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Atomic, Molecular and Plasma-Material Interaction Data Evaluation and Development

Summary Report of the Technical Meeting
IAEA Headquarters, Vienna, Austria
19 – 21 November 2018

Prepared by

C. Hill
Nuclear Data Section, International Atomic Energy Agency
Vienna, Austria

January 2019

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ABSTRACT

A Technical Meeting was held at IAEA Headquarters from 19 – 21 November 2018 to establish a Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP), a consortium of research groups working in the area of fundamental atomic and molecular physics relevant to plasma processes. Its focus is on promoting collaboration and communication between experimentalists and theoreticians to improve the quality and completeness of data used in modelling and interpreting fusion plasmas.

January 2019

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1. Introduction

A Technical Meeting was held in Room C0343 of the Vienna International Centre, Vienna from 19 – 21 November 2018 to establish the Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP), a consortium of research groups working in the area of fundamental atomic and molecular physics relevant to plasma processes. Its focus is on promoting collaboration and communication between experimentalists and theoreticians to improve the quality and completeness of data used in modelling and interpreting fusion plasmas.

18 participants from 11 Member States attended the meeting and presented their research in 20 – 25 minute talks. These presentations were followed by discussion sessions to lay out the scope, purpose and working practices of the Network.

This report outlines the proceedings of the meeting (Section 2), provides details on the GNAMPP project (Section 3 supplemented by Appendix 1), and summarizes the meeting's conclusions (Section 4). Appendices 2, 3, and 4 provide a list of participants' details, the meeting agenda and presentation abstracts respectively.

2. Proceedings

The meeting agenda is provided as Appendix 2 to this document. The first two days were devoted to 20 – 25 minute presentations from the meeting participants, in which they outlined the nature and scope of their research; 5 – 10 minutes at the end of each presentation were devoted to questions from the audience. This part of the meeting was divided into separate, thematically-coherent sessions encompassing experimental methods as well as theoretical techniques and modelling. The presentation abstracts are provided in Appendix 3.

The discussion sessions set out the scope of the GNAMPP network, its purpose, membership, working practices and administration, as described in the following section.

3. GNAMPP

As the number and size of experimental fusion reactors grow, there is an increasing need for accurate fundamental data to be used by the codes that model their properties and behaviour. By necessity, much of these data are calculated using theoretical models and codes, but benchmarking and validating these codes is difficult and costly. Comparison with high-quality experimental results is often patchy and reliant on difficult-to-obtain scientific literature that may be hard to interpret and/or published by researchers who can no longer be contacted.

GNAMPP facilitates the development of better theoretical data by creating a network of researchers in the experimental and theoretical domains whose complementary approaches can validate data sets, identify data needs and collaborate on complex projects towards the provision of data for modelling codes.

Specifically, the goals of GNAMPP were identified to be:

- To provide a forum for the exchange of ideas and data between researchers in plasma physics and communities of theorists and experimentalists.
- To foster collaboration between research groups towards a better understanding of the fundamental physics of plasmas and a quantification of the uncertainties in calculated data.
- To jointly express the importance of atomic and molecular processes to the quantitative understanding of plasmas and their properties.
- To identify priorities and missing experimental or theoretical data; in particular, to focus the community's effort on areas with the greatest impact.
- To outline missing or deficient understanding of many-body collisional processes in plasma.
- To assist and support funding applications.
- To encourage the development of key experimental facilities.

The IAEA is able to support these goals by arranging Consultancy Meetings, Technical Meetings and, within the mechanism of a Coordinated Research Project (CRP), Research Coordination Meetings. It is anticipated that by using the GNAMPP as a forum for interactions between research groups, these meetings will be accessible to a wider community of researchers and will benefit from a broader range of expertise.

Where feasible, and subject to the funding priorities of the IAEA, a biennial Technical Meeting on a topic within the scope of GNAMPP will be organised, to which Network members working in a relevant area may be invited. A newsletter will be produced and distributed (by email and through the website) on a regular basis.

Scope

Research topics that fall within the scope of the network include:

- Tokamak diagnostics
- Fundamental theory in the atomic and molecular physics of plasmas: the modelling of collisional and spectroscopic processes
- Edge-plasma physics
- Neutral beam modelling

- Experimental collisional and spectroscopic physics, particularly research groups with ion beams and EBIT devices
- Heavy ion reactions
- Small molecular species in the divertor region

To maintain the focus of the Network, and to make the project manageable within the resources available, the following topics are among those explicitly excluded from consideration:

- Industrial plasma processing (semiconductor etching, etc.)
- Medical plasmas
- Plasma-material interactions
- Radiation damage to materials
- Modelling of plasma dynamics; tokamak design

Website

The GNAMPP website is https://amdis.iaea.org/GNAMPP/. It is developed and maintained by the Atomic and Molecular Data Unit.

Scientific Advisory Committee

The Scientific Advisory Committee (SAC) of the GNAMPP consortium is:

- José Crespo López-Urrutia (Max-Planck-Institut für Kernphysik, Germany)
- Ursel Fantz (IPP-Garching, Germany)
- Xinwen Ma (Lanzhou Institute of Chemical Physics, China)
- Stefan Schippers (Justus Liebig University, Germany)
- Yaming Zou (Fudan University, China)

Administrative matters and the organisation of biennial meetings are the responsibility of the Atomic and Molecular Data Unit in the Nuclear Data Section of the IAEA.

