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### **INDC International Nuclear Data Committee**

### **19th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion**

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria 28-29 April 2014

> Report prepared by Bastiaan J. Braams IAEA Nuclear Data Section

> > July 2014

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Prepared by

Bastiaan J. Braams IAEA Nuclear Data Section

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#### **Executive Summary and Recommendations**

The International Fusion Research Council (IFRC) Subcommittee on Atomic and Molecular Data met at IAEA Headquarters in Vienna on 28-29 April 2014 to review the work of the Atomic and Molecular Data Unit (AMDU) within the Nuclear Data Section. The subcommittee heard presentations on the Unit's activities in the years 2012 and 2013 and discussed priorities for database development and evaluation, coordinated research projects and other meetings, and presentation on the web and elsewhere of the work of the Unit.

The IFRC Subcommittee offers the following specific recommendations.

- 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.
- 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.
- 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.
- 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 scientists users of A+M+PMI data and atomic, molecular and materials scientists data producers.
- 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. 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.
- 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.
- 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.
- 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.

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. 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.

#### 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 is selected to coordinate with 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 in August or September. 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 recommendations about the meeting programme and the programme of coordinated research activities of the Unit.

#### 2. Meeting Proceedings

#### Opening

Nuclear Data Section Head Dr Robin Forrest welcomed participants to the IAEA and briefly reviewed the position of Fusion activities within the Nuclear Data Section. The present meeting is concerned with activities of the A+M Data Unit, but in addition to its work on atomic and molecular data the Section also provides nuclear data libraries that are important for fusion research, notably the Fusion Evaluated Nuclear Data Library (FENDL) and the Ion Beam Analysis Nuclear Data Library (IBANDL). FENDL contains evaluated data for neutron-, proton- and deuteron-induced reactions at energy up to 60 MeV or more, as such energies are important for the International Fusion Materials Irradiation Facility (IFMIF). IBANDL contains experimental nuclear cross sections relevant to Ion Beam Analysis.

Dr Forrest noted that the Nuclear Data Section celebrates its 50th anniversary in 2014 while the Atomic and Molecular Data Unit was formed in 1977. The advice by the IFRC Subcommittee is important to the Agency. A special circumstance this year is that the work of the Section, including that of the Atomic and Molecular Data Unit, is subject to a review organized by the Agency's Office of Internal Oversight Services (OIOS), such as is done approximately once every 10 years. The report by the Subcommittee will be an important document to provide to this review.

Participants briefly introduced themselves. The Subcommittee has new members Dr Inga Tolstikhina (P. N. Lebedev Physical Institute), Dr Alexander Kukushkin (NRC "Kurchatov Institute"), Dr Guang-Nan Luo (IPP-CAS) and Dr Kyu-Sun Chung (Hanyang University). The Secretary Bas Braams asked Dr Remy Guirlet to stay on as Chair for the present meeting and this was accepted by Dr Guirlet and by the subcommittee.

#### 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 18th meeting, 26-27 April 2012. The following topics are covered.

- ALADDIN and other numerical datasets
- AMBDAS bibliographical database
- Knowledge Base
- Development of XSAMS
- GENIE Search Engine
- Data Centre Network
- Code Centre Network
- Coordinated Research Projects
- Publications
- Other meetings and workshops

The overview is presented in the format:

#### Advice from the IFRC Subcommittee meeting of 26-27 April 2012.

Actions by the Atomic and Molecular Data Unit in the period to April 2014.

Coordinated Research Projects: The subcommittee affirms the importance of the Light Elements CRP and the Tungsten in Plasma CRP. Development of a database for properties of BeH and  $BeH_2$  can be a good topic for a consultancy or consultants meeting in parallel or as a follow-up to the light elements CRP. The Tungsten in Plasma CRP should really lead to evaluated and recommended data for the principal collision processes of tungsten ions in plasma.

