

The meeting called for the fusion data community and e.g. the Data Centres Network to come up with list of characterisations for data evaluation and data production. This could be facilitated through a “data-share portal”, listing data priorities, the existing quality of data involving particular species (for example, tungsten), and identifying significant data gaps. On approach would be for the IAEA to host a resource where the experimentalists can list the data that they have produced, though this needs to be in a consistent format and readable by everyone, clearly identifying the devices and experiments which produced data. Where rough parameters are known, the contact details of data providers who would like access to insert their own benchmarking details will be provided. It was agreed that this requires a more focused meeting to decide which participants can provide that information (within GNAMPP or more broadly).

It was noted that one of the problems currently is to obtain the available data: a significant amount of duplicated work is involved in extracting truly valuable data and an open repository utilising a consistent format would be very valuable; failing that, just knowing whom to contact would be an improvement on the *status quo*.

Databases (for example CollisionDB and ALADDIN) of cross section and rate coefficient data for collisional processes make it easy to compare data from various source publications, but spectra taken by various experimental apparatus (including tokamaks and EBITs) are different because they depend on electron temperature and density (which can often be inhomogeneous along the spectrometer line of sight).

For example, obtaining and interpreting VUV spectral data in a form that is reliable requires considerable effort and at present “knowing what you have” is not the same as providing it. The issues are a deficit of expert knowledge and the large volume of unstructured data which makes it hard to find data concerning a particular element and particular conditions. A start would be a listing of what data are available in some defined format: only once it is decided for which processes particular cross sections are missing can the quality be discussed.

There exist many successful services, such as ADAS which has created data sets which are obtained from more fundamental cross section data through intermediate processing. Specifically, the condensed data from ADAS is based on rates: what is used in practice are the effective rates based on initial rates dependant on the collision strength, Ω_{ij}. It was noted that it is important to save the intermediate stages, which raises the question of who should be doing this: data producers whose code is developed with some particular functionality will perhaps not be keen to do something different than what their code has been optimised for.

An output of this Working Group will be for the GNAMPP network to put together people data needs with data providers who are able to calculate some (but often not all) data. A steering committee could be established, and expert volunteers are needed for that committee. A focus on particular processes will be maintained.

Session by WG2a on Plasma Experiments and Comparison Activities with Collisional-Radiative Models: W and Hydrogen Experiments with Fusion Devices and Linear Plasma Devices

Session by WG2b on Photon Opacity Models for Edge Plasmas

Excellent data exists on low ionisation stages of tungsten which are seen in tokamak spectra and it seems that more exchange of data is needed. Long-lived meta stables might also have an impact. There can be a very high population of such species, which are not well-understood; proper modelling becomes even more complex when considering surface physics in addition to plasma physics and collisional-radiative models. It was resolved that a smaller group should look into this.

It is reasonable to condense (bundle) the number of metastable species considered in a given model to make the data manageable and to stimulate a change in the mindset in researchers trying to model divertor edge plasmas with tungsten.

In practice, all lines are needed in order to accurately simulate the spectra and how they can change due to temperature changes; they cannot be bundled too much because this leads to poor reproduction of the observed spectra. Measurements at relevant temperatures indicate the presence of W VII at temperatures below 10 eV, and meta stables are known to be present in this and nearby ionisation stages which cannot be excluded. There are other codes that can be run unbundled, but we do need different ionisation stages. In practice, bundling was introduced more for pragmatism: it was needed to get things calculating.

The next technical meeting in the series is planned for 2023, but a virtual update of the profiles of the various research groups and an intermediate meeting should be organised virtually in 2022.

Working Group 2b, with Sven Wiesen as chair, discussed the JET: Lya/Lyb line ratios, found to be near-constant, although collisional-radiative models suggest dependent line ratios even with raised density. Also discussed were the main uncertainties of JET opacity (absolute) measurements; Lya/Lyb line ratios in D and H plasmas were summarized as deduced from an assumed line shape (instrument-broadening only), constant integration length, instrumental sensitivity, and assumed level populations and impurities.

The effects leading to line broadening are Doppler, “natural” (lifetime), isotope, Zeeman-splitting, and Stark broadening; many of these are included in the EIRENE MC code, along with their convolutions (Gaussian+Lorentzian=Voigt profiles).

It is important to define which processes are relevant in fusion: in devices with metal walls and better diagnostics this can now be better clarified. Furthermore, there exists a hierarchy of model complexity that should be formally established: detailed photon-tracing vs. simple models, escape factors, etc. as well as revised CR models (going beyond early works).

A possible topic for the next meeting is the wall reflection on metal surfaces and its link to CHERAB and the impact of reflections on diagnostics e.g. in ITER/DEMO.

Conclusions

GNAMPP currently has 37 members. Another intermediate virtual meeting should be organised in 2022 with possibly several invited presentations on the work and needs of different research groups. Each working group should have a steering committee and by early 2022 a summary report of this meeting should be ready with the future work plans (also updated on the AMD Unit's website, which also contains a summary of the individual data needs and priorities.)

All presentations for the meeting are available to all participants as videos, abstracts are available as attachment to this report and online as well.

