20th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria
25-26 April 2016

Report prepared by
Bastiaan J. Braams

September 2016
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Printed by the IAEA in Austria
September 2016
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IAEA Nuclear Data Section

Abstract
The 20th meeting of the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) was held on 25–26 April 2016 at IAEA Headquarters in Vienna, Austria. Activities of the Atomic and Molecular Data Unit for the period 2014–2016 were reviewed and recommendations were made for continuing activities in 2016–2017 and for possible new projects in the 2018–2019 budget cycle. The proceedings, conclusions and recommendations of the Subcommittee meeting are briefly described in this report.

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1. Introduction

The Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) meets biennially to advise on the work of the Atomic and Molecular Data Unit within the Nuclear Data Section. The meeting time in the Spring of the even years has been chosen to match the budget and policy preparations of the Agency; meeting and budget plans for the next year are developed over the summer and preliminary CRP proposals for the next biennium (which starts in an even year) are reviewed near the end of the previous even year. Therefore, in addition to providing advice about priorities in work on atomic, molecular and plasma-material interaction (A+M+PMI) data for fusion the subcommittee is asked for specific recommendations about the programme of major meetings and coordinated research activities of the Unit in the next biennium.

The proceedings of the meeting are summarized in Section 2 and the discussions and recommendations are summarized in Section 3. Appendix 1 provides an overview of the mission and general activities of the Unit and a detailed overview of activities in 2014–2015 is provided in Appendix 2. The list of participants is in Appendix 3 and the meeting agenda is given in Appendix 4.

2. Meeting Proceedings

Opening

The meeting was opened by the Head of the Nuclear Data Section, Arjan Konig, who welcomed the participants and introduced the work of the Section, noting the overlap of interest between nuclear and atomic and molecular data activities in the area of uncertainties, particularly the study of uncertainty propagation through Monte Carlo techniques.

The participants introduced themselves and various administrative matters were covered.

B. J. Braams: General report on Unit activities

Unit Head Bas Braams presented an overview of Unit activities and actions in the context of advice given by the IFRC subcommittee at their 19th meeting, 28–29 April 2014. The following topics are covered.

- Coordinated Research Projects
- Large “decennial” meeting; other meetings and workshops
- ALADDIN and other numerical datasets
- Data evaluation activities
- Development of XSAMS and of GENIE search engine
- AMBDAS bibliographical database
- Knowledge Base
- Data and Code Centre Networks
- Publications

The overview is presented in the format:

Advice from the IFRC Subcommittee meeting of 28–29 April 2014.

Actions by the Atomic and Molecular Data Unit in the period to April 2016.

The overview is followed by some remarks on staffing and about an award.

For Coordinated Research Projects in the area of plasma-material interaction highest priority goes to a CRP on erosion and tritium retention for steel surfaces, with emphasis on the kinds of low- or reduced-activation steels that may be used in a reactor.

A CM was organized in August 2014 to advise about the need and scope of possible CRP. Key recommendations:
Erosion and tritium retention are both important and erosion is much more complicated for steel
than for elementary metals due to differential sputtering.

The CRP has to arrange that different groups carry out experiments using the same target
materials, including pre-damaged targets.

Most of the work on PMI with steel is experimental; relevant modelling will need to be
couraged.

A proposal for the CRP was approved and the first meeting was held in December 2015 with seven
participating projects.

**In the area of atomic and molecular data it is recommended to initiate a new CRP on data for charge
exchange processes related to neutral beams. The main topic of interest will be beam interaction with
core plasma but processes relevant to generation of the beam may also be included.**

A CM was organized 17-18 March 2016 to advise about the need and scope of this CRP. The relevance
was affirmed, and we obtained good advice on the scope.

- Focus on core plasma processes, not on beam generation.
- Do not limit it to charge transfer processes but include data for electron collisions; state-to-state
  transitions. (This is important for beam attenuation.)
- Concentrate on beams of H/D/T, with only peripheral interest in He, Li, other.
- Include sensitivity studies of beam penetration, beam emission and charge transfer impurity
  spectra to uncertainties in atomic data.

The proposal for a CRP on “Data for Atomic Processes of Neutral Beams in Fusion Plasma” has been
submitted and we expect a positive review. (The proposal was approved by CCRA at their meeting on
2016-05-18.) Participants are to be assembled between May and August. The first meeting of the new
CRP is planned for December 2016. (Due to the staff transition this has since been moved to 2017.)

**Data for plasma interaction with liquid metals gallium and tin, certain salts and possibly also
aluminium, are needed in order to assess uses of these materials in a reactor environment. For a CRP
this topic has lower priority than one on steel surfaces, but it is recommended as a good topic for a
Technical Meeting.**

We have assembled information about this topic, including conference contributions and research
groups. A survey has been prepared by A. Botrugno (see Appendix 5). The field has its own biennial
meeting series (ISLA), but those meetings are dominated by technology and plasma physics aspects;
there is not much on fundamental data.

We did not organize our own meeting on the topic, but it remains in our mind. We would find it attractive
to combine a liquid metal event with broader interests in vapour shielding, also for solid targets, as will
be discussed later during this meeting.

**The Unit should organize again, in 2014 or early 2015, a large “decennial” meeting on atomic,
molecular and plasma-material interaction data for fusion science and technology to bring together
fusion scientist users of A+M+PMI data and atomic, molecular and materials scientists data
producers.**

The Decennial IAEA Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data
for Fusion Science and Technology was held in Daejeon, Korea, 15-19 December 2014. The meeting
was hosted by the Korean Government with generous support from the National Fusion Research
Institute (NFRI).

The meeting had 60+ participants, 40+ from outside Korea, and a good mix of fusion scientists and
atomic, molecular and PMI data researchers. Discussions were held on atomic and molecular data,
plasma-material interaction data, and database and resource issues. The meeting was much appreciated.

**The Unit has the mission to provide internationally recommended and evaluated data for atomic,
molecular and plasma-material interaction process and related materials structure properties for
fusion science and technology; this is the principal aim of the ALADDIN database. [...]**
We continue to add data to ALADDIN that were developed in connection with our CRPs. Data evaluation is an ongoing concern. We have organized several concrete data evaluations (electron collisions with Be and with W) and have contributed to others (eMOL activities on N₂ and N₂⁺; the NFRI activity on CH₄), always as a group project with a co-objective to build up a data evaluation network.

We have a separate presentation to review these concrete evaluations and also the effort to develop guidelines for uncertainty estimates for calculated data.

[...] The attention given in the past two years to data evaluation and uncertainty assessment for atomic and molecular data is appropriate and it is a topic for continued attention. This includes activities such as code comparison workshops and a technical meeting on uncertainties in calculated data.

We have continued those activities. We were involved in code comparison workshops for spectral lineshapes in plasmas (SLSP3) and for non-local thermodynamic equilibrium kinetics (NLTE9). The “Joint IAEA-ITAMP Technical Meeting on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data” was our major event on the fundamentals of uncertainty assessment. The topic of uncertainty assessment pervades our other work, including the Data Centres Network and the Code Centres Network activities.

The subcommittee is pleased with the continued success of XSAMS through the Virtual Atomic and Molecular Data Centre (VAMDC). For the Unit it is most important to see ALADDIN and other fusion A+M databases integrated into the VAMDC framework.

As a result of work carried out in consultancies with Dr Christian Hill (University College London) a subset of ALADDIN is accessible through the VAMDC interface. The ALADDIN2 subset contains gas-phase collisional differential and integrated cross sections and rate coefficients.

We have not tried to integrate our PMI data into VAMDC.

Astrophysics and astrochemistry remains the core community for VAMDC.

There is still an important role for bibliographical database AMBDAS and the subcommittee hopes that the provision of collisional and plasma-material interaction data in AMBDAS can be renewed in collaboration with DCN colleagues and others.

We have made progress on this through collaboration with DCN colleagues and others. For electron-atom and electron-molecule collisions AMBDAS was brought up-to-date through work by Dr Mi-Young Song of NFRI and a consultancy by Dr Wonwook Lee of KAERI. For PMI data we benefited from an internship by Ms Kyung-Mi Lim (recent graduate of SNU) in 2014. For heavy particle collision data we have an ongoing effort with Dr M. Imai of Kyoto.

It is an ongoing effort to maintain these collaborations and the work. Only for bibliographical data on spectroscopy is there a stable source; the NIST Atomic Spectroscopy Group.

The wiki-style Knowledge Base was initially meant to evolve as a community activity, but in practice all content has come from the Unit. The subcommittee is comfortable with that; the wiki pages are also valuable as one part of the Unit’s regular web presence.

The knowledge base continues to be a low-key effort for us, but they are the most visited pages under www.amdis.iaea.org.

We actively maintain a calendar of meetings as a part of the Wiki, and we intend to build up a collection of pages for relevant experimental programmes in A+M collision physics.

Our wiki effort (among other work) may benefit from the presence of a long-term (1-2 years) consultant, Dr Tapasi Das, from July 2016.