The Light Elements CRP has concluded and the final report has been assembled but not yet published. We want to pursue the data on beryllium hydride and incorporate the latest work done at UCL and at JET. Instead of BeH we took an opportunity to cooperate with the EMOL project in an evaluation of data for  $N_2$ .

The Tungsten in plasma CRP is planned to have its final meeting in October 2014. We will try hard to get a coherent database out of the tungsten CRP.

#### The subcommittee emphasizes that the new Hydrogen and Helium CRP should produce a comprehensive recommended standard database of isotope-resolved data for plasma modelling.

We have the principal modellers on this CRP (D. Reiter, K. Sawada, D. Wünderlich) together with data producers. In fact, even for these very small systems it is going to be very challenging to get a comprehensive database with proper treatment of rovibrational excited states.

## The subcommittee is pleased with the approval of the beryllium CRP, which will have its first RCM later in 2012. The subcommittee also reiterates its support for a CRP on irradiated tungsten as the highest priority.

The beryllium CRP was assembled and held its first meeting in Sep 2012. It is a small CRP due to the difficulty of working with Be. (We have PISCES and JET and are adding Troitsk.) We would have liked to find more contributions involving fundamental computations for this CRP, but the materials experts prefer to work on steel or other materials. Still, we assess that the CRP is relevant and is on the right track.

The irradiated tungsten CRP was approved and assembled and held its first meeting in Nov 2013. There is great interest in this CRP and we could not accommodate all interested and well qualified parties; there are 19 participating projects. The focus is on tritium retention as it is affected by radiation damage, both neutron and surrogate irradiation.

Priorities for CRPs to start in the 2014-2015 biennium: One possibility is a broad CRP on charge exchange, including cross sections and spectroscopic features related to diagnostic and heating neutral beams, although this topic may be more suitable for an incidental Technical Meeting or perhaps a Trieste Workshop. Another possible topic for a new CRP is the plasma material interaction properties of steel, which is once again being considered as plasma-facing material for a DEMO or a reactor.

We have preliminary approval for a CRP on plasma-material interaction with reduced-activation steels. If we go ahead with this then a detailed proposal could be submitted near the end of 2014 and the CRP could start in 2015.

We think that data on charge exchange processes in connection with diagnostic and heating neutral beams would be a good topic for a new CRP in the A+M area, starting in 2016.

ALADDIN and other numerical datasets: The Unit should work with DCN partners and others to realize the original ambition of ALADDIN to serve as an internationally recommended standard library of A+M+PMI data for fusion. For atomic and molecular data emphasis should shift from production of new data to evaluation of existing data. For plasma-material interaction processes there is still much need for new data, especially for fusion-relevant mixed materials.

We have put much effort into encouraging new work in data evaluation, both general principles of uncertainty estimation and evaluations for specific systems. This is really an effort to expand the community of A+M physicists that are interested in evaluations. An NFRI-IAEA TM in Daejeon had over 20 participants with proceedings in FST. In July 2014 we have an IAEA-ITAMP meeting on uncertainty assessment for calculated scattering data. For specific evaluations we have cooperations with the EMOL project (N. J. Mason) and with the NFRI data centre.

For plasma-material interaction we have new work on a Dust database following a CRP. There is SDTrimSP data from Greifswald on mixed materials ready to be added to ALADDIN, but we don't have new experimental data.

#### AMBDAS bibliographical database: The IFRC subcommittee agrees that AMBDAS remains valuable because of the ease with which one can search on specific processes. It is important to reinvigorate the provision of collisional and plasma-material interaction data in AMBDAS.

For spectroscopic bibliographical data we rely entirely on NIST. For bibliographical data on A+M collision processes we are now picking up the work jointly with DCN colleagues from NIFS, NFRI and KAERI. For bibliographical data on plasma-material interaction we are developing a partnership with Helsinki. It has taken longer than we would have liked to continue the work that used to be done at CFADC in Oak Ridge. We agree that AMBDAS still has a valuable role.