References:

[1] IAEA Summary Report INDC(NDS)-0848, "*Joint IAEA-FZJ Technical Meeting on the Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasmas of Fusion Devices*", 29 March – 1 April 2021, https://doi.org/10.61092/iaea.gt1c-hv9e

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2nd Meeting of the Global Network for the Atomic and Molecular Physics of Plasmas

6 – 9 December 2021

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Appendix II

2nd Meeting of the Global Network for the Atomic and Molecular Physics of Plasmas

6 – 9 December 2021

AGENDA

Monday, 6 December 2021

Session 1: WG1: Atomic and Molecular Data Recommendation and Validation with CR Models

Chairs: Ursel FANTZ and Dirk WÜNDERLICH

14:00 – 14:20	Christian HILL, Kalle HEINOLA and Arjan KONING: Opening of the meeting; Welcome and introductions
14:20 – 14:40	**Alisher KADYROV**, *Faculty of Science and Engineering, Curtin University, Australia* Charge exchange and ionisation in ion-atom collisions
14:40 – 15:00	**Nathan GARLAND**, *Griffith University, Australia* H, He and H_2 elastic scattering models for use in plasma kinetic models
15:00 – 15:20	**Ioan F. SCHNEIDER**, *Université le Havre Normandie, France* Recent results on the reactive collisions of electrons with H_2^+, BeH^+, ArH^+ and some of their isotopologues
15:20 – 15:40	Coffee Break
15:40 – 16:00	**DIPTI**, *IAEA, Austria* Kinetics of W ions for the charge exchange recombination spectroscopy diagnostic for ITER
16:00 – 16:20	**Bobby ANTONY**, *Indian Institute of Technology (Indian School of Mines) (IIT(ISM)), India* Electron impact scattering from beryllium and tungsten
16:20 – 16:40	**Yuri RALCHENKO**, *National Institute of Standards and Technology, United States of America* Inner-shell ionization in Maxwellian X-ray spectra of Ne-like W
16:40 – 17:00	**David TSKHAKAYA**, *Institute of Plasma Physics of the Czech Academy of Sciences, Czechia* Needs for W data for kinetic modelling of tokamak plasma edge

Tuesday, 7 December 2021

Session 2: WG1: Atomic and Molecular Data Recommendation and Validation with CR Models

Chairs: Ursel FANTZ and Dirk WÜNDERLICH

13:40 – 14:00	**Nupur VERMA**, *University of Delhi, India*
	Atomic structure calculations and electron impact excitation of chlorine-like tungsten ions
14:00 – 14:20	**MURAKAMI Izumi**, *National Institute for Fusion Science, Japan*
	Progress of collisional-radiative modelling for tungsten EUV spectra
14:20 – 14:40	**Duck-Hee KWON**, *Korea Atomic Energy Research Institute, South Korea*
	Collisional-radiative modeling for low temperature Ar, He, and H plasmas
14:40 – 15:00	**Dirk WÜNDERLICH**, *Max Planck Institute for Plasma Physics, Garching, Germany*
	Application of molecular convergent close-coupling cross sections in collisional radiative models for molecular hydrogen: current status and outlook
15:00 – 15:20	**Dmitry FURSA**, *Faculty of Science and Engineering, Curtin University, Australia*
	Electron impact dissociation of molecular hydrogen and its isotopologues
15:20 – 15:40	**Bowen LI**, *Lanzhou School of Nuclear Science and Technology, China*
	Electron-impact single ionization of tungsten ions
15:40 – 16:00	**David COSTER**, *Max Planck Institute for Plasma Physics, Garching, Germany*
	Exploration of the impact of uncertainty in atomic physics rates on the plasma
16:00 – 16:20	Coffee Break
16:20 – 17:20	Working Group 1 discussion and planning session

Wednesday, 8 December 2021

Session 3: WG2a: Plasma Experiments and Comparison Activities with CR Models: W and Hydrogen Experiments with Fusion Devices and Linear Plasma Devices

Chair: Sebastiján BREZINSEK

14:00 – 14:20	**PRITI**, *National Institute for Fusion Science, Japan* Spectral analysis of multiply-charged W^{6+} – W^{13+} in the EUV and visible range
14:20 – 14:40	**OISHI Tetsutarou**, *National Institute for Fusion Science, Japan* Spectroscopic observation of W I to W XLVII tungsten emission lines in visible, VUV and EUV wavelength ranges in the Large Helical Device for ITER edge plasma diagnostics
14:40 – 15:00	**Ewa PAWELEC**, *University of Opole, Poland* Spectroscopic observations of the hydrogen and tungsten hydride molecules in divertor plasma – isotope effect
15:00 – 15:20	**Rémy GUIRLET**, *IRFM, CEA Cadarache, France* Extreme UV spectroscopy measurements and analysis for Tungsten density studies in the WEST tokamak
15:20 – 15:40	**Jun XIAO**, *Fudan University, China* Experimental and Theoretical Study of Moderately Charged Tungsten Ions at the SH-HtscEBIT
15:40 – 16:00	Coffee Break
16:00 – 16:20	**Stefan SCHIPPERS**, *Justus Liebig University, Giessen, Germany* Experimental cross sections for atomic collision processes involving tungsten ions
16:20 – 17:20	Working Group 2a discussion and planning session