In conclusion the subcommittee emphasizes the continued high value to ITER and to the broader fusion programme of internationally evaluated and recommended data for atomic, molecular and plasma-material interaction processes and related materials structure properties for fusion. [..]

We are grateful for that emphasis.
There are two threads in our effort on provision of evaluated and recommended data. On the one hand we have our activities on methods (guidelines) for the provision of uncertainties for calculated atomic and molecular data, especially collision data. Our meeting at ITAMP in 2014 and follow-up activities (including a journal article now under review) are the high points of that effort to-date. On the other hand we have pursued concrete evaluations as a small group activities; data evaluations for electron collisions with N$_2$ and N$_2^+$; electron collisions with Be and its ions and most recently electron collisions with W and its ions.

We expect to continue in both directions. We also think of support for uncertainty assessment for simulations of PMI. (This is an active field in the USA already.)

"... The provision of such data is a designated task for the IAEA A+M Data Unit, while the evaluated and recommended data library must be the joint effort of an international network of data centres and researchers. In this regard the Unit’s ongoing efforts to strengthen community ties between researchers from basic atomic, molecular and materials science and researchers from fusion energy science are very important.

We appreciate those words too. Hyun Chung and I started here in 2009 (I arrived at the end of August, Hyun one month later) and it took some time for us to recognize how much we need to work on community building for the atomic and molecular data work. (PMI work is better integrated with fusion energy research.)

On the outreach front the biggest struggle is to retain access to relevant experimental A+M collision physics. We have access to good efforts in computational A+M physics and in that community we continue to emphasize the interest in methods and tools for uncertainty assessment.

In our CRP and meeting programmes we always try to bring together fusion energy scientists and A+M+PMI scientists.

Remarks on staffing

The Agency has a rotation policy by which the normal maximum length of appointment is 7 years and it has a retirement policy with retirement age 62 for staff that arrived before 2014; for newer staff it is age 65. For the Unit Head Bas Braams, the contract ends at the end of November 2016 when both policies apply, so there will not be an extension. For the atomic physicist Hyun Chung, the contract ends at the end of September 2017 after a one-year extension to an 8th year. A further extension would be highly unusual. Therefore, we expect to have two new staff by the time of the next IFRC Subcommittee meeting in 2018.

The advertisement for the Unit Head position should appear within a few weeks. (It appeared on 2016-05-26.) This is an honest opening; we do not have a designated candidate (and it would not be allowed). Seeking: A respected and well-connected research scientist from fusion energy science, plasma physics, atomic and molecular physics or plasma-material interaction; and really from more than one of the above. The advertisement for the Atomic Physicist position should appear before the end of 2016.

Consultant (P0) position: Starting 01 July 2016 we have a Consultant, Dr (Ms) Tapasi Das, on an appointment for one year (with the possibility to extend to two years max). Dr Das obtained a Ph.D. in 2014 from IIT Roorkee with R. Srivastava and is currently in the Atomic Spectroscopy Group at NIST as a guest researcher.

John Dawson Award 2015 to Hyun Chung

Citation. 2015 John Dawson Award for Excellence in Plasma Physics Research: “For creative and novel use of the hard x-ray free electron laser to isochorically create high density plasmas and accurately measure the ionization potential depression, and for new theory that addresses discrepancies with long standing models and provides stimulus for continued developments.”

H.-K. Chung: Review of Data Centre Network and Code Centre Network activities

Atomic Physicist Hyun-Kyung Chung reviewed the activities of these two networks, which hold biennial meetings to review data needs and priorities in the fields of fundamental data for fusion plasma-
relevant processes and in computational techniques and codes for their calculation. The meeting reports and further details are available online at https://www-amdis.iaea.org/DCN/Presentations/2015/ and https://www-amdis.iaea.org/CCN/Meetings4/.

B. J. Braams: Review of Coordinated Research Projects; contribution from G. Mazzitelli on liquid metals and vapour shielding; discussion

Coordinated Research Projects (CRP) are the main mechanism that is used by the Unit for data development. Over the years the Unit has initiated about one new CRP every year or a bit less frequently than that. Here is the timeline of recent CRPs.

- 2010-2015: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV.
- 2011-2016: Data for Hydrogen and Helium and Their Isotopes in Fusion Plasma.
- 2015-2020: Plasma-wall Interaction with Reduced-activation Steel Surfaces.
- 2016-2021: Data for Atomic Processes of Neutral Beams in Fusion Plasma.
- For consideration: Data for Plasma Interaction With Liquid Metal Surfaces.
- For consideration: Atomic Models and Data for Vapour Shielding in Fusion.

See https://www-amdis.iaea.org/CRP/

The presentation started with an overview of the existing CRPs. Please see the Unit’s web pages for more information about these and see Appendix 2 for a very brief description. At the Subcommittee meeting the discussion was focussed on the newest CRP about neutral beams and on the possible future CRP or CRPs about liquid metal surfaces and about vapour shielding.

https://www-amdis.iaea.org/CRP/NeutralBeams/

Objective: Provide evaluated and recommended data for the principal atomic processes of heating and diagnostic neutral beams in fusion plasma.

- Data for beam penetration, BES, MSE and CXRS/CHERS spectroscopy.
- Excitation and ionization in collisions between electrons and H/D/T neutrals.
- Excitation, ionization and charge transfer in collisions between hydrogen neutrals and fuel and selected impurity ions.
- (Lower priority:) collision processes in the hydrogen beam neutralizer; atomic processes of neutral beams of helium and lithium in fusion plasma.

Electron energy from 100 eV to 100 keV, neutral energy from 1 keV to 1 MeV.

Schedule: An advisory CM was held 17-18 March 2016. The detailed proposal for the new CRP has been submitted to the Committee on Coordinated Research Activities. Participants are to be identified and approved May-August 2016 and the first RCM is planned for December 2016. (Note after the meeting: The CRP has been approved, but we have allowed the schedule to slip to let the project start in 2017.)

In conjunction with the Neutral Beams CRP two code and method comparison activities are under discussion with potential co-organizers and participants.

We are thinking about a code comparison workshop for beam penetration and beam-based photoemissions.
https://www-amdis.iaea.org/meetings/CCW2017NeutralBeamEmissions/

For such a workshop the organizers would specify a set of simple uniform plasma conditions and beam parameters. Contributors perform their best calculations before the workshop, put their results into a
standard format, and at the meeting the results are compared in fine detail and one tries to understand the sources of all significant differences.

We are also thinking about a code comparison workshop for electronic transitions in atomic collision processes.

https://www-amdis.iaea.org/meetings/CCW2017AtomicCollisions/

The principal test cases for such an event are collision of H with a highly charged ion in an approximation of straight line motion at a fixed relative velocity and even a fixed impact parameter; one wants to compare results for state resolved charge transfer, ionization, and change of state of the H neutral.

Under consideration: CRP on Data for Plasma Interaction with Liquid Metal Surfaces

At the IFRC Subcommittee meetings in 2012 and 2014 a CRP on liquid metal surfaces had been discussed and had been found to be of possible interest, but in the area of plasma-material interaction priority was given to the topics of plasma interaction with beryllium, tungsten and steels. However, liquid metal surfaces remain of interest in the fusion programme. The topics for such a CRP would be impurity production (erosion), hydrogen retention and migration, and material ablation, evaporation and vapour shielding under intense pulsed power loads. Relevant materials include lithium, tin, gallium, perhaps aluminum, perhaps also some salts. Present experiments mainly involve liquid lithium; reactor considerations may favour Ga and Sn.

The discussion about a possible CRP or other activity on plasma interaction with liquid metal surfaces was supported by a survey produced by Dr Antonio Botrugno (Consultant in the Physics Section) of related plasma experiments and facilities. This document is reproduced as Appendix 5.

Further discussion was introduced by Dr Giuseppe Mazzitelli. He reviewed the interest in liquid metals lithium, gallium, tin, lithium-tin alloy and (mainly as a surrogate) aluminum. Good atomic data are available for Li for erosion, retention and charge transfer, but for Ga and Sn all the atomic and plasma-material interaction data need to be reviewed. Many present experiments are concerned with technological issues of creating the flowing liquid and Dr Mazzitelli provided an overview. The presentation then moved on to atomic physics relevant to ablation, but in the low density regime where the rate coefficients for ionization and recombination only depend on temperature. It was emphasized that ablation involves atomic physics beyond the coronal approximation and also involving radiation transport. For the work of the A+M Data Unit there is a close connection between work on data for liquid metal surfaces and data for vapour shielding. The discussion then moved to a possible activity on vapour shielding.

Under consideration: CRP on Atomic Models and Data for Vapour Shielding in Fusion Devices

Vapour shielding is of interest for pulsed heat loads (disruptions, large ELMs) on plasma-facing materials and also the process of pellet ablation. The process involves conversion of energy from energetic electrons into photons and partial reflected of the energy back into the plasma. For easily ablating materials such as Li the process sets in at relatively low heat loads; there is even a notion of continuous vapour shielding in a box enclosure. The atomic data needed for simulation of vapour shielding are those associated with radiation hydrodynamics in warm and hot dense matter: non-LTE kinetics, line shapes, opacities.