## The wiki-style Knowledge Base can be valuable for dialog and qualitative information that doesn't fit well into the numerical databases. In the spirit of wikis and in order not to overwhelm Unit resources it will be necessary to find colleagues willing to contribute to the Knowledge Base.

The Wiki has remained a low-key Unit activity. After our server shutdown (security incident) it became difficult to maintain open access for editing to the Wiki, and we did not try to reopen it to the outside world for editing. The Wiki is only edited by us. We think that we are not losing much by having it blocked for outside editing.

# Data Centre Network: The subcommittee emphasized ITER's need for standard and recommended data as a focal point for the work of the DCN. Quality control of data and the provision of recommended data remain the most important issues for the network. A network of data evaluators should be developed in close connection with the Data Centre Network.

With support from the DCN we have put much effort into developing a network of data evaluators and promote structured small group evaluations. Of special note:

- Joint IAEA-NFRI TM on Data Evaluation for Atomic, Molecular and Plasma-Material Interaction Processes in Fusion, 4-7 Sep 2012, Daejeon, Korea. (Papers in Fusion Science and Technology).
- Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data, 7-9 July 2014, Cambridge, MA, USA.
- Cooperation with EMOL network on evaluations of data for H<sub>2</sub>O and N<sub>2</sub>.
- Cooperation with NFRI on evaluations of data for methane.

One objective is to obtain guidelines agreed by the community for uncertainty assessment and data evaluation.

# Code Centre Network: The subcommittee agrees that CCN should emphasize documentation of codes for the benefit of fusion plasma researchers. A suitable focused topic for the next meeting of the CCN would be the evaluation of accuracy and uncertainty in theoretical atomic collision data. Another CCN meeting could focus on codes for plasma-material interaction.

The CCN meeting in 2013 (held over from 2012) was meant to help develop guidelines for uncertainty assessment of calculated scattering data. (Besides, the meeting was coupled to an EMOL project meeting on evaluation of e-H<sub>2</sub>O scattering data.) The effort will continue at the meeting at ITAMP in July. For a possible CCN meeting in 2014 or early 2015 we are thinking to focus on codes for interpretation of PMI data, for example simulations of thermal desorption spectroscopy. We would want to bring fusion researchers together with code authors in the materials field.

# Development of XSAMS: The subcommittee is very pleased with the adoption of XSAMS by the Virtual Atomic and Molecular Data Centre (VAMDC). The Unit should continue to support XSAMS activities, but with priority for adoption of XSAMS by the fusion community rather than for extensions to the Schema.

For the past 2-3 years we have really left leadership of XSAMS to VAMDC. We adopted the final VAMDC XSAMS as the international standard version of XSAMS. It means that atomic and molecular data (small molecules) are very well covered. Particle-surface interaction processes are covered in a rudimentary way and we are not going to change that.

At this time a key issue for XSAMS is the success of the VAMDC effort to establish a long-term sustained infrastructure including a legal entity. It is hoped to achieve this before the end of 2014.

ALADDIN can produce output in XSAMS format. We would like to make ALADDIN a proper VAMDC node.

### GENIE Search Engine remains valuable, but the Unit should let its extension to other databases depend on the development of the XSAMS-based portal.

Indeed we continue to support GENIE, but we have not tried to expand it to further databases. (Open-ADAS and Spectr-W3 were added before 2012.) At this time, databases that might be a candidate to be added to GENIE (e.g. DREAM and DESIRE) are also part of VAMDC or at least working with VAMDC.

GENIE was an excellent concept and it is a valuable lightweight tool. However, with the success of VAMDC and its extension (at least for now) in Sup@VAMDC we don't find it so useful to put new effort into GENIE.

#### Publications: The subcommittee is very pleased with the plans to produce future instances of Atomic and Plasma-Material Interaction Data for Fusion (APID) as volumes in the IOP open access Journal of Physics Conference Series. The subcommittee also recommends to pursue the publication route of a joint survey article in a major journal, as was done following the Tritium Inventory CRP. This would be in addition to the preparation of the APID/JPCS collection of articles.