Thursday, 9 December 2021

14:00 – 14:20	**Somsak DANGTIP**, *Thailand Institute of Nuclear Technology, Thailand* Potential studies on plasma behaviours with reconstructed limiter-type tokamak of Thailand

Session 4: WG2b: Photon Opacity Models for Edge Plasmas

Chair: Sven WIESEN

14:20 – 14:30	**Sven WIESEN**, *Forschungszentrum Jülich (FZJ), Germany* Working Group 2b: Photon opacity models for edge plasmas
14:30 – 15:10	**Kerry LAWSON**, *Culham Centre for Fusion Energy, United Kingdom* Opacity measurements in the JET divertor
15:10 – 15:30	**Joël ROSATO**, *Physique des Interactions Ioniques et Moléculaires (PIIM), Aix-Marseille Université (AMU), France* Development of accurate hydrogen line shape models for Lyman radiation transport calculations in edge plasmsas
15:30 – 15:50	Coffee Break
15:50 – 16:50	Working Group 2b discussion and planning session
16:50 – 17:10	AOB, Meeting conclusion

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Electron impact scattering from beryllium and tungsten

Bobby Antony
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Interaction of charged particles, especially electrons, with plasma wall and divertor plate is a hot topic due to their significance in modeling plasma for fusion reactors. The choice of an appropriate element for the plasma wall or divertor plate is critical in its design [1]. The phenomena like erosion of wall material, transport of impurities, and redeposition of these impurities on the walls are imperative in any plasma reactor [2] and hence need to be considered in any model. The elements of interest for such studies are Li, Be, W, etc. Tungsten is an apparent choice for wall coating element due to its high temperature survivability, high neutron irradiation and low hydrogen retention [3]. These elements, along with their oxides or clusters with other element, are found to be impurities in the fusion edge plasma [4]. Due to the need for collision data on these elements and their molecules or clusters, a method for calculating various cross section is presented here. These data are presented for energy range from the ionization threshold of the atom/molecule/cluster to 10 keV.

References

[1] F.Maviglia *et al*, *Nucl. Mat. Ener.* **26** 2021 100897; https://doi.org/10.1016/j.nme.2020.100897
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[3] V.Philipps, *J Nucl. Mat.* **415** 2011 S2; https://doi.org/10.1016/j.jnucmat.2011.01.110
[4] L.Chena *et al*, *Nucl. Mat. Ener*. **16** 2018 149; https://doi.org/10.1016/j.nme.2018.06.021

Exploration of the impact of uncertainty in atomic physics rates on the plasma

David Coster[1]

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The EasyVVUQ framework has been used to explore the impact of uncertainty in the ionization and recombination rates on the resultant plasma state in a simple coronal model. If this is felt to be of broader interest, the impacts could be examined in the future in an edge/SOL transport code.

Kinetics of W ions for the charge exchange recombination spectroscopy diagnostic for ITER

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Charge-exchange recombination spectroscopy (CXRS) remains one of the most important diagnostic methods for existing and future magnetic fusion devices. In particular, the CXRS with energetic neutral beams of hydrogen will be a key diagnostic tool for ITER where interactions with its important impurity, namely, tungsten, should result in new spectral features to be analyzed. The results of the present spectral synthesis are based on the new set of *nl*-resolved CX cross sections for recombination of the W^{q+} ions (q = 61-66) with atomic hydrogen calculated using the classical trajectory Monte Carlo method for the planned ITER neutral beams (diagnostic beam of 100 keV/u and heating beam of ~ 1 MeV/u). These calculated CX cross sections, along with the atomic data needed for other relevant physical processes, were used in a large-scale collisional-radiative model to study the population kinetics of atomic states of the tungsten ions and to generate the synthetic spectra across a wide range of photon energies. The simulations show that the CX-induced emission may drastically modify the observed spectrum in the visible and VUV ranges, which can provide important predictions for interpretation and evaluation of the CXRS diagnostics on ITER. Details of the theoretical calculations and results will be presented and discussed.

Abstract ID : **6**

Electron impact dissociation of molecular hydrogen and its isotopologues

Content

Dissociation processes play significant roles in the modeling of hydrogenic plasmas. An accurate description of dissociation processes requires a comprehensive set of electron-impact excitation cross sections that are fully resolved in transitions between vibrational levels of the ground and excited electronic states. Such data set has recently been produced by the Curtin University research group using the Molecular Convergent Close-Coupling (MCCC) method for molecular hydrogen and all isotopologues, and contains more than 60,000 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).

The MCCC cross section dataset was used to determine cross sections of dissociation into neutral fragments for electron scattering on the ground and vibrationally excited states of molecular hydrogen and isotopologues [2]. The radiative cascade from the excited bound vibrational levels can lead to dissociation via the vibrational continuum of lower electronic states. For triplet states, the radiative cascade terminates on the dissociative $b\ ^3\Sigma_u^+$ state. For singlet states, it terminates on the ground state leading to a population of the bound vibrational levels and dissociation via the ground state vibrational continuum. We have produced a comprehensive set of cross sections for vibrational excitations and dissociation of molecular hydrogen and isotopologues via electron-impact excitation and radiative cascade [3].