For an activity by the Unit on vapour shielding the relevant materials would be any first wall and divertor plasma-facing materials; maybe also hydrogen pellets end maybe “killer” impurity pellets. There are many studies already for Li and W, fewer for Sn and Al. There is possible interest in Be, C, Fe wall material, in H for pellet ablation, and maybe in Ne or other for impurity pellet injection.

Discussion about future CRPs

The Subcommittee quickly agreed that the proposed CRPs on liquid metals and on vapour shielding should be discussed together as one coordinated project.
The Unit needs to ask what is the added value that it can bring to work that is already done in the area of liquid metals and vapour shielding. This was discussed and it is agreed that (as with other activities of the Unit) a key objective is to bring together people from the plasma physics and the atomic physics communities. Present studies of vapour shielding in the fusion energy community are focussed on the plasma physics aspects (for example, physics of the electrostatic sheath under vapour shielding conditions) and our CRP would emphasize the atomic physics that is important for radiation transport.

It is pointed out that there are similar data needs for lithography and the Unit may keep that in mind; there can be useful data or other contributions from that community.

In the discussion it was also emphasized that vapour shielding must be taken into account for spectroscopic diagnostics. In the proposed CRP we should make sure to include data that are important for correct interpretation of spectroscopy when there is vapour shielding.

The discussion led to a recommendation to the Unit to pursue a CRP on atomic data for vapour shielding with emphasis on plasma-wall interaction with likely wall materials including relevant liquid metals. Therefore, the two proposed CRPs that the Unit might start in the 2018-2019 biennium are combined into one and for liquid metals the interest is specifically in the physics of ablation, not in the hydrogen retention issues or in impurity production under routine steady heat loads. The CRP should bring together people from the field of radiative properties of warm and hot dense plasmas with people from fusion energy research.

Discussion was started about possible topics for another CRP to start in the 2018-2019 biennium. With present CRPs on beryllium, tungsten, steels and now liquid metals (as a part of vapour shielding) the Unit has the plasma-material interaction bases covered. In the area of atomic and molecular physics there would be interest in a CRP or other activity on spectroscopic measurements of erosion or, somewhat broader, edge plasma spectroscopy. The Subcommittee returned to this topic on the second day. (See below.)

B. J. Braa ms: Other activities (Workshops, meeting cooperation, other meetings, committee service, publications)

2014 Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices, ICTP, Trieste, Italy, 3-7 November 2014

This conference (or workshop) brought together researchers from the areas of fusion energy science and materials science in order to review advances in computational studies of plasma-material interaction processes and the evolution of material microstructure in fusion devices. The programme emphasized work that is relevant to hydrogen (tritium) trapping and transport in candidate fusion reactor wall materials, including effects of radiation damage. Participants came from fusion energy science and materials science. The conference had 35 oral presentations, 16 poster presentations, 3 formal discussion sessions and good time for free discussion. Output includes a special section of Journal of Nuclear Materials (Vol 467, 2015) and as follow-up there is the International Workshop on Models and Data for Plasma-Material Interaction (MoD-PMI 2015), Marseille, France, 25-27 May 2015 and MoD-PMI 2016 to be held in Loughborough, UK, 22-24 June 2016.

Web page: https://www-amdis.iaea.org/Workshops/ICTP2014/


This was a two-week event. The Advanced School in the first week brought together experts in experimental and theoretical plasma spectroscopy to train early-career plasma scientists in the most recent developments and results in the field. The Workshop in the second week provided opportunities for participants to present their work, discuss current needs in plasma diagnostics, and motivate further developments. Participants were plasma physicists, plasma spectroscopists, and other users of atomic data for fusion, astrophysics and laser and plasma applications. The school was designed for advanced PhD students or post-docs while the workshop attracted more senior scientists in the field. The combined event had 26 lecturers and invited speakers plus 3 directors and 35 participants by application. The
school included an introduction to 4 codes: GRASP2K, LANL Atomic codes, CRETIN and FLYCHK. There are plenty of schools on plasma physics, but this school on plasma spectroscopy is special and it was much appreciated. Follow-up includes a proposal (meanwhile approved) to hold a similar school on atomic processes in plasmas at ICTP in 2017.

Web page: https://www-amdis.iaea.org/Workshops/ICTP2015/

2016 Joint ICTP-CAS-IAEA School and Workshop on Plasma-Material Interaction in Fusion Devices, Hefei, China, 18-22 July 2016, hosted by CAS IPP and ISSP

This one-week advanced school, hosted by the CAS Institutes of Plasma Physics (ASIPP) and of Solid State Physics (ISSP), will be devoted to computational methods and their application for the study of plasma-material interaction processes in fusion devices and of related material properties.

Web page: https://www-amdis.iaea.org/Workshops/ICTP2016Hefei/

General remark on our ICTP events: We always try to attract a highly qualified mix of participants from developing and developed countries. It requires extensive advertising through our own channels.

Cooperation: Radiative Properties of Hot Dense Matter, Vienna, Austria, 29 Sep – 03 Oct 2014

This was the 16th meeting in a biennial series for which the topics include dense plasma spectroscopy, radiation heating, spectral line shapes, opacities, non-equilibrium atomic kinetics, breakdown of the isolated atom picture, and detailed x-ray spectra simulation; also experiments using high-intensity short-pulse lasers, Z-pinch type discharges, VUV-FEL and XFEL experiments, and warm dense matter studies. The conference venue was next to Schönbrun palace. There were 105 scientific participants. Hyun Chung served as local organizer and served on the programme committee.

Web page: https://www-amdis.iaea.org/meetings/RPHDM2014/

Cooperation: The 3rd Spectral Line Shapes in Plasmas (SLSP) code comparison workshop, Marseille, France, 2-6 March 2015

The SLSP workshop series was created by E. Stambulchik (WIS, Israel) with a major role for Hyun Chung as the local person for SLSP1 and SLSP2 in Vienna (2012 and 2013). The main organizer of SLSP3 was Annette Calisti of Aix-Marseille University (AMU).


This was an immediate outgrowth of our ICTP conference (workshop) in 2014 on models and data for plasma-material interaction. The main organizer was Yves Ferro of AMU; Bas had an active role on the scientific committee.

Web page: https://mod-pmi.sciencesconf.org/

Other service; programme committees

Linac Coherent Light Source (LCLS). Hyun served on the Proposal Review Panel for the LCLS facility at the Stanford Linear Accelerator Center, 2012-2015, where she reviewed proposals to use the XFEL to study matter at extreme conditions.

ICAMDATA 2014, Jena, Germany. Bas served on the programme committee.

Workshop on Sensitivity, Error and Uncertainty Quantification for Atomic, Plasma, and Material Data, Stony Brook University, NY, USA, 7-9 November 2015. This meeting was organized to bring together people from mathematics, fusion and materials science. Bas served on the programme committee; Hyun was invited speaker. We provided a lot of inspiration for this meeting through our events at ITAMP and ICTP in 2014.

NLTE9 code comparison workshop 2015, Paris, France. Hyun served on the programme committee.
Atomic Processes in Plasmas (APiP) 2016, Paris, France. Bas served on the programme committee; Hyun was a lecturer, invited speaker and she led a FLYCHK code session.

ICAMDATA 2016, Gunsan, Korea. Bas is on the programme committee.

Radiative Processes of Hot Dense Matter (RPHDM) 2016, Santa Barbara, USA. Hyun is on the programme committee.

Atoms journal. Hyun is on the editorial board.

Atomic Data and Nuclear Data Tables journal. Hyun is on the editorial board.

**Our meetings in 2014–2016**

See the list in Appendix 2.

**Highlights of Decennial Meeting (Dec 2014)**

The meeting was hosted by National Fusion Research Institute, Daejeon, Republic of Korea, in the context of “Practical Arrangements” for cooperation between IAEA and NFRI in the area of the evaluation of atomic molecular and plasma material interaction data relevant to fusion. The objective of the meeting was to review the current status of activities in atomic, molecular and plasma-material data for fusion applications, identify priorities for data-oriented work and recommend future activities for the IAEA. Discussion topics were:

- Atomic and Molecular Data Review
  - Atomic data status and requirements
  - List of relevant metastable levels
  - Molecular data status and requirements
- Plasma-Material Interaction Modelling and Data
  - Erosion and deposition
  - Hydrogen retention and transport
- Databases, Policy issues
  - Database issues
  - Resources

The meeting had more than 60 participants from 16 Member States and two from the ITER organization.

**Meetings Attended and other Duty Travel (2014–2016)**

See the list in Appendix 2.