Joining the network

The application requirements are:

Prospective research groups are invited to submit a short written profile of their expertise, experimental apparatus and current area of interest. They are encouraged to include images where relevant.

Each research group should have a name and a primary point of contact (usually a group leader / principal investigator with an email address and maybe other contact details).

A bibliography of up to 10 recent, relevant, peer-reviewed articles should be provided (*identified by DOI*).

Any existing collaborations with other GNAMPP members should be highlighted

A selection of keywords, chosen from those listed on the GNAMPP website, should be selected to classify the research interests of the prospective member. An initial list of keywords, decided at the November 2018 meeting is given in Appendix 1.

Collaborations

Details of collaborations between network members are provided on the GNAMPP website, at https://amdis.iaea.org/GNAMPP/collaborations/. During the initial meeting described in this report, a collaboration between the research groups of Dmitry Fursa (Curtin University, Australia) and Ursel Fantz (University of Augsburg and ITER Technology and Diagnostics Division (ITED) and the Max Planck Institute for Plasma Physics (IPP), Garching, Germany) to provide higher-quality H_2 collisional cross sections for fusion applications was initiated.

4. Conclusions

The first meeting of the GNAMPP consortium established the Network and set out its purpose, membership, working practices and administration. The interests of its founding research groups were described and discussed, and the scope of future GNAMPP activities laid out.

It is hoped that GNAMPP will facilitate much-needed cooperation and collaboration between experimentalists and theoreticians with the goal of improving the quality of the fundamental atomic and molecular data used in modelling fusion plasma processes.

Appendix 1: Keywords

The following table lists the keywords chosen by participants of the meeting to classify research falling within the scope of the Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP).

ADAS
Ammonia
Argon
Associative Reactions
Astrophysics
Auger Processes
Beryllium
Carbon
CCC
Charge-Exchange Processes
Collisional-Radiative Processes
COLTRIMS
Cross Section Measurements
Crossed Beams
CTMC
Dense Plasma Physics
Density Functional Theory
Deuterium
Dielectronic Recombination
Dissociative Attachment
Dissociative Charge-Transfer
Dissociative Excitation
Dissociative Ionization
Distorted-Wave Approximations
EBIT
ECRIS
Edge Plasma
EELS
Elastic Scattering
Electron – Ion Collisions
Electron – Ion Recombination
Electron – Molecule Collisions
Electron Capture
Electron Impact Dissociation
Electron Impact Excitation
Electron Impact Ionization
Electron Microscopy
Electronic Structure Calculations
Experiment
Heavy Particle Collisions
Helium
Highly Charged Ions
Hydride Molecules
Hydrogen (1H)
Hydrogen Isotopes
Inelastic Scattering
Ion Beams
Ion Impact Processes
Ion Storage Ring
IR Spectroscopy
Iron
Iron Spectroscopy
IXS
Laser-Plasma Interactions
Line Shapes
Lithium
Low Temperature Plasmas
Many-Body Interactions for Dynamics
MCDF
Merged Beams
Molecular Dynamics
Molecular Interactions
Molecular Spectroscopy
Molybdenum
Motional Stark Effect
Neon
Neutral Beams
Nitrogen
Non-LTE Processes
Non-Perturbative Treatments
Optical Spectroscopy
Oxygen
Photoionization
Photon – Ion Interactions
Photon Scattering
Plasma Density Diagnostics
Plasma Diagnostics
Plasma Impurities
Plasma Temperature Diagnostics
Proton-impact ionisation
Quantum Dynamics
R-Matrix calculations
Radiation Transport
Radiative Cooling
Reaction Dynamics
Reactive Scattering
Relativistic Quantum Mechanics
Relativistic Theories
Semi-Classical Approach
Spectral Line Intensities
Spectral Line Positions
Spontaneous Emission
Storage Ring
Synchrotron Radiation
Tandem Accelerator
TDCC
Theory
Trapped Ions
Tritium
Tungsten
Uncertainty Quantification
UPS
VUV/EUV Spectroscopy
Warm Dense Matter
X-Ray Spectroscopy

Appendix 2: List of Participants

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Appendix 3: Agenda

1st Meeting of the Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP)

IAEA Headquarters, Vienna, Austria
19 – 21 November 2018
Meeting room: C0343

Monday, 19 November 2018

09:30 – 10:00	**Christian HILL**, *IAEA* Welcome, introduction of the participants, adoption of the agenda

Session 1: Experimental Methods I

10:00 – 10:30	**José Ramon CRESPO LÓPEZ-URRUTIA**, *Max-Planck-Institut für Kernphysik (MPIK), Germany* Reliable atomic data for fusion research and astrophysics: Benchmarking calculations for highly-charged ions
10:30 – 11:00	**Pedro AMARO**, *Faculty of Science and Technology, Nova University of Lisbon, Portugal* Atomic processes relevant for high-temperature plasmas
11:00 – 11:30	Coffee Break
11:30 – 12:00	**Nobuyuki NAKAMURA**, *Institute for Laser Science (ILS), University of Electro Communications (UEC), Japan* Recent results on tungsten spectra obtained with a compact electron beam ion trap
12:00 – 12:30	**Baoren WEI**, *Fudan University, China* Absolute charge-exchange cross section measurement in heavy ion interaction with atom and molecule
12:30 – 13:00	**Ke YAO**, *Fudan University, China* Studies of tungsten spectroscopy and resonant electron ion recombination at Shanghai-EBIT
13:00 – 14:00	Lunch