Electron-impact dissociation proceeds almost exclusively via excitation of the dissociative $b\ ^3\Sigma_u^+$ state in low-temperature plasmas. The latest measurements for dissociation of the ground vibrational level of H_2 are in excellent agreement with MCCC calculations [4]. However, in the absence of similar measurements for vibrationally-excited or isotopically substituted H_2, 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 three) between MCCC cross sections and the recommended and widely used R-matrix cross sections [6] for dissociation of vibrationally-excited H_2, D_2, T_2, 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.

We have conducted a Monte-Carlo simulation of electron beam propagation in a gas of molecular hydrogen [7]. Ab-initio estimates have been obtained for energy deposition parameters and dissociation probabilities due to the primary and secondary electrons. The uncertainty of the collisions cross section dataset leads to uncertainties of the derived collision data. We have developed a computational framework for propagating uncertainties for such derived collision data using the Total Monte-Carlo method.

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[7] R. K. Horton et al., Plasma Sources Sci. Technol. 30, in press (2021)

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Presenter: Prof. FURSA, Dmitry (Curtin University)

Submitted by **FURSA, Dmitry** on **Thursday 14 October 2021**

Abstract ID : **2**

Statistical Property of Complex Spectra from Many-electron Atomic Ions

Content

Many-body interactions among valence electrons make the emission spectra from many-electron atomic ions, such as tungsten ions in fusion plasmas, very complex. Such spectra consist of thousands of discrete lines and frequently show quasi-continuum profiles. Therefore, it is often difficult to follow a typical plasma-spectroscopic strategy, where a few emission lines of such systems are deeply investigated and utilized as plasma diagnostics. Instead, it may be reasonable to study their statistical properties. However, few properties have been known for many-electron atom spectra.

One of such properties is the power-law intensity distribution of the spectra. In 1982, Learner has reported that the number of emission lines from many-electron atoms with given intensity follows a power-law distribution of the intensity [1]. This law has been known only empirically and its theoretical explanation has been missing. Here, we report that by combining two well-known statistical models — an exponential increase in the level density of many-electron atoms and local thermal equilibrium of the excited state population — produces a surprisingly simple analytical explanation for this power-law dependence [2]. We find that the exponent of the power law is proportional to the electron temperature. This dependence may provide a useful diagnostic tool to extract the temperature of plasmas of complex atoms without the need to assign lines.

1. R. C. M. Learner, *J. Phys. B* **15**, L891 (1982).
2. K. Fujii and J. C. Berengut, *Phys. Rev. Lett.* **124**, 185002 (2020)

Primary authors: FUJII, Keisuke (Kyoto university); Dr BERENGUT, Julian C. (University of New South Wales,)

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Submitted by **FUJII, Keisuke** on **Monday 04 October 2021**

Abstract ID : **8**

Proposed recommendations for analytic anisotropic elastic scattering models for electron-neutral collisions in edge plasma modelling

Content

Modelling tokamak edge plasmas require accurate techniques to understand the interplay between microscopic and macroscopic processes. A prime example of this interplay is how particle and Monte Carlo simulation codes use angular scattering information of electrons following scattering events within a simulation. It is well known that the forward peaked nature of high energy electron elastic scattering is relatively trivial to accurately describe in plasma simulations. However, for lower energy collisions, which can produce near isotropic or even backward peaked differential cross sections, there is not a strong consensus among the plasma modelling community on how to best describe these angular scattering trends. Resolution of this anisotropic scattering behaviour is important to ensure simulated macroscopic properties, such as particle and heat fluxes delivered to device walls, are based on physically reasonable data assumptions. In this study we propose a systematic method to approximate the aforementioned non-trivial angular scattering behaviour with a formula that can be readily implemented in Particle-in-Cell and/or Monte Carlo plasma simulation codes. Specific application of this method is demonstrated for targets relevant to the edge modelling problem of tokamaks such as ITER, with recommendations provided for atomic hydrogen and helium, as well as for molecular hydrogen.

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Submitted by **GARLAND, Nathan** on **Thursday 21 October 2021**

Extreme UV spectroscopy measurements and analysis for Tungsten density studies in the WEST tokamak

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The VUV emission of tungsten in WEST is measured by an absolutely calibrated grazing incidence spectrometer of the Schwob-Fraenkel type which can scan the lower half of the plasma. We have analysed the detected spectral lines in the range 120-140 Å and compared their behaviour with calculations and published information. We obtained an unambiguous identification of four intense and well resolved spectral lines emitted by W^{42+}-W^{45+} close to the magnetic axis in the analysed experiments. The W^{44+} 132.88 Å line is very intense and thus probably particularly useful for core W monitoring in plasmas with temperatures above 3 keV. The measured spectral line brightnesses are used to assess the Tungsten density in the emission region. For the ions of interest, the emission location can be very sensitive to the ionisation equilibrium while the W density is very sensitive to the photon emission coefficients, hence the importance of using high quality calculations for the latter.