**Publications**

IAEA-INDC (NDS) Reports

- Reports are published for every meeting

International Bulletin on Atomic and Molecular Data for Fusion

  - Volume 70 in press

- Atomic and Plasma-Material Interaction data for Fusion (APID Series)
- Data and papers related to results produced by CRPs and Consultants groups
- All volumes are available on-line
- Edition in preparation

Volume 17: CRP on “Atomic Data for Heavy Element Impurities in Fusion Reactors

- CRP publications elsewhere—will be published in APID volumes

CRP on “Light Element A & M and Radical Behaviour in the Divertor and Edge Plasma Regions”

CRP on “Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV”
• Special issues
• Spectral Line Shapes in Plasmas, Atoms (March 2014)
• Journal of Nuclear Materials, Volume 467 (November 2015) - 12 articles

Considerations about future other activities

The Unit is dedicated to data that are relevant for fusion energy development, but we could be involved in an occasional other activity that matches the goals of the Nuclear Data Section or of the Division of Physical and Chemical Sciences.

One item that we have in mind is a possible outreach to the broader electron-molecule collision community. We find that many of the groups that were once devoted to electron-molecule collision processes in a plasma environment are now primarily doing research for biologically inspired molecules and are studying, for example, damage by low-energy electrons.

We have worked with our nuclear data colleagues on Auger emission for medical applications (CM in May 2013).

We have talked with colleagues about a possible event on the interface between atomic and nuclear data, thinking of the role of atomic and molecular spectroscopy in measurements of nuclear parameters (magnetic dipole moment, electric quadrupole moment), the effect of atomic structure on certain nuclear excitation and decay rates, and the Auger emission that may follow a nuclear capture or decay process. We might cooperate in a satellite of ICPEAC 2017 on these topics. T. Kibédi (ANU) would be the lead person.

Review and discussion. Data needs, recommendations and priorities for Unit activities. All.

The Subcommitte returned to the topic of future CRPs or other data development activities and at first the discussion narrowed down to topics in plasma spectroscopy, both for edge and core plasma.

One topic is atomic data for spectroscopic measurements of erosion. Basically, this means comprehensive data for atomic processes of the lowest charge states of the eroding material, but if the material can erode as molecules then one needs data for the molecular break-up in addition to the atomic data. Instead of focussing the CRP (or other activity) on spectroscopic measurements of erosion one can consider edge plasma spectroscopy more broadly. For spectroscopic measurements of erosion the impurities are in an ionizing regime and one cares for a more limited class of processes than for edge plasma spectroscopy in general.

For the broader topic of edge plasma spectroscopy tungsten is once again singled out as the species for which new work remains most wanted; there is still a big need for spectroscopic data for the lowest charge states of tungsten. Fusion experimentalists should be asked to advise about their data and data needs, both for discrete lines and for quasicontinuum emissions.

For tungsten in both edge and core plasma conditions it looks appropriate to have another evaluation of data and data needs in the 2017-2018 timeframe. Core plasma spectroscopy is often confounded by “nuisance lines”: unidentified lines that confuse the CXRS or CHERS diagnostics. On JET these lines are generally attributed to tungsten, but they are not properly identified. For the edge plasma the problem is that there are so many lines of low charge states of tungsten, the spectra are very difficult to analyze. One needs a good CR model and not just the line identifications, and one needs a treatment of the quasicontinua.

The conclusion of this discussion about spectroscopy is that the community needs a continued effort on spectroscopic and CR data for tungsten, with special interest in the lowest charge states but also with interest in the many unidentified core plasma lines and continuum emissions.
Some other topics besides spectroscopy were discussed with a view towards future Unit activities including Consultancies, Technical Meetings or even a CRP.

For the neutral gas divertor scenarios data are needed for molecular collisions $\text{H}_2 + \text{H}_2$, isotopically and vibrationally resolved. (In the recent CRP on processes of hydrogen and helium these neutral-neutral collisions were not considered.) As a start it must be inventorized what data are available in other communities, for example in the field of rarefied gas dynamics.

More data are needed for elastic and other collisions of the $\text{H}^-$ anion for negative ion beam generation and beam neutralization. The ITER negative ion-based neutral beam will rely on collisional detachment, but photodetachment is of high interest too. Data for photodetachment of negative ions for neutral beams should be inventorized and evaluated. These topics (collision processes of $\text{H}^-$ and photodetachment) could also be covered together in an activity devoted to data needs for negative ion-based neutral beams.

The discussion then turned to topics in plasma-material interaction (other than the spectroscopic measurements of erosion). Recent and present CRPs are concerned with beryllium, tungsten, steels and the ablation process for liquid metals, and there is no particular interest to initiate a similar activity for carbon-based materials or any other possible wall material. The subcommittee does not recommend any particular CRP in the area of plasma-material interaction other than the one on the atomic physics of vapour shielding. However, there is interest in some smaller activities.

A plasma-material interaction topic that looks attractive for the A+M Data Unit is that of code comparison and experiment comparison of temperature programmed desorption spectroscopy (TPS/TDS). The Unit is already planning an experimental comparison in conjunction with the CRP on irradiated tungsten and this may be followed by a similar comparison activity for steels. The subcommittee appreciated these activities and it would be good to follow up with a comparison of simulations of the TDS process.

The closing topic for discussion was that of data formats and data exchange. There is increased emphasis in the ITER and ITPA activities on integrated modelling, in the USA since a long time and increasingly so in Europe. The subcommittee recommends that the Unit should look more closely at the data formats selected for the Integrated Modelling & Analysis Suite (IMAS) by the ITER Integrated Modelling Expert Group. We recall the Atoms, Molecules, Nuclei and Solids (AMNS) interface, which is a set of code protocols or language bindings rather than a storage format; the AMNS standards are being developed in connection with ITER integrated modelling. The Unit’s activities on data exchange need to take account of AMNS and of the IMAS standards.

3. Recommendations and Conclusions

- The Unit is encouraged to continue to pursue the satisfaction of the data needs of Member States through the Data Centres Network, interaction with ITER and national experimental fusion energy laboratories and publicising its activities at international conferences and the scientific literature.
- Consideration should be given to the initiation of two new CRPs, on the vapour shielding phenomenon in fusion devices (high priority) and the prospects and data for novel liquid metal wall concepts for plasma-facing components in such devices (lower priority).
- A CRP on spectroscopic measurements of erosion (focussing on the fundamental data needs relating to the “S/XB” (inverse efficiency) topic); a Technical Meeting or Consultancy might also be considered.
- There are large gaps in the available data for modelling tungsten ions (particularly in relation to dielectronic recombination) in its “middle-to-low” charge states ($Z < +20$); this could be the topic of a data evaluation meeting or Technical Meeting, with the participation of modellers working in the edge plasma region of magnetic confinement fusion energy devices.
- Further data needs were identified in the areas of:
  - elastic collisions among $\text{H}_2$ molecules (isotopically and vibrationally resolved)
  - elastic and other collisions for $\text{H}^-$ for negative ion-based neutral beam (NB) generation
o data for photodetachment relevant to negative-ion based neutral beams (present NB designs rely on collisional neutralization)
o edge plasma spectroscopy, with a special tie to erosion measurements for studying plasma-material interaction.

- A follow-up activity relating to the Irradiated Tungsten CRP (F43021) could focus on experimental data comparison for time-programmed or thermal desorption spectroscopy (TDS), possibly including a code comparison workshop to compare and validate the computational models used in this area.
Appendix 1: Mission and General Activities of the Atomic and Molecular Data Unit

Version of April 2016

The mission of the Atomic and Molecular Data Unit (AMDU) is to support the development of fusion energy by providing internationally evaluated and recommended data for atomic, molecular and plasma-material interaction (A+M+PMI) processes and for related materials properties.

The work on atomic data is primarily concerned with spectroscopy and electron-atom (ion) collisions. We emphasize the elements that are important as an impurity in fusion plasma.

The work on molecular data is concerned with electron-molecule and ion-molecule collisions. The work is focussed on the molecules and molecular ions that determine the condition of the edge and divertor plasma.

The work on plasma-material interaction data is focussed on erosion and tritium retention in the wall materials used or foreseen for fusion: beryllium, carbon, tungsten and steels.

The work on materials properties data (very limited to-date) is concerned with surface and materials microstructure in relation to erosion and tritium retention.

Nature of our work

There are three formal components to our work: data development, data evaluation and database maintenance (data dissemination). These activities are carried out in cooperation with an international network of data centres and researchers. Data development is primarily carried out through our CRPs. We support data evaluation through technical meetings. Database management is done by us with support from our data centres network.

There is an informal component to our work that is perhaps the most important. All our activities have the effect and the aim to build a community across disciplines of researchers working towards fusion energy. The data and databases are the interface between atomic, molecular and materials scientists as producers and fusion scientists as users. Our CRPs and meetings bring together researchers from basic atomic, molecular and materials science with researchers from fusion energy science.

Our most important asset is the reputation of the Agency. We cannot pay for research, but we are able to offer highly valued recognition to A+M+PMI data producers that their work is important for fusion energy.

Relevance

The Agency’s support for fusion energy development is a part of its work to assist Member States in planning for and using nuclear science and technology for purposes including the generation of electricity.

Atomic data are primarily relevant for spectroscopic diagnostics of the core plasma and for simulations of the global energy balance of fusion plasma.

Molecular data are critical for simulations of the divertor and edge plasma and in thereby for the assessment of the feasibility of cold divertor plasma solutions to the power exhaust problem.