Session 2: Experimental Methods II

14:00 – 14:30	**Xavier URBAIN**, *Université Catholique de Louvain, Belgium* Low energy ionization, charge transfer and reactive collisions for ion source and edge plasma chemistry
14:30 – 15:00	**Stefan SCHIPPERS**, *Justus Liebig University (JLU), Giessen, Germany* Single and multiple ionization of ions by electron and photon impact
15:00 – 15:30	**Daniel W. SAVIN**, *Columbia University, United States of America* Ion-neutral reactive scattering studies
15:30 – 16:00	Coffee Break
16:00 – 16:30	**Andreas WOLF**, *Max-Planck-Institut für Kernphysik (MPIK), Germany* Electron-ion collision experiments with merged beams in storage rings: General aspects and research at the cryogenic electrostatic storage ring CSR
16:30 – 17:00	**Dirk WÜNDERLICH**, *Max Planck Institute for Plasma Physics (IPP), Garching, Germany* Atomic and molecular data for collisional radiative modelling relevant to fusion
19:00	Social Dinner: Griechenbeisl, Fleischmarkt 11, 1010 Wien

Tuesday, 20 November 2018

Session 3: Theory and Modelling

09:00 – 09:30	**Raúl BARRACHINA**, *Centro Atómico Bariloche, Argentina* Atomic, molecular and optical research in Argentina
09:30 – 10:00	**Dmitry FURSA**, *Faculty of Science and Engineering, Curtin University, Australia* Electron-impact excitation of molecular hydrogen: dissociation and vibrationally resolved cross sections
10:00 – 10:30	**Grzegorz KARWASZ**, *Nicolaus Copernicus University, Toruń, Poland* Electron (and positron) scattering cross sections needed for low temperature plasmas
10:30 – 11:00	**Martin G. O'MULLANE**, *Department of Physics, University of Strathclyde, United Kingdom* Transformation of fundamental atomic data for use in interpreting diagnostics and plasma modelling
11:00 – 11:30	Coffee Break

Session 4: Experimental Methods III

11:30 – 12:00	**Yang YANG**, *Fudan University, China* High-resolution tungsten spectroscopy relevant to the diagnostic of high-temperature tokamak plasmas and Researches on magnetic field induced transition
12:00 – 12:30	**Xinwen MA**, *Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, China* Experimental potentials for atomic data for fusion research and astrophysics at Lanzhou
12:30 – 14:00	Lunch

Session 5: Experimental Methods III

14:00 – 14:30	**Michael SCHULZ**, *Missouri University of Science and Technology, United States of America* The few-body problem in simple atomic systems
14:30 – 15:00	**Carmen CISNEROS**, *Universidad Nacional Autónoma de México (UNAM), Mexico* Some aspects of atomic, molecular and plasma physics in Mexico
15:00 – 15:30	**Lin Fan ZHU**, *University of Science and Technology (USTC), Hefei, China* Benchmark dynamic parameters of atoms and molecules determined by the fast-electron and inelastic X-ray scattering
15:30 – 16:00	Coffee Break
16:00 – 17:30	Discussion session 1 (all participants)

Wednesday, 21 November 2018

09:00 – 10:30	Discussion session 2 (all participants): Research group profiles and prospects for collaboration
10:30 – 11:00	Coffee Break
11:00 – 12:30	Discussion session 3 (all participants)
12:30 – 13:00	Concluding remarks; any other business; closure of the meeting

Appendix 4: Presentations

Atomic processes relevant for high-temperature plasmas

Pedro AMARO, Universidade Nova de Lisboa, Portugal

In this meeting I will present the projects of the group LIBPhys-UNL that are relevant for high-temperature plasma physics, particularly, of high interest for fusion-plasma research.

We performed high-precision measurements of X-ray transitions in a high-temperature plasma generated by an electron cyclotron resonance ion source (ECRIS). High-precision measurements were performed with a vacuum double flat crystal spectrometer that, due to its geometrical setup, provides accurate (few ppm at few keV) and absolute measurements [1, 2]. I present briefly the spectrometer and latest measurements [3]. This spectrometer provides accurate x-ray standards in narrow transitions of highly charged ions that can be used to energy-calibrate microcalorimeters dedicated for diagnostic x-ray lines in a fusion-generated plasma.

We measured the details of electron collision and recombination cross-sections of highly charged iron and tungsten produced by an electron beam ion trap (EBIT). Typical measurement cycles compressed a wide range of electron beam energies (300 eV to 1150 eV), which probed many atomic processes, including radiative recombination, dielectronic recombination, collisional excitation and resonant electron scattering. I present the latest results of experimental cross-sections for this range electron of beam energy of atomic lines in iron that are of astrophysical interest [4]. Preliminary results and discussion concerning fusion-plasma research are also provided for tungsten, giving special attention to the less-known atomic process of resonant electron scattering.