The final report of the Light Elements CRP is prepared as a special issue of JPCS; I hope that the contract with IOP is imminent. For a future CRP, however, we would like an open access journal that provides more service, has perhaps a higher reputation, and provides rolling electronic publication in a single special issue. The new "Atoms" journal looks attractive for the final report of the Tungsten CRP.

We did not get a joint article out of recent CRPs. A serious effort was made for the Dust CRP, but in the end the contributions were not adequate. The Light Elements CRP was too broad for one article. The Tungsten CRP may be focused enough.

APID Volumes 15 and 16 have appeared in print. APID 17 is still not finished.

#### The subcommittee reinforces its support for holding another broad Technical Meeting in 2013 covering atomic, molecular and plasma-material interaction processes and data and materials properties data inasmuch as they are relevant for plasma-material interaction. The subcommittee suggests an effort to make it a joint ITER-IAEA meeting.

Not done in 2013 due to a busy schedule. We had a tentative agreement to hold this meeting near the end of 2014 with NFRI as the local organizer. However, we have a conference at ICTP in November 2014 that covers much of the PMI/PSI ground that belongs to the intended broad meeting and we hope for a good participation from fusion scientists there.

We do want to hold the broad A+M+PMI meeting in Q1 or Q2 of 2015.

(Addendum: Following the meeting of the Subcommittee this broad A+M+PMI meeting was restored to the meeting agenda and is now being organized in cooperation with NFRI to be held 15-19 December 2014 in Daejeon, Korea.)

## The subcommittee views the two recent Code Comparison Workshops as a worthwhile outreach activity at relatively low cost for the Unit. The subcommittee supports the interest of the Unit to co-operate in future similar code comparison workshops.

Following those two meetings (Non-LTE in 2011, Spectral Line Shapes in 2012) we cooperated in the Second Spectral Line Shapes in Plasma workshop in 2013 and we granted cooperation to the Third SLSP that is to be held in 2015 in Marseille.

## The subcommittee encourages the Unit to seek to continue the joint IAEA-ICTP workshops with a next instance in 2014 or 2015. It is noted that the ICTP is also an excellent venue for advanced workshops.

We were granted a one-week slot in Nov 2014 for an advanced event (conference) on "Models and Data for Plasma-Material Interaction in Fusion Devices." The early organization is very encouraging. We had a very good response to our invitations and obtained a list of 34 invited speakers.

For 2015 we have requested support for a two-week "Advanced School on Modern Methods in Plasma Spectroscopy". First week for advanced training, second week a conference on plasma diagnostics. Yu. Ralchenko (NIST) would be co-Director.

(Addendum: In June 2014 we learned that this request was awarded. We have accommodation at ICTP for a two-week workshop in March 2015 and financial support from ICTP for effectively one week.)

Conclusion: The subcommittee offers the broad recommendation to the Unit to use its influence and its meetings to strengthen the community that is involved in data production and data evaluation for atomic, molecular and plasma-material interaction processes. The international Data Centres Network, broadly defined, needs the support and visibility that is brought by the A+M Data Unit of the IAEA.

We strongly agree and this remains a driver of our activities.

#### H.-K. Chung: Review of Data Centre Network, Databases and Data Evaluation

Atomic physicist Hyun-Kyung Chung described the Unit's web-based data services, databases, activities of the Data Centre Network and collaborative activities on data evaluation.

#### Data services

The Unit home page, <u>http://www-amdis.iaea.org/</u>, is the portal to the Atomic and Molecular Data Information System (AMDIS). It provides prominent links to our numerical and bibliographical databases and other data collections, to online computing capabilities for A+M data, to the Wiki-style knowledge base on atomic, molecular and plasma-material interaction data for fusion and to our meetings and other activities.