Plasma-material interaction data, including data for sputtering, trapping and reflection, are critical for the assessment of first wall and divertor erosion and lifetime and for loss of tritium fuel into the wall.

Materials structure data are required by us inasmuch as the materials structure influences erosion and tritium retention properties.
The international fusion energy programme is at present dominated by construction of ITER. However, parties are also planning for the next step fusion nuclear science facility (FNST) or demonstration reactor (DEMO) and for a power plant. The most important physics issue for next-step devices is power exhaust; more specifically this means the physics of the divertor plasma and of plasma-material interaction. Our data work is strongly tied to the needs of ITER, FNST, DEMO and the fusion power plant.

Areas of emphasis

In our work and meetings we give special emphasis to uncertainty assessment and data evaluation of atomic and molecular data. We encourage specific carefully documented evaluations. We have found that new work is needed on methods for uncertainty assessment of calculated cross section data for atomic and molecular processes and we encourage such work through our meetings.

We continue to emphasize development of new data for plasma-material interaction processes and the related materials structure properties. For these data we find it not yet possible to insist on careful uncertainty assessments.

We coordinate the development of standards for data exchange in the form of the XML Schema for Atoms, Molecules and Solids (XSAMS).

We maintain the ALADDIN numerical database, AMBDAS bibliographical database, GENIE database search engine and a wiki-style Knowledge base.

Recent and planned CRPs

**Light elements:** Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions (2009-2014).

**Tungsten in plasma:** Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV (2010-2015).

**Hydrogen and helium:** Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma (2011-2016).


**Irradiated tungsten:** Plasma-wall interaction for irradiated tungsten and tungsten alloys in fusion devices (2013-2018).

**Steel surfaces:** Plasma-wall interaction with reduced-activation steel surfaces in fusion devices (2015-2020).

**Neutral beams:** Data for Atomic Processes of Neutral Beams in Fusion Plasma (planned for 2016-2021).

The Light Elements and H/He CRPs address A+M data for divertor plasma modelling and the beryllium, irradiated tungsten, and steel surfaces CRPs address PMI data including erosion and tritium retention for these critical materials. The CRP on tungsten in plasma is concerned with data for the most dangerous core plasma impurity and the CRP on neutral beams is concerned with atomic data for heating and diagnostic neutral beams.

Selected recent meetings

The International Fusion Research Council (IFRC) subcommittee on atomic and molecular data for fusion meets every two years to review and advise about the work of the A+M Data Unit. They are especially concerned with current and future CRPs of the unit.

The International Atomic and Molecular Data Centre Network (DCN), meets every two years to review progress in the collection, evaluation and dissemination of A+M+PMI data and to discuss priorities for new work on data development.
The new A+M Code Centre Network meets approximately every two years to review issues related to codes that are shared between the A+M+PMI and the fusion communities. Meetings have a focus topic and involve a subset of the network. In 2013 the meeting focussed on uncertainty assessment of calculated scattering data and in 2015 it focussed on uncertainties in plasma-material interaction data.

The Joint IAEA-NFRI Technical Meeting on Data Evaluation for Atomic, Molecular and Plasma-Material Interaction Processes in Fusion took place 4-7 Sep 2012 in Daejeon, Korea with approximately 30 participants from 11 countries. Topics included error propagation and sensitivity analysis, current status of evaluated databases, evaluation of theoretical and experimental data sets, evaluation methods and the role of semi-empirical fits. The meeting has an important role in rejuvenating the international work on data evaluation for A+M processes in fusion.

The unit has cooperated in several code comparison workshops: the 7th Non-Local Thermodynamic Equilibrium (NLTE) Code Comparison Workshop, the First Spectral Line Shapes in Plasmas (SLSP) code comparison workshop, and the Second SLSP code comparison workshop, all held off-site in Vienna and the Third SLPS code comparison workshop in 2015 in Nice.

In July 2014 the Unit worked with the Institute for Theoretical Atomic, Molecular and Optical Physics (ITAMP) to hold the Joint IAEA-ITAMP Technical Meeting on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data at the Harvard-Smithsonian Center for Astrophysics in Cambridge, MA. The primary goals are to come up with reasonable uncertainty estimates and related computational procedures for calculations using the various methods of collision physics: perturbative, nonperturbative, time-independent, time-dependent, semi-classical, etc..

The Unit cooperated in the 16th International Workshop on Radiative Properties of Hot Dense Matter (RPHDM), in Vienna 29 September – 3 October 2014 with Hyun Chung as as local organizer. This biennial meeting brings together leading researchers in radiative transfer, line shapes, dense plasma spectroscopy, non-LTE population kinetics, opacity studies and plasma processes, to identify current problems in these fields and directions for future research.

The Unit has organized relatively advanced events at ICTP in Trieste. In November 2014 we organized the 1-week Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices, focussed on computational studies of plasma-material interaction processes and evolution of material microstructure in fusion devices, including effects of radiation damage and with special interest in hydrogen (tritium) trapping and transport in wall material. In March 2015 we organized the 2-week Joint ICTP-IAEA Advanced School and Workshop on Modern Methods in Plasma Spectroscopy, bringing together experts and young researchers in experimental and theoretical plasma spectroscopy for fusion, astrophysical and industrial plasma and warm and hot dense matter. In July 2016 we will have the 1-week Joint ICTP-CAS-IAEA School and Workshop on Plasma-Material Interaction in Fusion Devices, hosted by the Chinese Academy of Sciences Institutes of Plasma Physics (IPP) and of Solid State Physics (ISSP).

In December 2014 the Unit organized the Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology, hosted by the Korean Government through the National Fusion Research Institute (NFRI) in Daejeon, Korea. This approximately decennial meeting brought together fusion plasma modellers and diagnosticians and atomic, molecular and materials scientists to review production and uses of A+M+PMI data for fusion.
Appendix 2: Activities of the Unit, 2014–2015

(Much of the following was also presented in report INDC(NDS)-07xx, “Report of the IAEA Nuclear Data Section to the International Nuclear Data Committee for the period January 2014 – December 2015”, April 2016.)

Overview

The mission of the Atomic and Molecular Data Unit (AMDU) is to establish and maintain internationally recommended databases on atomic, molecular and plasma-material interaction (A+M+PMI) processes and related materials structure data for use in fusion energy research and other plasma science and technology applications. These databases and other information are accessible through the Unit’s web pages at http://www.amdis.iaea.org/. (AMDIS stands for Atomic and Molecular Data Information System.)

The Unit maintains a numerical database (ALADDIN) and other numerical datasets, a bibliographical database (AMBDAS), a search engine (GENIE) to find and access numerical data hosted elsewhere, and a Wiki-style Knowledge Base on A+M+PMI data for fusion. Coordinated Research Projects (CRPs) are organized to encourage worldwide collaboration in the production and validation of new data. Technical Meetings and Consultants’ Meetings are held to support the activities of the Unit and coordinate database activities throughout Member States. Among the recurring meetings of that kind are the coordination meetings of the International Atomic and Molecular Data Centres Network (DCN), those of the Code Centres Network (CCN) and meetings devoted to quality assessment of A+M and PMI data. In cooperation with ICTP the Unit regularly organizes a workshop addressed primarily to young researchers in an area such as plasma modelling with use of A+M+PMI data, plasma spectroscopy, plasma-material interaction, or atomic processes in plasmas. The Unit also cooperates in more advanced code and data-oriented workshops.

The AMDU is advised by the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC). Priorities for data evaluation are also assessed by the DCN. The IFRC Subcommittee on Atomic and Molecular Data and the DCN each meet biennially, in alternate years.

Numeric databases

ALADDIN is the principal numeric database maintained by the unit. The interface is split into two broad categories of data: atomic and molecular collisions, which include photon impact processes, electron impact processes and heavy particle collisions, and particle-surface interaction, which includes reflection, penetration, physical sputtering, chemical sputtering and radiation-enhanced sublimation. Data in ALADDIN come largely from coordinated research projects, consultancies and other activities of the AMDU and are recommended data at the time of their compilation.

In 2015, an entire collection of heavy particle collision data sets compiled by Japan Atomic Energy Agency (JAEA) and Kyoto University published in the periods from 1980 to 2008 was uploaded to ALADDIN.

Several further numerical datasets that do not fit well into the ALADDIN framework are accessible through the AMDU home page. This includes a comprehensive collection of rate coefficients calculated by the FLYCHK code for processes of direct collisional ionization, excitation autoionization, radiative recombination, dielectronic recombination and radiative cooling for each atomic and ionic system up to Z=79 (Au).