Of interest in fusion-plasma research, I also present a compact and simple theoretical expression for evaluating ionization cross sections for a wide range of energies and charge states. This expression is based on the binary-encounter Bethe model [5, 6] and requires only incident energy and shell information (binding energy and quantum numbers). Work is in process to provide a user-friendly website with this data accessible for the plasma and atomic scientific community.

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Atomic, molecular and optical research in Argentina

Raúl O. BARRACHINA, Comisión Nacional de Energía Atómica, Argentina

The first laboratory in Argentina dedicated to Atomic, Molecular and Optical (AMO) Physics was created in 1960 by Prof. Wolfgang Meckbach. It is located at the Bariloche Atomic Centre (CAB) and depends on the National Atomic Energy Commission (CNEA). Today, the "Department of Interaction of Radiation with Matter" (DIRM) includes three divisions in AMO Physics, Fusion Research and Surface Science. Among its experimental facilities we should mention a 1.7 MeV Tandem accelerator with PIXE, RBS, ERDA and channelling capabilities, and a chamber for Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS). There are also two electrostatic accelerators of 100 and 300 keV, a time-of-flight system for ISS spectroscopy, a surface analysis equipment for XPS, UPS, AES and SIMS spectroscopy, and STM and atomic force AFM microscopes.

Other AMO institutes in Argentina, as for instance the Institute of Astronomy and Space Physics (IAFE) in Buenos Aires, the Rosario Institute of Physics (IFIR) in Rosario, and the Southern Physics Institute (IFISUR), created in Bahía Blanca in 2008, are mostly devoted to theoretical research.

The AMO community in Argentina study a large range of processes, with different projectiles (ions, electrons, positrons, photons, etc.), targets (atoms, molecules, surfaces, etc.) and outgoing channels (elastic and inelastic collisions, charge exchange, ionization, transfer ionization, etc.), usually at intermediate and large impact energies. From the theoretical point of view, we employ Continuum Distorted Wave models, Classical Trajectory Montecarlo, Sturmian functions, and time-dependent close coupling, among other techniques.

CNEA also counts with a 20 MeV tandem accelerator at the Constituyentes Atomic Centre (CAC), and an Accelerator Mass Spectroscopy (AMS) facility at the Ezeiza Atomic Centre (CAE), both located in Buenos Aires.

Argentina participates in the Management Board for the Development, Application and Validation of Nuclear Data and Codes (MBDAV) of the Nuclear Energy Agency (NEA-OECD), and -in particular- in the Joint Evaluated Fission and Fusion (JEFF) collaboration. Furthermore, through the Radioisotope Metrology Laboratory (LMR) and the Ionizing Radiation Dosimetry Laboratory at the CAE, Argentina is part of the Ionizing Radiation Advisory Committee of the Bureau International des Poids et Mesures (BIPM) and the International Committee for Radionuclide Metrology (ICRM).

At present, CNEA is creating the "Argentinean Network for Nuclear, Atomic, Molecular and Optical Data and Codes", or DINAMO (for to its acronym in Spanish). Its objectives are to provide fundamental data for nuclear and non-nuclear science and technological projects (for example in nuclear medicine, radioisotope production, radioactive waste management, uranium enrichment, and fusion), and to coordinate the generation, collection and critical assessment of data by the different groups in Argentina. In particular, this network is intended to act as a point of contact and liaison with the nuclear data section and the atomic and molecular data unit of IAEA, the data bank of NEA-OECD and BIPM.

Therefore, based on our 50 years of experience in AMO research, we are willing to contribute with the international atomic and molecular data centre network. We can certainly provide numerical and bibliographic data, direct contact for any expertise needed -especially in relation with ion impact atomic processes and surface science- and collaborate with ongoing and future coordinated research projects.

Some aspects of atomic, molecular and plasma physics in Mexico

Carmen CISNEROS, Universidad Nacional Autónoma de México

The field Atomic, Molecular and Plasma Physics (AMP) in Mexico encompasses the study of atoms, molecules, and light, among those are the studies of fundamental and applied aspects as well as from the experimental and theoretical points of view.

There are groups of different institutions dedicated to AMP studies. The main groups are at diverse institutes in the Universidad Nacional Autónoma de México, besides there are also laboratories in other institutions were AMP research is performed. Regarding particular laboratories it is worth to mention Collisions Laboratory, Laboratory of Low Temperature Plasma, Spectroscopies Laboratories: FTIR and Mass, Optical Emission, Raman and Atmospheric Plasma, Molecular Photodynamics Laboratory, Cold Atoms and Quantum Optics Laboratory , Plasma Physics and Radiation Interaction with Matter and Multiphotoionization and Multiphotondissociation of PHA and Organic Molecules, all these laboratories have strong inter collaborations and with groups from all over the world.