For several months, December 2012 through March 2013, the A+M Data Unit web services were severely disrupted due to security breaches and a subsequent complete reorganization of the server system. Instead of a single server under control of the Nuclear Data Section the system now involves three servers: an internal development server and a staging server that are accessible only within the Agency and a Cloud server that provides public access. The Cloud server is under strict control of the IT Division and the core software on the other servers is that of the Cloud server. The migration has been disruptive; however, it has led to an upgrade and unification of database systems and data services and to a more secure environment.

Google Analytics is used across the Section to keep track of web visits and the evolution of patterns in the visits. Except for the gap in early 2013 the visits to AMDIS are stable over the two-year period

and the most visited parts below the main AMDIS page appear to be the ALADDIN numerical database, the Knowledge Base Wiki, the GENIE search engine, the CRP pages, the FLYCHK data collection, and then the pages on meetings organized by the unit, the AMBDAS bibliographical database, the pages on our Workshops (ICTP events and code comparison meetings) and the Unit publications. The data from Google Analytics also provide geographic information and information about the web origin of a visit; the web origin is Google search in 41% of cases and direct access (e.g. bookmarked page) in 31% of cases; all other sources much less. The data are tabulated in the presentation.

#### Databases

The numerical ALADDIN database contains evaluated and compiled data since 1980 and in recent years largely data produced in CRPs or consultancies of the Unit. In connection with XSAMS (see under Other Activities) and with the Virtual Atomic and Molecular Data Centre (VAMDC) and with support through consultancies by Ch. Hill (UCL and VAMDC) we are working to modernize the database and its interface. Data in ALADDIN are organized in different ways (tables in various formats and also fit functions) and we wish to normalize this. Unofficially the A+M data part of ALADDIN is now also accessible through VAMDC, but the access is via a copy of the database not located on our Cloud server. It needs further work with our IT services to make the appropriate software available on our own server.

A critical issue for ALADDIN now is to review data quality and to renew the effort to make ALAD-DIN the repository for evaluated and recommended data compilations for fusion.

The bibliographical database AMBDAS has been updated with data for spectroscopy and structure provided by NIST, as they have done in the past. Volume 69 of the International Bulletin on Atomic and Molecular Data for Fusion ("the Bulletin") was produced in 2013; this is the hardcopy version of AMBDAS updates. However, there has not been an update to AMBDAS in the area of atomic and molecular collision processes and particle-surface interaction since 2010. These sections of AMBDAS had been for many years provided by the Oak Ridge Controlled Fusion Atomic Data Center (CFADC), which closed in 2012; efforts there to retain or recreate the bibliographical data work were not successful. Instead we are now working with Data Centre Network colleagues from NFRI, KAERI and NIFS to resume the A+M collisions part of AMBDAS and with the Helsinki group (consultancy with A. Lasa) to resume the collection of PSI data in AMBDAS.

As an outgrowth of the CRP on "Characterization of Size, Composition and Origins of Dust in Fusion Devices" a database on properties of dust particles has been developed at IPP Garching and is now being standardized for international use with the intent that it will be hosted at IAEA. The interest in quantified properties of dust is entirely due to the needs of ITER: dust, and especially tritiated dust, provides serious safety and operational issues; the amount of dust on hot surfaces in ITER is limited to 6 kg due to a strong chemical reactivity with air and stream (ITER accident scenario), and dust particles can be accelerated to velocities up to several km/s and damage the first wall or diagnostics. This makes it valuable to have a database of physical and chemical properties of dust in present fusion devices, in dependence on location in the device and operating conditions of the machine.

The starting point for the dust database are Scanning Electron Microscopy (SEM) measurements. These measurements (images) are analyzed by a public-domain program ImageJ, which returns geometric and other parameters for a database. This work was initiated by V. Rohde at IPP Garching and is now being pursued through consultancies with us by S.-H. Hong at NFRI. His work has led to recommendations for standard procedures in collection and analysis, for example with respect to settings of contrast and resolution, so that database entries from different devices are properly comparable. The objective is to have a standardized database hosted at IAEA with contributions from major fusion and laboratory experiments.