A comprehensive collection of calculated data based on the Flexible Atomic Code (FAC) [Can. J. Phys. 86: 675-689 (2008)] is available for energy levels, radiative transition rates, collisional excitation cross sections, radiative recombination and photoionization cross sections, autoionization rates and collisional ionization cross sections for atoms and ions from Z=2 (He) to Z=14 (Si). A data set of the fine-structure levels of the ground and excited configurations, oscillator strengths and electron-impact excitation cross-sections, photo-ionization and electron-impact ionization cross-sections provided by Los Alamos National Laboratory (LANL) is also available for Ar, Cl and Si ions.
Bibliographic database

AMBDAS, the Atomic and Molecular Bibliographic Data System, contains about 50,000 entries going back to 1950s of articles and reports on atomic, molecular and particle-material or plasma-surface interaction data relevant to fusion energy research. The broad categories in AMBDAS are structure and spectra, atomic and molecular collisions and surface interactions. Entries are classified by process and reactants and classified as experimental or theoretical. Relevant energy values or energy ranges are also provided.

During 2014-2015 the structure and spectra part of AMBDAS was updated with bibliographical data obtained from the NIST Atomic Spectroscopy Group. The electron collisions part was updated due to compilations by DCN collaborators from KAERI and National Fusion Research Institute (NFRI, Korea).

Knowledge Base Wiki

The Unit uses Wikimedia technology to maintain a Knowledge Base on data sources, data production, data needs, applications of data and related information about atomic, molecular and plasma-material interaction data in fusion energy research and related fields. These wiki pages are among the most visited area of the AMDU website. The information on the wiki is addressed to fusion plasma researchers and atomic, molecular and materials physicists in a way that complements our traditional databases with the aim to encourage collaboration and initiate relevant new research. We had hoped that the maintenance of these pages would become a community effort, but in practice all the editing is done within the Unit and the development has been rather low key in 2014-2015. A new list of researchers and research group in A+M/PMI collision experiments and theory is being compiled.

Coordinated Research Projects (CRP)

The final report of the CRP on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions was produced in 2014 and appeared in the IOP Journal of Physics: Conference Series in January 2015. This CRP was concerned with data on processes including excitation, ionization, recombination and heavy particle collisions for ions of hydrogen, helium, lithium, beryllium, boron, carbon, nitrogen and oxygen and molecules of these atoms.

The CRP on Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV had its 3rd and final RCM in October 2014. Tungsten is the wall material in the regions of high heat and particle flux in JET and in ITER. As an impurity in the plasma, tungsten radiates very strongly, because it does not get fully stripped of electrons. The main objective of this CRP was to provide atomic data to support transport modelling and the interpretation of spectroscopic measurements of tungsten in all regions of the plasma from the wall to the core. The final report of this CRP appeared in 2015 as a special issue “Atomic Data for Tungsten” of the Atoms journal (published by MDPI). As a follow-up to the CRP a consultancy meeting on Recommended Data for Atomic Processes of Tungsten Ions was held in September 2015.

The CRP on Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and their Isotopes in Fusion Plasma is continuing but did not meet in 2014–2015. It has its 3rd and final meeting in March 2016. This CRP is devoted to the development of data for collisional, photon-induced and radiative processes for species H, H+, H-, He, He+, He2+, He-, H2, H2+, H3+, HeH+, He2+ and their isotopic variants. The principal focus is on data that are resolved with respect to the vibrational (in the case of molecules) excited state of the incoming and outgoing particles. In addition, the data should be complete and consistent for hydrogen isotopes H, D and T.

The CRP on Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials had its second meeting in August 2014. Beryllium is used on the JET tokamak and is planned to be used on ITER. Because of its toxicity the experimental database on beryllium is sparse. Key processes studied in this CRP are physical and chemical sputtering by H, He and Be, trapping and reflection of hydrogen (H, D, T) on beryllium surfaces in the plasma environment, the transport of hydrogen in beryllium and means to extract trapped tritium. In addition the CRP is concerned with data for mixed materials, especially Be-(H,D,T,He), Be-C, Be-N, Be-O and ternary and higher mixtures, and data for the principal plasma impurities as projectiles.
The CRP on Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices had its second RCM in September 2015. The critical issue for this CRP is tritium retention and how it is influenced by radiation damage. Pure crystalline tungsten has an extremely low affinity for tritium, but this good property is impacted the wrong way by the neutron fluency in DEMO or in a fusion reactor. Investigations into properties of irradiated fusion materials are hampered by the unavailability of an adequate neutron source and by the great difficulty of relevant first principles computations. Therefore the material properties, the resistance to sputtering and ablation, and the behaviour of trapped tritium in tungsten-based materials after neutron irradiation are still poorly known.

The new CRP on Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices had its first RCM in December 2015. This CRP has the objective to enhance the knowledge base and develop new databases on interaction of fusion plasma with reduced activation steel alloys that are considered for fusion. The CRP will seek to quantify the erosion due to exposure to plasma and to quantify the retention and transport properties of tritium in the surface.

**Data and Code Centre Network meetings**

The International Atomic and Molecular Data Centre Network (DCN) meets every two years to discuss data needs and coordinate activities. At the DCN meeting in Vienna in November 2015 activities of 8 data centres in the network were presented and in addition there were presentations from guests of 4 data projects oriented towards astrophysical and industrial plasma applications. Discussions were held and recommendations developed on current activities in data development and data exchange, data evaluation, data exchange formats, maintenance of bibliographical databases and on priorities for data development and evaluation, new meetings and information exchange. The shared goal is provision of a comprehensive curated, evaluated and recommended database for A+M+PMI processes relevant in fusion devices.

The Code Centre Network (CCN) had its fourth meeting in July 2015 at the IAEA in Vienna. The CCN has a different focal topic at different meetings and this time the meeting was concerned with uncertainty assessment of data for plasma-material interaction, including uncertainties associated with interatomic potentials, density-functional theory (DFT) simulations, molecular dynamics (MD) simulations, kinetic Monte Carlo (KMC) simulations and rate equation simulations for hydrogen retention and migration in fusion materials.

**Other AMDU meetings**

The Unit organized the IAEA decennial Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology, hosted by NFRI in Daejeon. There were 68 participants (44 from outside Korea) including the organizers and the meeting had 36 talks and 12 posters. NFRI made all local arrangements and also supported the participation by 9 invited speakers plus air travel by one of the organizers. This is one of the fruits of the Practical Arrangements on “Cooperation in the area of the evaluation of atomic, molecular and plasma-material interaction data relevant to fusion” that were established between IAEA and NFRI in early 2013 with a duration of 3 years.

Several meetings were held on topics connected to data evaluation and uncertainty estimates. The most important of these was the “Joint IAEA-ITAMP Technical Meeting on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data” held in July 2014 at the Institute of Theoretical Atomic, Molecular and Optical Physics (ITAMP), Harvard-Smithsonian Center for Astrophysics, in Cambridge, Massachusetts, USA. This meeting brought together a total of 26 people working on electron collisions with atoms, ions, and molecules, heavy-particle collisions, and electronic structure of atoms and molecules to discuss ways to obtain reasonable uncertainty estimates for calculations using the various methods of collision physics. There was also a consultancy meeting on “Guidelines for Uncertainty Quantification of theoretical atomic and molecular data” (June 2015), one on evaluation of data for electron collisions with Be and other light elements, and one (already mentioned) on data for processes of tungsten ions in plasma.
The Unit organized 2 events in cooperation with ICTP and held at ICTP in Trieste. The one-week Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices in November 2014 brought together researchers from fusion energy science and materials science in order to review advances in computational studies of plasma-material interaction processes and evolution of material microstructure in fusion devices, including effects of radiation damage and with special interest in hydrogen (tritium) trapping and transport in wall material. The two-week Joint ICTP-IAEA Advanced School and Workshop on Modern Methods in Plasma Spectroscopy in March 2015 was designed to provide training and information exchange for plasma physicists, plasma spectroscopists, and other users of atomic data for fusion, astrophysics and laser and plasma applications. Both ICTP events were aggressively advertised by us and attracted a highly qualified mix of participants from developing and developed countries.

**Other AMDU activities**

The Unit cooperated in the organization of the 16th International Workshop on Radiative Properties of Hot Dense Matter (RPHDM 2014) that was held 29 September through 3 October in Vienna. Hyun Chung served on the Organizing Committee and as local contact. There were 105 scientific participants and the meeting was very successful.

The Unit cooperated in the Third Spectral Lineshapes in Plasmas (SLSP) code comparison workshop that was held in Marseille, France, 2-6 March 2015. Line shapes are used in plasma diagnostics, hence our interest. This workshop followed the model of the well-established Non-local Thermodynamic Equilibrium code comparison workshops in which we have cooperated earlier. Test cases are specified about 6 months in advance, participants prepare their calculations and at the workshop the results are compared in detail with the objective of understanding differences among codes. The Unit also cooperated in the International Workshop on Models and Data for Plasma-Material Interaction (MoD-PMI) in Marseille in May 2015; a meeting that developed out of our ICTP conference 6 months earlier.

Special issue publications: In addition to the final reports of 2 CRPs the Unit helped to produce a special issue “Spectral Line Shapes in Plasmas” in the Atoms journal (MDPI) based on the first and second SLSP code comparison workshops and a special issue “Critical Assessment of Theoretical Calculations of Atomic Structure and Transition Probabilities” also in the Atoms journal was published after the 3rd CCN meeting. A special issue of Journal of Nuclear Materials on “Models and data for plasma-material interaction” (2015) was developed based on the ICTP-IAEA event on PMI in 2014.