Some faculty members have been involved with AMP for fusion, collaborated on Atomic data for fusion. Volume 1: Collisions of H, H_2, He and Li atoms and ions with atoms and molecules (still revered). They also participated in the Coordinated Research Program on Atomic Data for Medium and High - Z Impurities in Fusion Plasmas "resulting in the report Electron Capture Collision Processes involving multiple charged ions: Si, Ni, Ti, Mo, and W ions with H. H_2 and He Targets. Results on hydrogenic negative ion formation have been generated with proposes of plasma heating and electron capture and striping of Tl and K for plasma diagnostics were also obtained. More recently they had collaborated in ground breaking advances on atomic and molecular physics, including studies of ion-photon experiments at the Advanced Light Source in Berkeley.

There are also projects related to Atomic and Molecular Theoretical Physics that go to the theories of the first principles (electronic structure of atoms and molecules, theory of functional density, production and characterization of ultra-cold atomic and molecular gases and their interaction with electromagnetic radiation, Bose-Einstein condensates and degenerated Fermi gases), Group Theory applied to the molecular structure, to very specific applications to particular problems (conversion of hydrocarbons into energy, study of the nucleic bases of DNA). Topics in which very important contributions have been made.

We are open to undertake and collaborate with new projects related with the present Network.

Reliable atomic data for fusion research and astrophysics: Benchmarking calculations for highly charged ions

José R. CRESPO LÓPEZ-URRUTIA,
Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Fusion research relies on spectroscopic diagnostics and modelling of atomic processes in plasmas. Similarly, astrophysics also requires large atomic databases to interpret observations. Due to continuous improvements of diagnostic systems in terms of both resolution and accuracy, the perspective of further developments in this field emphasizes the need for accurate and reliable atomic physics data. This is crucial for highly charged ions (HCI), a huge class of atomic systems of which the sheer size precludes full experimental coverage. Reliance on calculations based on state-of-the-art atomic structure codes such as Flexible Atomic Code (FAC) and other widely used packages implies a necessity for systematic benchmarking of their results against accurate laboratory data. Transition energies and cross sections for excitation, ionization, recombination and charge transfer have to be provided. Their accuracy has to enable discriminating between various theoretical models and finding the most appropriate ones. Establishing solidly founded standard benchmarks is thus essential. This applies to elements used in the wall materials of fusion reactors, those investigated in present and future astrophysics missions, as well as in other technological applications.

In terms of both variety of investigated species and data accuracy, the electron beam ion trap (EBIT) has proven to be the most efficient workhorse for HCI applications. Emission lines ranging from the X-ray to the optical domain for ionic species from lowly charged ions of light elements to the highest charge states of the heaviest elements have been measured and compared to theory. Cross sections and lifetimes have been studied in great detail. However, recent developments in spectroscopic equipment and theoretical methods call for even more accurate and systematic work. At synchrotron radiation sources and free-electron lasers, there is a need for more precise X-ray photon-energy standards. Moreover, several proposals regarding the use of HCI for atomic clocks in the optical and the vacuum-ultraviolet regions have been put forward in the last decade. I will present some of those results, compare them with theory and discuss the need for further research in the fields of experiment and theory, accompanied by the establishment of an expanded data base for accurate benchmarked reference data supported by IAEA.

Electron-impact excitation of molecular hydrogen: dissociation and vibrationally resolved cross sections

Dmitry V. FURSA
Department of Physics and Astronomy, Curtin University, Perth, Australia

Molecular hydrogen and its isotopologues (D_2, HD, etc.) are present in a range of vibrationally excited states in fusion, atmospheric, and interstellar plasmas. Electron-impact excitation cross sections resolved in both final and initial vibrational levels of the target are required for modeling the properties and dynamics, and controlling the conditions of many low-temperature plasmas. Recently, the convergent close-coupling (CCC) method [1] has been utilized to provide a comprehensive set of accurate excitation, ionization, and grand total cross sections for electrons scattering on H_2 in the ground (electronic and vibrational) state [2,3,4], and calculations are being conducted to extend this data set to include cross sections resolved in all initial and final vibrational levels [5]. In this talk I will review the available e-H_2 collision data, discuss the resolution of a significant discrepancy between theory and experiment for excitation of the $b^3\Sigma_u^+$ state [6], and present estimates for dissociation of H_2 [7].

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Electron (and positron) scattering cross sections needed for low temperature plasmas

Grzegorz KARWASZ, Nicolas Copernicus University, Toruń, Poland

High power output in the ITER tokamak requires an efficient cooling. This is done mainly via electron and atomic collisions. As far for carbon-lined tokamaks, the modeling of the edge plasma reproduces well its temperature and density, this is not the case of plasmas containing beryllium and tungsten - atoms and ions, that appear in the plasma via wall-sputtering [1].

The differences between modeling and experimental checks are to be attributed mainly to the poor knowledge of cross sections for atomic targets like metal vapors and their molecules, differently from carbon-containing molecules [2]. Therefore, some extrapolation and semi-empirical analysis of cross sections is to be done in order to derive unknown data [3].

We will compare existing experiments, theories and semi-empirical estimates of cross sections, for total and partial processes, in electron (and positron) scattering on atoms, molecules, radicals and ions. The goal is to guide the choice of data for modeling the edge tokamak plasmas. A by-product of this analysis will be cross sections for the use in modeling industrial (and research) low temperature plasmas.