Abstract ID : **3**

Charge exchange cross sections for plasma-impurity ions

Content

Single electron capture cross sections for slow (0.5 - 32 keV) Be, B, C, Fe, Ni, and W ions (q = 1, 2) on gaseous He, Ne, Ar, Kr, H_2, D_2, CO, N_2, CO, CO_2, CH_4, C_2H_6, and C_3H_8 targets were measured[1,2]. An attempt to draw an empirical behavior for such slow low-q ions on target species will also be presented.
We have started another attempt to derive charge-exchange cross sections for collisions of NBI H atom (1 MeV/u) and impurity W^{q+} ions by using 1.0 MeV/u W^{q+} ion collisions on H atomic targets. The present status for this measurement will also be presented.

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Charge exchange and ionisation in ion-atom collisions

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We review recent progress in applications of the wave-packet convergent close-coupling (WP-CCC) approach to ion-atom collisions relevant to plasma modelling and diagnostics. In particular, we present

- A computationally more efficient one-centre approach to two-centre rearrangement collisions involving single and multielectron targets [1]. The method is tested on proton-hydrogen system and then applied to proton-lithium collisions.
- The angular differential cross sections of elastic scattering, excitation, and electron capture, as well as the ionisation cross sections singly differential in the ejected-electron angle, and in the ejected-electron energy [2] in proton-hydrogen collisions.
- The angular differential cross sections for direct scattering and electron capture [3], and various singly differential cross sections for ionisation [4] in proton-helium collisions.
- An effective single-electron treatment of ion collisions with multielectron targets that does not use the independent-event model [5]. The method is applied to calculate single-electron capture and single-ionisation cross sections for proton collisions with alkalis.
- We also report on calculations of the total and state-selective cross sections for bare beryllium ion collisions with hydrogen in its ground state [6], and update on the status of similar calculations for the excited states of hydrogen.

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Abstract ID : **9**

Collisional-radiative modeling for low temperature Ar, He, and H plasmas

Content

Collisional-radiative (CR) modeling for low temperature Ar [1], He [2], and H plasmas was developed, which solves nonlinear steady-state balance equations including radiation trapping and heavy particle collisional ionization, and considers non-Maxwellian electron energy distribution function. The electron temperature and density diagnostics by the CR modeling and optical emission spectroscopy was compared with Langmuir probe measurements for the capacitively-coupled plasma, inductively-coupled plasma, and a novel applied-field MagnetoPlasmaDynamc (AF-MPD) thruster [3,4] devices in KAERI. The AF-MPD thruster device has been constructed and developed to generate high particle beams and heat fluxes relevant to divertor plasma which can be used for the plasma surface interaction study. The detailed population kinetics and spectra intensities by the CR modeling are presented and discussed.

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D and He Lyman series line intensity ratios measured in the JET divertor

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Abstract

Discrete spectral lines are the dominant component of radiation emitted by the hydrogenic ionization stages of D and He fuel in large plasma machines. Their intensities are determined by collisional-radiative population models and it is important that these are confirmed by comparisons with experiments, if the plasmas are to be reliably modelled in the next step machines such as ITER. This is particularly important for the transport modelling of divertor plasmas. The most stringent test of the models is to compare line intensity ratios, since this avoids having to measure the density of the emission region and simplifies the analysis in that an absolute sensitivity calibration of the observing spectrometer is not required. The comparison between measurements and theory can also be complicated by the occurrence of reabsorption of the radiation along some lines-of-sight when the plasma is optically thick. Measurements of line intensity ratios of VUV Lyman series radiation from D and He have been made in the JET tokamak. The observed ratios tend to be approximately constant and do not appear to show the expected temperature dependence. Examples for both hydrogenic D and He are presented and comparisons with theory given.

**See author list of J. Mailloux et al., 2021, Nuclear Fusion Special issue, 28th Fusion Energy Conf. (Nice, France, May, 2021)*

Opacity measurements in the JET divertor

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Abstract

The combination of plasma density and path lengths encountered in divertor plasmas can lead to significant reabsorption of Lyman series radiation of the hydrogen fuel and its isotopes. It is crucial that the reabsorption or opacity of the divertor plasmas is understood, if they are to be reliably modelled in the next step machines such as ITER. Previous work on JET has included analyses by Lachin (1988) and Lomanowski *et al.* (2020). The present analysis relies on the observed near-constant ratios between the Lyman series line intensities and assumes that these ratios persist as the density changes. With this assumption a direct measurement of the absorption of the affected lines can be made and has been applied to JET pulses in which a density limit is achieved. Additional population due to molecular processes (Verhaegh *et al.,* 2021) will lead to an increase in the presently derived values of opacity.

As an example, in a H-fuelled L-mode density limit pulse, 91294, reabsorption is observed in the Lyman alpha, beta, gamma and delta lines with, respectively, opacities of 2.5, 1.5, 0.3 and 0.04 being reached along the VUV spectrometer's line-of-sight. Emission and absorption coefficients, together with the source functions are illustrated and populations of the ground and first four excited states determined. Differences in the ground state populations calculated using the different spectral lines are understood in terms of the reabsorption occurring at different points along the line-of-sight as well as the omission of population contributions from molecules in the present analysis.