The Unit's Wiki-style Knowledge base is found at <u>https://www-amdis.iaea.org/w/</u>. The content was mainly created in 2010 by us based on INDC reports, APID volumes and presentations at our meetings. The main sections within the Knowledge base Wiki are concerned with A+M+PMI data needs for fusion, sources of data, places and tools for data exchange, fusion research more broadly (in relation to A+M+PMI data) and special topics in the area of atomic, molecular and plasma-material interaction data in fusion energy research and related fields. The information on the wiki is addressed to fusion plasma researchers and atomic, molecular and materials physicists. It is part of our effort to bring these communities together.

Development of the Knowledge base has been a low-key effort in 2012-2013. Before the server disruption the Wiki pages were open to editing from outside the Agency (a password was still required), but in practice we did not find outsiders interested to contribute to these pages. After the restructuring of our web services it is no longer possible to edit from outside the Agency and we don't really mind it. Maintenance is now entirely done by us.

The GENIE search engine was maintained but no new databases were added in 2012-2013. At present GENIE provides access to 9 databases in the area of structure and spectra and to 6 databases in the area of collision processes. For structure and spectra the databases are: the NIST Atomic Spectra Database, Kurucz's CD-ROM 23, Atomic Line List v. 2.04, TOPbase (Opacity Project), Kelly Atomic Line Database, the MCHF/MCDHF Collection, KAERI AMODS Spectral Lines, CAMBD Atomic Spectra and Spectr-W3. For collision processes they are: the IAEA ALADDIN Database, NIFS AMDIS Database, CAMBD Collisional Processes, NIST Atomic Cross Sections, Open-ADAS and Spectr-W3 collisions. In the area of structure and spectra the Chianti database could be added; however, at this time we favour further database integration through the Virtual Atomic and Molecular Data Centre (VAMDC) infrastructure.

#### **Data Centres Network**

The International Atomic and Molecular Data Centres Network (DCN) is a cooperation through the IAEA of centres that are active in the domain of atomic, molecular and plasma-material interaction data for fusion and related plasma applications. The nature of activities varies, but each participating centre should have an established programme in collection, dissemination, evaluation and/or generation of A+M+PMI data. The participating centres are NIST (USA), CRAAMD (China), JAEA (Japan), NIFS (Japan), KAERI (Korea), Kurchatov Institute (Russian Federation), NFRI (Korea), FZJ (Germany), ADAS (UK-based) and IAEA.

The DCN normally meets biennially to discuss coordinated activities among the centres on data issues for fusion and other plasma applications. Topics at the most recent meeting in September 2013 were:

- XML Schema for Atoms, Molecules and Solids (XSAMS)
- Bibliographical data compilation
- New work on data evaluation
- Priorities in A+M+PMI data compilation and evaluation

The DCN meeting may have some outside guests and in 2013 we had Dr Christian Hill (University College London and VAMDC) to describe what is involved in setting up a database node as a part of the Virtual Atomic and Molecular Data Centre and Dr Hossein Sadeghpour of the Institute for Theoretical Atomic, Molecular and Optical Physics (ITAMP) to discuss A+M areas of current interest.

The topic of bibliographical data compilation was discussed and plans were made between IAEA, NIFS, NFRI and KAERI to renew the collection and indexing of bibliographical data for A+M collision processes. In the area of numerical databases there is interest to establish a database of parameters that describe interaction potentials and surface binding energies for BCA (binary collision approximation) calculations of plasma-material interaction. Also interest was expressed in a database of diatomic potential energy curves for molecules and molecular ions that are of interest for edge plasma studies (primarily light element hydrides and N<sub>2</sub>, O<sub>2</sub>).