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Experimental potentials for atomic data for fusion research and astrophysics at Lanzhou

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In this report I will first introduce the experimental facilities for atomic ions/molecular ions colliding with atoms and molecules. The facilities cover accelerator such as high energy storage rings, 320 kV platform for multiple disciplinary research with highly charged ions, very low energy EBIS, and experimental setups for differential data measurements in ion-atom collisions. Second, I will present some typical results obtained at these facilities related to the atomic data for fusion research and astrophysics. Last but not least, I will give a brief description of the near future working plans concerning atomic ion collisions investigations and collective collection of data for fusion research and astrophysics.

Recent results on tungsten spectra obtained with a compact electron beam ion trap

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In this contribution, we present tungsten spectra obtained with a compact electron beam ion trap. Visible and EUV spectra of tungsten ions with charge states 6-27 are presented and compared with collisional radiative model calculations.

Ion-neutral reactive scattering studies

Daniel Wolf SAVIN, Astrophysics Laboratory, Columbia University

The Savin group has long-standing expertise in reactive scattering studies involving neutral atoms and atomic or molecular ions. The measurements are performed using either a single-source or dual-source merged-fast-beams apparatus, enabling us to measure absolute integral cross sections (ICSs) for translational collision energies E_T from ~ 2 meV to ~ 20 eV. In recent years we have measured the reactive scattering ICS for associative detachment of H(D) + $H^-(D^-)$ → $H_2(D_2)$ + e^- [1-4], proton- and H_2^+-transfer from H_3^+ onto C and O [5,6], and isotope exchange of D with H_3^+, H_2D^+, and D_2H^+ [7,8]. Our studies are motivated by astrophysical questions, but the techniques and some of the reactions are also relevant for fusion studies. In my presentation, I will discuss some of our recent work, illustrating our experimental capabilities, and highlight some of the shortcomings in state-of-the-art reactive scattering theory.

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Single and multiple ionization of ions by electron and photon impact

Stefan SCHIPPERS, Justus-Liebig-University, Giessen, Germany

The Giessen Atomic and Molecular Physics group (http://www.uni-giessen.de/amp) has long-standing expertise in electron-ion and photon-ion collisions employing crossed-beam and merged-beams experimental methods. In recent years, we have measured *absolute* cross sections for electron impact single and multiple ionization of fusion relevant ions such as tungsten [1,2] and xenon [3] ions, and have developed a new high-current electron gun [4] facilitating electron-ion crossed beams experiments at electron energies of up to 3.5 keV (previously, the electron energy had been limited to 1 keV). In addition, we carry out experiments on photoionization of ions [5,6], which, although no being directly relevant to fusion plasmas, nevertheless provide important benchmarks for the further development of the theoretical methods. In particular, we have performed joint experimental and theoretical studies of valence shell ionization of tungsten ions as well as and of inner-shell ionization of, e.g., negatively charged oxygen ions [8] and singly charged iron ions [9]. In my talk, I will present selected examples from our recent work, which illustrate our capabilities to challenge state-of-the-art atomic collision theory in various aspects.

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The few-body problem in simple atomic systems

Michael SHULZ, Missouri University of Science and Technology, USA

In controlled fusion research reliable transition rates for various processes occurring in ion-atom collisions, like ionization and capture, are needed. To obtain such data is tedious and costly and the results are often afflicted with large experimental uncertainties. Furthermore, it is not always straight forward to account for e.g. the thermal energy distribution of the ions, plasma density effects etc. in a collision experiment. Therefore, the development of accurate theoretical models is essential. The major challenge such efforts are facing is presented by the few-body problem (FBP). The essence of the FBP is that the Schrödinger equation is not analytically solvable for more than two mutually interacting particles even if the underlying forces are precisely known. Thus, theory has to rely on heavy numeric modelling. The assumptions entering in these models have to be tested by detailed experimental data. In this talk, kinematically complete experiments on ionization and capture processes, which offer the most sensitive tests of theory, will be discussed.

Low energy ionization, charge transfer and reactive collisions for ion source and edge plasma chemistry

Xavier URBAIN
Université Catholique de Louvain

A review of our recent measurements in merged- and crossed-beam geometry will be given. We shall discuss the adverse role of mutual neutralization in volume negative hydrogen production on the basis of our latest kinetic energy release measurements. The interest of low- to medium energy collisions for the interpretation of molecule-assisted recombination will be stressed, together with the problematics of plasma detachment by nitrogen and deuterium puffing. Quantitative metastable helium production, as demonstrated in a recent electron-impact ionization experiment, should allow us to measure cross sections at play in pure or mixed helium plasmas. Helium dimer and helium hydride ions may also enter the composition of edge plasmas, and preliminary results on electron-impact dissociation of the dimer will be presented.