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**See author list of J. Mailloux et al., 2021, Nuclear Fusion Special issue, 28th Fusion Energy Conf. (Nice, France, May, 2021)*

Atomic physics data requirements for low ionization stages of tungsten

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Abstract

A detailed analysis is described of JET VUV spectra in which low ionization stages of W are observed as discrete spectral lines. This extends the study presented by Pawelec *et al*. (2021). The analysis indicates which ionization stages are expected to be observed in a large plasma machine. Observation of discrete lines is valuable both for diagnosing plasma parameters, determining W concentrations and consequently in transport analyses. Spectral line blending is a significant problem in any analysis of VUV spectra and these data will allow an assessment of the spectral lines that are useful for diagnostic purposes given the spectral resolution of the observing spectrometer. Of importance is that the analysis indicates where further line identifications are needed and highlights the transitions for which atomic data are required. As noted by Pawelec *et al*. the highest quality atomic data is desirable and it is expected that the present study will allow effort to be focussed on where it is most useful.

Pawelec E. et al., 2021, Joint IAEA/FZJ Technical meeting on CR properties of W and Hydrogen in edge plasmas.

**See author list of J. Mailloux et al., 2021, Nuclear Fusion Special issue, 28th Fusion Energy Conf. (Nice, France, May, 2021)*

Electron-impact single ionization of tungsten ions

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Tungsten is being considered as a plasma-facing material in magnetically confined fusion devices, such as ITER, because of its low sputtering rate, high temperature characteristics and low tritium absorption. Considerable effort has been made to obtain reliable atomic data to enable identification of reference lines for plasma diagnostics and to reliably estimate radiative cooling rates. A number of publications about electron-impact single ionization (EISI) processes have been published for tungsten. However, reliable EISI data are not available for many tungsten ions. Moreover, the effect of long-lived excited states in low charged ionic stages need to be investigated.

We used the flexible atomic code (FAC) in the distorted-wave approximation method to calculate electron-impact single ionization cross sections for tungsten ions. Contributions from direct ionization (DI) and excitation-autoionization (EA) processes are taken into account. Comparison between the previous experimental measurement results and present calculation show a prominent contribution of metastable states in low charged states such as W^{7+}-W^{8+} ions. We also performed ab initio calculation for other moderate charged ions.

In this report, I will present an overview of our recent progress in EISI for tungsten ions.

Abstract ID : **7**

Accurate atomic data of Helium-like ions with Z = 5 – 9 deduced from the Relativistic Configuration Interaction Theory calculations.

Content

We provide accurate energy levels for the lowest singly excited 70 levels among $1snl(n \leq 6, l \leq (n-1))$ configurations and the lowest doubly excited 250 levels arising from the K-vacancy $2ln'l'(n' \leq 6,\ l' \leq (n'-1))$ configurations of helium-like ions with $Z = 5-9$. Wavelengths, weighted oscillator strengths and transition rates for all E1, E2, M1 and M2 transitions are also calculated. The calculations were performed using the Relativistic Configuration Interaction (RCI) method implemented in the Flexible Atomic Code (FAC). The second set of calculations was obtained with other packages of programs for relativistic atomic structure calculations (AMBiT) based on a method combining many-body perturbation theory and configuration interaction (CI). Comparisons have been made with the compiled data from the NIST ASD and other calculations and a good agreement was found which confirms the reliability of our results.

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Submitted by **MANAI, Soumaya** on **Tuesday 19 October 2021**

Abstract ID : **4**

Progress of collisional-radiative modeling for tungsten EUV spectra

Content

Spectroscopic modelling for tungsten ions is highly demanded to examine tungsten behavior in fusion plasmas as an impurity to cause high radiation power loss. Collisional-radiative models for highly charged tungsten ions have been constructed by several groups, but models in mid- and low-charged tungsten ions are not well studied yet and measured extreme ultraviolet (EUV) and vacuum ultraviolet spectra are not fully explained by models since atomic structure of such tungsten ions are very complex and the atomic data are not easily calculated. We have developed a collisional-radiative (CR) model for tungsten ions to explain EUV spectra measured in plasma with electron temperature ~1 keV – 2 keV, where continuous two-peak broad structure, so-called unresolved transition array (UTA), is seen at 4.5-7 nm wavelength region [1-3]. The UTA is produced by overlapped numerous lines of 4d-4f and 4p-4d transitions of open 4f- and 4d-shell ions, but any current CR models do not reproduce the UTA well [1-5]. We included recombination processes to the CR models for W^{25+} - W^{39+} ions, but still the models were not enough to reproduce the UTA well, since the width of the first peak at 5nm is narrower and the second peak at 6 nm was still weaker than measured spectra. We have tried to extend the CR model to lower charged tungsten ions in order to reproduce the UTA. We will report the contribution of such lower charged tungsten ions to the spectra at 4.5-7nm region in plasma with electron temperature less than 1 keV.