The Unit supported the atomic physics codes widely used by fusion and plasma community. FAC (Flexible Atomic Codes), cFAC (a modified version of FAC) and GRASP2K (an atomic structure code package) are made available through the Unit’s home page. In order to facilitate the use of FAC and cFAC data, a FLYFAC code to take cFAC data and produce ionization distributions and spectroscopic properties is under the development. The FLYFAC code will be freely available with training material. A project to make the SCFLY code, a version of FLYCHK code for plasma spectroscopy publically available is on the way.

Unit staff participated in international meetings and we highlight only 2 such events. AMDU was invited to speak about uncertainty estimates for calculated data at the Workshop on Measurement Uncertainty organized at the Bureau International des Poids et Mésures (BIPM) in Sèvres, France, in June 2015. AMDU was also invited to a workshop on “Sensitivity, Error and Uncertainty Quantification for Atomic, Plasma, and Material Data” held in Stony Brook University, Institute for Advanced Computational Science, in USA, in order to discuss the uncertainty quantification of A+M/PMI data for fusion applications.

One noteworthy honour: atomic physicist Hyun Chung shared the 2015 John Dawson Award for Excellence in Plasma Physics Research of the American Physical Society. The citation reads: “For creative and novel use of the hard x-ray free electron laser to isochorically create high density plasmas and accurately measure the ionization potential depression, and for new theory that addresses discrepancies with long standing models and provides stimulus for continued developments.”
Meetings organized by us in 2014–2015

TM of the International Fusion Research Council Subcommittee on A & M Data for Fusion (28-29 April 2014)

Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical A & M Scattering Data (7-9 July 2014)

2nd RCM on Data for Erosion and Tritium Retention in Beryllium Plasma Facing Materials (18-19 August 2014)

CM on Plasma Interaction with Steel Surfaces (20-22 August 2014)

29 September – 3 October 2014, Vienna, Austria: 16th International Conference on Radiative Properties of Hot Dense Matter (RPHDM)

6-8 October 2014: 3rd RCM on Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV

3-7 November 2014, Trieste, Italy: Joint ICTP-IAEA Conference on Models and Data for PMI in Fusion Devices


2-6 March 2015, Marseille, France: The 3rd SLSP Code Comparison Workshop

16-27 March 2015, Trieste, Italy: Joint ICTP-IAEA Advanced School and Workshop on Modern Methods in Plasma Spectroscopy

22-23 June 2015: CM on Guidelines for Uncertainty Quantification of theoretical atomic and molecular data

13-15 July 2015: CM on Evaluation and Uncertainty Assessment for Be, C, Ne Atomic Data

29-31 July 2015: TM of the Code Centres Network on Simulation of PMI Data

8-11 September 2015, Seoul National University, Seoul, Korea: 2nd RCM on PWI for Irradiated Tungsten and Tungsten Alloys in Fusion Devices

14-16 September 2015, Korea Atomic Energy Research Institute, Daejeon, Korea: Joint IAEA-KAERI

CM on Recommended Data for Processes of Tungsten Ions


9-11 December 2015, IAEA Headquarters: 1st RCM on Plasma Interaction with Reduced-Activation Steel Surfaces in Fusion Devices

Meetings planned for 2016

(Status of August 2016.)

14-16 March 2016: 3rd RCM of CRP on Atomic and Molecular Data for State-Resolved Modeling of Hydrogen and Helium and Their Isotopes in Fusion Plasma

17-18 March 2016: CM on Data Evaluation for Heavy Particle Collision Processes

25-26 April 2016: TM of the 20th IFRC Subcommittee on Atomic and Molecular Data for Fusion Research

15-17 June 2016: 3rd RCM of CRP on Data for Erosion and Tritium Retention in Beryllium Plasma Facing Materials

18-22 July 2016, Hefei, China: Joint ICTP-CAS-IAEA School and Workshop on Plasma-Material Interaction in Fusion Devices

28-29 July 2016: CM on Developments in Data Exchange
Meetings attended and other duty travel in 2014–2015

9-21 March 2014, Rehovot, Israel: Visit Dr E. Stambulchik on CR modeling using FAC data.

5-7/8-9 May 2014, Livermore/Palo Alto, USA: Visit Dr H. Scott at LLNL and participate in the proposal review panel meeting at Linac Coherent Light Source (LCLS).

19-24 May 2014, Daejeon/Gwangju, Korea: Visit different institutes to give lecture/presentations.


7-10 July 2014, Cambridge, Massachusetts, USA: Attend Joint IAEA-ITAMP Technical Meeting on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data.

22-25 September 2014, Jena, Germany: Attend 9th International Conference on Atomic and Molecular Data and their Applications (ICAMDATA).


13-15/16-17 October 2014, Livermore/Palo Alto, USA: Visit Dr H. Scott at LLNL and participate in the PRP meeting at LCLS.

3-7 November 2014, Trieste, Italy: Organize the Joint IAEA-ICTP Conference on Models and Data for Plasma-Material Interaction in Fusion Devices.


15-17 June 2015, Paris, France: Attend a Workshop on Measurement Uncertainty organized at the BIPM and visit the Observatoire de Paris.

6-8 July 2015, Greifswald, Germany: Visit Prof Ralf Schneider at University of Greifswald and Max Planck Institute for Plasma Physics to discuss computational work on PMI.


21-28 July 2015, Toledo, Spain: Attend the Int. Conf. on Photonic, Electronic and Atomic Collisions.

8-11 September 2015, Seoul, Korea: Organize the 2nd RCM on PWI with Irradiated Tungsten.

14-16 September 2015, Daejeon, Korea: Organize the CM on Data for Processes of Tungsten Ions.

7-9 November 2015, Stony Brook, USA: Attend the workshop on Sensitivity, Error and Uncertainty Quantification for Atomic, Plasma, and Material Data.

16-20 November 2015, Savannah, USA: Attend the APS-DPP meeting.

1-4 December 2015, Paris, France: Attend the 9th NLTE Code Comparison Workshop.
Appendix 3: Meeting Participants

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IAEA, Baastian Braams – Scientific Secretary
E-mail: b.braams@iaea.org

IAEA, Hyun-Kyung Chung, Atomic and Molecular Data Unit
E-mail: h.chung@iaea.org
Appendix 4: Meeting Agenda

Monday 25 April 2016

09:30 – 09:45  **A. Koning and B. J. Braams:** Welcome, introduction of participants, election of a Chair.

09:45 – 10:45  **B. J. Braams:** General report on activities.

11:15 – 12:30  **H.-K. Chung:** Review of Data Centre Network and Code Centre Network activities; discussion.

12:30 – 14:00  Lunch

14:00 – 16:00  **B. J. Braams:** Review of Coordinated Research Projects; discussion (includes contribution by G. Mazzitelli).

16:30 – 17:15  **H.-K. Chung:** Review of evaluation activities; discussion.

19:00 – ...  Social dinner (Gmoakeller)

Tuesday 26 April 2016

09:00 – 10:30  **B. J. Braams:** Other activities (Workshops, meeting cooperations, other meetings); discussion.

11:00 – 12:30  **All:** Broad review and discussion. Data needs. Areas of emphasis for A+M Data Unit and new unit staff, 2016-2024.

12:30 – 14:00  Lunch

14:00 – 15:30  **All:** Discussion, recommendations and priorities for Unit activities.

16:00 – 17:00  **All:** Any other business, meeting conclusions.

17:00  Close of meeting
Appendix 5: Survey of Liquid Metal Experiments for Fusion
(Survey prepared by A. Botrugno, Consultant in the Physics Section.)

Introduction

Material components on the interior of the vessel of a fusion device are continually destroyed and reformed by the interactions with particles exhausted from the machine core which include both ions and energetic neutrals.

Several ITER and DEMO studies show that application of solid metal (mainly W, but also Be and C in support of ITER) for in-vessel elements including plasma facing components (PFCs) such as first wall and divertor, causes serious difficulties for long term operations. Several challenges are related to power load, permanent damage (e.g. melting, degradation, erosion and re-deposition) and tritium retention.

While efforts continue in the search for solutions to the PFC-related challenges from the plasma side (e.g. advanced magnetic topologies, radiative divertor operation), on the other hand, from the material side the only potential alternative is a liquid metal PFC. The PFC-related challenges may be overcome using liquid metal. Most studies and experimental activities focus on Lithium (Li) as the best candidate for fusion applications because of its low Z and because it is compatible with steel over a wide temperature range. Other studies consider tin (Sn), gallium (Ga) using chromium plating to prevent liquid tin or gallium from attacking steels. The main advantage of tin and gallium over lithium are the melting temperature that is higher than lithium, and a wider operation window. Only few studies consider Aluminium (Al).