Absolute charge-exchange cross section measurement in heavy ion interaction with atom and molecule

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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 quantities for checking many-body theories. 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 experimental measurements, cross sections for highly charge ions interacting with atoms/molecules are still limited. In the near future, we plan systematic studies of the interactions between ions and atoms/molecules based on the highly charged ion collision platforms in Lanzhou and Shanghai. By measuring single and multiple electron capture absolute cross sections, we aim to determine electron capture cross sections as a function of impact energy. Using a reaction microscope, the three dimension momenta of the projectile ions, the recoil ions and the free electrons can be measured in multi-coincidence for the interaction of ions with atoms/molecules. Then both the transfer ionization cross sections and state-selective differential cross sections can be deduced. The systematic results expected from this project can help theorist to check the validity of their many-body theories and also can provide high accuracy atomic data for plasma physics.

The project will be performed in an international collaboration. They are:
Long WEI, Yu ZHANG, Roger HUTTON, Yaming ZOU, and Baoren WEI from Fudan University, Shanghai.
Yong GAO, Shuncheng YAN, Shaofeng ZHANG, Xiaolong ZHU, and Xinwen MA from Institute of Modern Physics, Lanzhou.
Junwen GAO, Yong WU, and Jianguo WANG from Institute of Applied Physics and Computational Mathematics, Beijing.
Hongqiang ZHANG and Ximeng CHEN from Lanzhou University, Lanzhou.
Michael R FOGLE from Auburn University.

Electron-ion collision experiments with merged beams in storage rings: General aspects and research at the cryogenic electrostatic storage ring CSR

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The role of experiments in strengthening application-oriented knowledge on atomic and molecular collision processes is twofold: (a) to directly determine rate constants and (b) to verify the theoretical assumptions and methods required to predict rate constants from many-body quantum calculations. In both cases, it is important that measurements define as precisely as possible the projectile and the target regarding chemical composition, charge state, internal structure and internal excitation state. Moreover, studies with angular resolution or in external fields can be important for additional benchmarking of the theory and for enabling predictions in anisotropic environments.

For studies of this type, beam experiments with well-defined collision energy and geometry, as well as with stored and state-controlled targets are particularly powerful.

In our laboratory we apply the technique of merged electron and ions beams using a collinear electron-ion interaction zone in an ion storage ring. The cryogenic electrostatic storage ring CSR was designed and taken into operation for this purpose recently. Long storage times in extreme vacuum allow the relaxation of internal excitation for many atomic and molecular ions, as well as measurements with good control of the internal excitation during the relaxation process. Through electrostatic ion storage and by suitable ion sources, electron collisions can be also studied for complex atomic ions and heavy di- and polyatomic molecular ions.

Measurements of low-energy recombination between electrons and small molecular ions under rotational-level control were performed recently at the CSR. The study of atomic ions with complex configurations (singly and multiply charged systems) is soon to start. The planned projects will involve collaboration with other laboratories. First electron collision results with the Heidelberg CSR will be presented. Regarding recombination studies for complex atomic ions, the status of scientific understanding as well as the perspectives for measurements at the existing ion storage ring facilities will be discussed.

Atomic and Molecular data for collisional radiative modelling relevant to fusion

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Population models, predicting population densities of excited atomic or molecular states in dependence of the plasma parameters, are typically used for plasma diagnostics. One specific type of population models that can be applied over a wide range of plasma parameters are Collisional Radiative (CR) models. In CR models, exciting and de-exciting reactions for excited states in the atom or molecule are balanced. As a result, a huge number of input parameters (reaction probabilities) are needed; this number increases even more in the case of molecules where vibrational or rotational sublevels are present.

The plasma parameters of plasmas used in fusion research can cover a wide range. For example, the transition from the attached to the detached mode of the divertor plasma in tokamaks results in a strong reduction of the electron temperature (from ≈ 50 eV to below 1 eV) which implies the transition from an ionizing to a recombining plasma. The situation is similar in the negative hydrogen ion sources for neutral beam injection (NBI) at ITER. An ionizing plasma ($T_e > 10$ eV) in the driver region is cooled down by a magnetic filter field to a recombining plasma with ≈1 eV close to the extraction system.

Consequently, the reaction probabilities included in CR models for these plasmas need to cover an energy range starting from close to the excitation threshold up to energies of more than 100 eV. Additionally, the transition from an ionizing to a recombining plasma can drastically shift the relevance of different excitation channels. Both, fusion machines itself and ion sources for NBI can be operated in different hydrogen isotopes. Different other particle species like He, Ar or N_2, Cs may be present in the plasmas, either as diagnostic gas or for modifying the properties of the plasma or the surfaces. It may additionally be necessary to include into the models processes including photons; for example in the case of a high ground state density self-absorption caused by optical thickness is significant.

CR models based on the flexible solver Yacora are available for several atomic and molecular species used in plasmas for fusion. The presentation discusses the available atomic and molecular data used as input in these CR models. While the general situation for light atoms is good, for molecules large gaps exist in the data basis of excitation cross sections. Even for the hydrogen molecule, the simplest existing molecule, no complete data set of cross sections exists that includes vibrational sublevels, excited state-excited state reactions and the isotope effect. The present available data set for the H_2 molecule is presented, including corrections and extensions performed in the last years. For the first time, cross sections calculated at Curtin University, Perth, Australia, using the Convergent Close- Coupling (CCC) method have been implemented into the Yacora CR model for H_2. The high relevance of the isotope effect will be highlighted. Additionally, a new service is introduced: Yacora on the Web is a web application, providing online access to the Yacora CR models for atomic and molecular hydrogen as well as for the helium atom.