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Submitted by **Prof. MURAKAMI, Izumi** on **Wednesday 06 October 2021**

Abstract ID : **1**

Spectroscopic Observation of WI to WXLVII Tungsten Emission Lines in Visible, VUV and EUV Wavelength Ranges in the Large Helical Device for ITER Edge Plasma Diagnostics

Content

Spectroscopic studies for emissions released from tungsten ions have been conducted in the Large Helical Device (LHD) for contribution to the tungsten transport study in tungsten divertor fusion devices and for expansion of the experimental database of tungsten line emissions [1-3]. Tungsten ions are distributed in the LHD plasma by injecting a pellet consisting of a small piece of tungsten metal wire enclosed by a carbon tube. The electron temperature of the LHD core plasmas with a tungsten pellet injection ranges from 0.5 keV to 3.5 keV, which is close to that of the edge plasmas in ITER around the last closed flux surface, including the scrape-off layer. Thus, observation of tungsten lines in LHD could improve the tungsten diagnostics in ITER edge plasmas. The current status of tungsten emission lines observed in LHD using visible, vacuum ultraviolet (VUV), and extreme ultraviolet (EUV) spectroscopy can be summarized as follows. The line emissions from the neutral atoms, WI, as well as the singly ionized ions, WII, were observed using visible spectroscopy in the wavelength range of 4000–4400 Å [2]. The visible spectroscopy has also observed magnetic dipole (M1) forbidden transition lines from WXXVII and WXXVIII in the wavelength range of 3300–3900 Å [4,5]. The line emissions from tungsten ions in low charge states, WIII–WVII, have been identified in the VUV range of 500–1500 Å [6]. Recently, several M1 lines of WXXX–WXL were successfully observed in the VUV wavelength range of 500–900 Å [7]. Additionally, in the EUV range of 5–500 Å, tungsten ions in low charge states, WV–WVIII, medium charge states, WXXV–WXXXIV in the structures of the unresolved transition array (UTA), as well as high charge states, WXLII–WXLVII, have been identified [8,9]. Measurements of emissions from WIX to WXXIV are still insufficient, which is addressed as a future task.

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Spectroscopic observations of the hydrogen and tungsten hydride molecules in divertor plasma – isotope effect

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Last campaigns in JET concentrated on isotope effects – there were (light) hydrogen, deuterium and tritium campaigns, with many pulses of mixed isotope plasmas, including current campaign in deuterium-tritium mixture. This situation made possible observations of hydrogen molecules with varying isotopic composition – H_2, HD, HT, D_2, T_2 and DT Fulcher band spectra were recorded during those experiments and their lines can be identified in the recorded spectra. Problems with analyses of those spectra are:

- complexity of the Fulcher band spectra in themselves
- fact, that for the isotopic mixtures the recorded spectrum consists of overlapping spectra of two "pure" and one "mixed" molecules, complicating the analysis enormously
- fact, that for some of those molecules, especially DT, there are next to no molecular data in literature.

This contribution presents which of the isotopic versions of hydrogenic molecules and spectra can be identified in the visible-region spectra of divertor plasma and how the available transition data fit the experimental results.

In the regions where plasma is touching the tungsten-covered plasma vessel we expect also observation of the tungsten hydride molecules, created during chemically-assisted physical sputtering. Spectra of those at ~675 nm was reportedly recorded in hydrogen and deuterium plasmas containing tungsten, and spectra in appropriate regions were reported also in deuterium fusion plasmas in TEXTOR, ASDEX and JET. Here we present spectra from this wavelength region recorded in different isotope fusion plasmas – from hydrogen to tritium. For those molecules, diatomic data for WT are absent; and in the case of WH and WD our results do not completely agree with existing sparse diatomic constants, which shows the importance of providing a theoretical input into this problem.

* See the list of authors of E. Joffrin et al, Nucl. Fusion 59 (2019) 112021 and J. Mailloux et al to be published

Abstract ID : **5**

Spectral Analysis of Multiply Charged W6+-W13+ in the EUV and Visible range

Content

Spectroscopy of few times ionized tungsten is a very useful tool to diagnose the ITER divertor plasma. Since the temperature of the diverter region of ITER is expected to be a few hundred eV, a large fraction of the plasmas is expected to contain tungsten ions in charge states mainly from three to fifteen times ionized W^{3+}-W^{15+}. Moreover, line identification of these ions is challenging as these ions have very complex atomic structures with the open $4f$ sub-shell, and competition of orbital energies between $4f$, $5s$, and $5p$ electrons. Therefore, due to a lack of reliable analysis, there is still no data available for W^{8+} to W^{12+} in the Atomic Spectra Database of the NIST [1]. To fill this void multiply charged tungsten ions (W^{6+}-W^{13+}) spectra were recorded in visible and EUV regions using a compact electron beam ion trap (CoBIT) at the University of electro-communications, Tokyo [2,3]. The analysis of the observed spectra is based on the collisional-radiative (CR) modeling with fine structure sub-levels atomic kinetics. The model includes basic kinetic processes such as electron impact excitation (de-excitation) and radiative decay. All the atomic data for energy levels, transition probabilities, and cross-sections are calculated using the wave function obtained within the relativistic configurational interaction (RCI) method [4]. In the present talk, we will present an investigation of previously unidentified lines in the visible and EUV range for W6+ and W13+. Details of the model and analysis will be presented in the meeting.