Lithium has been considered for a long time as wall conditioning material, only recently some studies have started to investigate the use of lithium as PFC. The advantages of using Lithium (and maybe other liquid metals) in a fusion device can be divided into two main categories: (i) Plasma facing component challenges, such as heat exhaust, tritium retention, surface damage, sputtering and re-deposition; all these issues influence the reactor’s operational duration and its maintenance; (ii) Plasma operation performances, such as enhanced confinement, suppression and control of edge localized modes (ELM), lower hydrogen recycling and indeed impurity suppression.

The specific case of liquid metal used as PFC is at an earlier stage of development around the world, but there are already several laboratories and several institutes with active experimental and theoretical programs on liquid metal as PFC. These programs are using D-D tokamak plasma in not fully steady-state operations, and they are using usually a small section of facing surface. The most promising system seems to be a capillary porous system which allows obtaining stable liquid metal surfaces and counteracting disruptions and j x B forces.

Issues related to the study of lithium as PFC include liquid metal stability and flow in the divertor and first-wall, mitigation of lithium ejection under quiescent and transient events, control of evaporation and condensation, operation for long-term, plasma response (mainly MHD effects) and impurity production.

Active Main Experiments

<table>
<thead>
<tr>
<th>Experiment and Institute</th>
<th>Tokamak: T-11M and T-3M</th>
</tr>
</thead>
<tbody>
<tr>
<td>Troitsk Institute of Innovative and Thermonuclear Research (TRINITI) 142190, Moscow Region, Troitsk, ul. Pushkovykh, vladenie 12.</td>
<td>RUSSIA</td>
</tr>
<tr>
<td><a href="http://www.triniti.ru/Triniti_eng/index.html">http://www.triniti.ru/Triniti_eng/index.html</a></td>
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</tr>
</tbody>
</table>
### Status and activities

- Experiment on lithium extraction from the chamber in support of Li closed loop circulation.
- Investigation on long term effects of lithium in plasma in support of steady state operations using capillary pore systems.
- Ga droplet limiter experiment in tokamak T-3M.

### People and contacts

S.V. Mirnov


### Experiment and Institute

**Tokamak: EAST**

- Lithium injection with different systems (vaporisation with a Lithium Limiter and pellet)
- Experiment with stationary H mode up to 400 s with Lithium conditioning.
- Lithium is used to induce ELMs.

**People and contacts**

J. S. Hu

J.S. Hu, J. Ren, An overview of lithium experiments on HT-7 and EAST during 2012, Fusion Engineering and Design Volume 89, Issue 12, December 2014, Pages 2875–2885


**Experiment and Institute**

National Spherical Torus Experiment (NSTX),
<table>
<thead>
<tr>
<th>Experiment and Institute</th>
<th>Lithium Tokamak Experiment (LTX)</th>
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<tbody>
<tr>
<td></td>
<td>Princeton Plasma Physics Laboratory (PPPL)</td>
</tr>
<tr>
<td></td>
<td>P.O. Box 451, Princeton, NJ 08543-0451</td>
</tr>
<tr>
<td></td>
<td>100 Stellarator Road Princeton, NJ, 08540</td>
</tr>
<tr>
<td></td>
<td>UNITED STATES</td>
</tr>
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<td></td>
<td><a href="http://nstx-pppl.gov/">http://nstx-pppl.gov/</a></td>
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<td><a href="http://www.pppl.gov/LTX">http://www.pppl.gov/LTX</a></td>
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**Status and activities**

- In NSTX the divertor heat load has been reduced by increased lithium evaporation.
- Increasing plasma performance
- In LTX, nearly 90% of the first wall is coated with lithium in either solid or liquid form; studying the low-recycling regime

**People and contacts**

M. Ono


<table>
<thead>
<tr>
<th>Experiment and Institute</th>
<th>Tokamak: FTU</th>
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<tbody>
<tr>
<td></td>
<td>Associazione EURATOM-ENEA sulla Fusione, Centro Ricerche di Frascati, C.P. 65</td>
</tr>
<tr>
<td></td>
<td>00044 Frascati, Rome,</td>
</tr>
<tr>
<td></td>
<td>ITALY</td>
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<td></td>
<td><a href="http://www.fusione.enea.it/FTU/index.html.it">http://www.fusione.enea.it/FTU/index.html.it</a></td>
</tr>
</tbody>
</table>

**Status and activities**

- Liquid Lithium Limiter based on capillary pore system
- Withstand heat loading up to 10 MW m$^2$
- High lithium evaporation over 550 C degrees.
- A new system, named Cooled Lithium Limiter (CLL), has been recently used in order to prevent evaporation
<table>
<thead>
<tr>
<th>People and contacts</th>
<th>G. Mazzitelli</th>
</tr>
</thead>
</table>

G. Mazzitelli et al. “Experiments on FTU with an actively water cooled liquid lithium limiter” Journal of Nuclear Materials Volume 463, August 2015, Pages 1152–1155

G. Mazzitelli et al. “FTU results with a liquid lithium limiter 2011” Nucl. Fusion 51 073006

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<tr>
<th>Experiment and Institute</th>
<th>Heliac Flexible TJ-II</th>
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<tbody>
<tr>
<td></td>
<td>Ciemat. Av Complutense 40, Madrid 28040</td>
</tr>
<tr>
<td></td>
<td>SPAIN</td>
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</tbody>
</table>

| Status and activities | • Recent experiments with lithium limiter  
• Studies on lithium evaporation aimed at understanding the effects of material properties on plasma edge parameters |

| People and contacts | F.L. Tabares |

F.L. Tabares et al. “First liquid lithium limiter biasing experiments in the TJ-II stellarator “ Journal of Nuclear Materials, Volume 463, August 2015, Pages 1142–1146

<table>
<thead>
<tr>
<th>Experiment and Institute</th>
<th>Tokamk: KTM</th>
</tr>
</thead>
</table>
|                          | IAE National Nuclear Center of the Republic of Kazakhstan (NNC RK),  
071100, Kurchatov, st.Krasnoarmeyskaya, 2 buil.54 B |
|                          | KAZAKHSTAN |

| Status and activities | • capillary porous system  
• study of the processes of plasma interaction with lithium surface; study of lithium influence on plasma parameters; study of the shielding effects of receiving divertor surface due to re-emitting on lithium |

| People and contacts | I. Lyublinski |

Irina TAZHIBAYEVA , “Results of KTM Lithium Divertor Model Testing on the Tokamak KTM and Future Plans” poster at the 2014 FEC

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<tr>
<th>Experiment and Institute</th>
<th>Tokamak ISTTOK</th>
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<tbody>
<tr>
<td></td>
<td>Instituto de Plasmas e Fusão Nuclear</td>
</tr>
<tr>
<td></td>
<td>Av. Rovisco Pais, 1049-001 Lisboa</td>
</tr>
<tr>
<td></td>
<td>PORTUGAL</td>
</tr>
<tr>
<td></td>
<td><a href="http://www.ipfn.ist.utl.pt/isttok/">www.ipfn.ist.utl.pt/isttok/</a></td>
</tr>
</tbody>
</table>

| Status and activities | Gallium and Tin: jets of Ga and Sn to reduce MHD effects |

| People and contacts |


### Laboratories With Test Activities on Gallium and Tin

<table>
<thead>
<tr>
<th>JSC STAR</th>
<th>“RED” Russian Federation</th>
<th>Li Ga Sn with capillary pore system</th>
<th>I.E. Lyublinski</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIFFER (part of FOM)</td>
<td>Netherland</td>
<td>Sn using a pilot linear device with H2 plasma</td>
<td>T.W. Morgan</td>
</tr>
<tr>
<td>University of Illinois</td>
<td>USA</td>
<td>Li as PFC using a theta pinch and a plasma accelerator</td>
<td>D.N. Ruzic</td>
</tr>
</tbody>
</table>

### Other Research Activities (and related articles)

In addition to the institutes that carry out experimental activities (they conduct also theory and modelling activity) on liquid metal, there are several other institutes around the world which conduct theory and modelling studies on the use of Li, Ga and Sn. Here is a partial list of institutes and some articles.

#### US
- Purdue University *Fusion Engineering Sciences, MAE Department*,
- *UCLA, Los Angeles CA 90095, USA* (Manmeet Narula, Alice Ying)
- Center for Energy Research, University of California–San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0417

#### JAPAN
- National Institute for Fusion Science, 322–6 Oroshi-cho, Toki 509–5292, Japan

#### INDIA

35
• Bhabha Atomic Research Centre, Mumbai 400085, India

ITALY
• Consorzio RFX, Corso Stati Uniti 4, 35127 Padova,

GERMANY
• Institute of Energy and Climate Research—Plasma Physics, Forschungszentrum Jülich GmbH,

FINLAND
• EURATOM/Tekes, Department of Physics, PO Box 43, FI-00014 University of Helsinki,

Articles:
Michiya Shimada and Yoshi Hirooka Actively convected liquid metal divertor, Nucl. Fusion 54 (2014) 122002 (7pp)

Conferences
• International Conference on Plasma Surface Interactions in Controlled Fusion Devices
• International Symposium on Lithium Applications for Fusion Devices
  3rd - 2013 - Italy  http://www.isla2013.enea.it/
• Fusion Energy Conference