Concluding, the presentation presents modelling activities with the focus on the low-temperature region of plasmas for fusion. Different CR models are available based on different sets of input data. The used input data is benchmarked at different plasma experiments.

High-resolution tungsten spectroscopy relevant to the diagnostic of high-temperature tokamak plasmas and Researches on magnetic field induced transition

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The X-ray transitions in Cu- and Ni-like tungsten ions in the 5.19–5.26Å wavelength range that are relevant as a high-temperature tokamak diagnostic, in particular for JET in the ITER-like wall configuration, have been studied. Tungsten spectra were measured at the upgraded Shanghai- Electron Beam Ion Trap operated with electron-beam energies from 3.16 to 4.55 keV. High-resolution measurements were performed by means of a flat Si 111 crystal spectrometer equipped by a CCD camera. The experimental wavelengths were determined with an accuracy of 0.3–0.4 mÅ. All measured wavelengths were compared with those measured from JET ITER-like wall plasmas and with other experiments and various theoretical predictions. It was found that such an extension brings the calculations closer to the experimental values in comparison with other calculations.
Magnetic field induced transition was studied systematically, especially with Ne-like and Cl-like isoelectronic ions. And an accidental degeneracy of quantum states in Fe^{9+} was found which induced a novel method to determine magnetic fields in low density plasma.

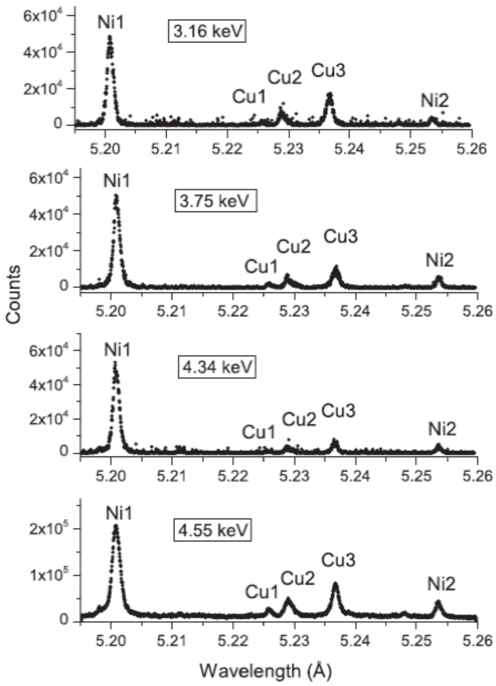

Figure 1. X-ray spectra of Cu- and Ni-like tungsten ions measured on the upgraded Shanghai EBIT for electron-beam energies of 3.16, 3.76, 4.34, and 4.55 keV.

Studies of tungsten spectroscopy and resonant electron ion recombination at Shanghai-EBIT

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Tungsten will be used as the divertor material of the future TOKAMAKS, for the reason of its high melting point, low sputtering, corrosion resistance, and low hydrogen retention characteristics. As a heavy impurity element, it is ionized but not fully stripped in the fusion plasma. Its radiation will lead to a huge amount of energy lose, while its spectra is a useful diagnostic tool for key plasma parameters.

In the past few years, Shanghai-EBIT [1] dedicated to study the atomic process for application of fusion research. In our EBIT, tungsten spectroscopies from visible to EUV region were observed for the charge states of W^{7+}- W^{28+} [2-6]. Many of these lines were identified for the first time.

Dielectronic recombination (DR) plays an important role in the high temperature plasma. It significantly affects the plasma temperature, the charge state distribution, and the ion level population. The *K*-shell excitation DR of He-like to O-like tungsten [7-9] was carefully studied at the EBIT. The cross sections were measured at an accuracy level of about 10%. In *L*-shell excitation DR process, metastable states were observed [10]. The processes were also studied for a few other elements, e.g., argon, xenon [11, 12]

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Benchmark dynamic parameters of atoms and molecules determined by the fast-electron and inelastic X-ray scattering

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Electron energy loss spectroscopy (EELS) and inelastic X-ray scattering (IXS) have been developed as powerful tools to investigate the dynamic parameters of atoms and molecules, e.g., optical and generalized oscillator strengths, squared form factors, Compton profiles and etc. The intrinsic relationship between these two experimental techniques makes them suitable to determine and crosscheck the same dynamic parameters, which provides an opportunity to exclude the possible experimental systematic errors and obtain the experimental benchmarks. Herein we present some recent results of N_2, CO_2 as well as H_2 and its isotopic substitutes measured by the EELS and IXS. The crosschecked results constitute a series of benchmark data for use in astrophysics, fusion science, atmospheric physics and plasma physics. Furthermore, vibronic effect in CO_2 and isotope effect in H_2, HD and D_2 have also been elucidated.

Relevant ongoing activities:
[1] Benchmark dynamic parameters, including the differential cross sections, optical and generalized oscillator strengths, integral cross sections, of the valence-shell excitations of atoms and molecules measured by the fast electron and inelastic x-ray scattering techniques
[2] Dielectronic recombination rate coefficients of Ni ions studied by the merged beam based on CSRm in Lanzhou

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