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Inner-shell ionization in Maxwellian x-ray spectra of Ne-like W

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Unlike low- and mid-Z ions, the most abundant highly-charged high-Z ions are known to be produced at electron temperatures on the order or even higher than their ionization energies (see, e.g., [1]). Therefore the Maxwellian plasmas of modern and future magnetic fusion devices are expected to contain a large fraction of hot electrons that should inevitably affect population kinetics and, in particular, the ensuing x-ray spectra. Such spectra will be an important diagnostic tool for tokamak and stellarator plasmas of the nearest future [2]. We will discuss this effect for the x-ray radiation of Ne-like W which is expected to be the most abundant ion in the ~20-keV core plasma of the ITER tokamak.

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Experimental cross sections for atomic collision processes involving tungsten ions

Stefan SCHIPPERS
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For several years the Giessen Atomic and Molecular Physics group has pursued measurements on cross sections for atomic collision processes of tungsten ions in plasmas [1,2]. In my talk, I will summarize our most recent results on electron-impact ionization [3-7] and photoionization [8,9] and present comparisons with results from theoretical calculations where available.

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Recent results on the reactive collisions of electrons with H_2^+, BeH^+, ArH^+ and some of their isotopologues

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Molecular cations of hydrogen and hydrides are important in the kinetics of the fusion plasma, close to the wall and/or the divertor. Their collisions with electrons result in dissociative recombination, ro-vibrational excitation and dissociative excitation [1]:

$$AB^+(N^+,v^+) + e^- \rightarrow AB^*, AB^{**} \rightarrow A + B,\ AB\,(N^{+\prime},v^{+\prime}) + e^-\ ,\ A + B^+ + e^- \qquad (1)$$

Here N^+/v^+ stand for the rotational/vibrational quantum numbers of the cation, whereas AB^* and AB^{**} for a bound excited (mostly Rydberg) state and for a dissociative (mostly doubly- or multiply-excited) state respectively of the neutral.

We will show our recently-computed cross sections for the collisions of H_2^+, HD^+, D_2^+, ArH^+, ArD^+, BeH^+, BeD^+ and BeT^+ with electrons of energy up to 12 eV, computed with our method based on the Multichannel Quantum Defect Theory (MQDT) [2-4]. The major physical features characterizing the extreme energies – rotational effects at very low energy, infinite series of dissociative channels and vibrational continua at high energy – will be illustrated.

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ATOMIC STRUCTURE CALCULATIONS AND ELECTRON IMPACT EXCITATION OF CHLORINE LIKE TUNGSTEN IONS

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Abstract

Extensive calculations of energy levels and radiative data such as transition wavelengths, transition rates, oscillator strengths and line strengths for electric diploe (E1) transitions are performed for chlorine like Tungsten ions WLVIII using Flexible Atomic code (FAC).These calculations include the major correlation effects. Comparisons are made with the available experimental results and theoretical data in the literature. Close agreement has been found ensuring the accuracy and reliability of our results. We have studied collisional excitation cross section and presented magnetic sublevel cross sections for excitations from ground state $3s^2\ 3p^5\ {}^2P^o_{\ 3/2}$ to the first excited sate $3s^2 3p^4 3d\ {}^4D_{3/2}$ of W^{57+}as a function of incident electron energy. We predict new data for several levels where no other theoretical and/or experimental results are available which will form basis for future experimental work. Our work will help develop diagnostics to measure tungsten concentrations in fusion plasmas and provide support for modeling predictions.

Application of MCCC cross sections in collisional radiative models for molecular hydrogen: current status and outlook

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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. In plasmas used in fusion research the particle temperatures and densities can cover a wide range. Typically, the edge plasma of fusion devices is much cooler than the core plasma, resulting in the presence of atoms and molecules and thus a high complexity of the reaction kinetics. Together with the presence of strong density gradients, processes like Molecular Assisted Recombination or the transition from an ionizing to a recombining plasma regime can play a crucial role. Strong parameter gradients are also present in the negative hydrogen ion sources for neutral beam injection (NBI) at ITER. An ionizing plasma (T_e>10 eV) in the driver region is cooled down by a magnetic filter field to a recombining plasma with T_e≈1 eV close to the extraction system. 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.

In the last years large gaps in the available set of excitation cross sections for molecular hydrogen needed as input for CR models have been filled by a set of electron collision excitation cross sections, recently calculated by using the Molecular Convergent Close-Coupling (MCCC) method at Curtin University, Perth, Australia. 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.

Further planned extensions made possible by the MCCC cross sections are the development of CR models for the isotopomeres of hydrogen, being of high relevance for fusion plasmas. Additionally planned is the development of ro-vibrationally resolved molecular CR models. Such models will be an important tool for determining – e.g. by means of emission spectroscopy – the rotational and vibrational temperature of the molecule which are important parameters for characterizing the plasma properties.

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