Past DCN meetings usually produced an update to a list of priorities for A+M+PMI data compilation and evaluation. However, we found that the list was not really helpful to the A+M+PMI community; the information is too generic. Dr A. Kukushkin of the Kurchatov Institute showed responses to a questionnaire about data needs for ion and neutral beam development and this looks like an attractive model. The results of the questionnaire are presented as items that show a physics application, some representative literature, specific A+M processes of interest, available data sources and a description of data needs. We regard this as a model to be followed. One should try to add information about the required data accuracy. The IAEA Wiki pages would be a good home for a description of these data needs. To extend the list it is recommended to work with ITPA or ITER domestic agencies.

#### Data evaluation

Since 2012 the A+M Unit has organized multiple meetings on evaluation. An overview is maintained at the web page <u>https://www-amdis.iaea.org/DCN/Evaluation/</u>. The meetings are:

- CM on "Procedures for Evaluation of Atomic, Molecular and Plasma-Material Interaction Data for Fusion", 7-9 February 2012, NIFS, Toki, Japan;
- CM on "Data Evaluation and the Establishment of a Standard Library of A+M/PMI Data for Fusion", 20-22 June 2012, IAEA Headquarters, Vienna, Austria;
- Joint IAEA-NFRI TM on "Data Evaluation for Atomic, Molecular and Plasma-Material Interaction Processes in Fusion", 4-7 September 2012, NFRI, Daejeon, Republic of Korea;
- 3rd TM on "International Code Centres Network", 6-8 May 2013, IAEA Headquarters, Vienna, Austria;
- CM on "Evaluation of Data for Collisions of Electrons with Nitrogen Molecule and Nitrogen Molecular Ion", 5-6 December 2013, IAEA Headquarters, Vienna, Austria;
- Joint IAEA-ITAMP TM on "Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data", 7-9 July 2014, Cambridge, MA, USA.

Two of these meetings stand out from our regular roster: the IAEA-NFRI TM in Daejeon, Korea, September 2012 and the IAEA-ITAMP TM in Cambridge, USA, in July 2014.

The IAEA-NFRI meeting in 2012 had more than 20 participants from Australia, China, Germany, India, Japan, Korea, Poland, Russia, UK, USA and IAEA. The meeting was focused on reaction data (as opposed to structure and spectra), with subtopics Current Evaluated Databases (Kramida, Landi, Mason); Evaluation Methods and Experiences (Itikawa, Kumar, Cho, Karwasz); Error Propagation and Sensitivity Analysis (O'Mullane, Ballance, Reiter, Krstic); Theoretical Data Evaluation (Aggarwal, Liang, Takagi, Song); Experimental Data Evaluation (Nakamura, Buckman, Shevelko, Imai); and Data Centres Evaluation Activities (Yoon, Murakami, Mason, Chung). Proceedings papers were published as a special issue of Fusion Science and Technology (2013).

Discussions at the IAEA-NFRI meeting covered a wide range, from ways to encourage more community activities in data evaluation to technical aspects of uncertainty assessment. It is found important to present database work as "data research" with its own scientific content, and being a critical part of scientific work. The terminologies of VIM (Vocabulaire International de Métrologie, 2007) and GUM (Guide to the expression of Uncertainty in Measurement, 2008) are adopted by major international organizations such as IAEA, IUPAC, IUPAP, BIPM, ISO, WHO, FAO, but they need to be much better disseminated in our community. The community needs to adopt evaluation procedures towards standard reference data for A+M processes. There was much exchange of ideas about these topics, including the development of workflow guidelines and procedures for structured group evaluation. On the more technical side the major issue appears to be the need to assign uncertainties to calculated cross sections. At present there are no good criteria for assessing theoretical data, which may be presented as "best possible" without proper uncertainty assessment. There is a real need to develop systematic ways to assess the propagation of uncertainties from atomic and molecular structure calculations to cross sections and rate coefficients. The long term goal is to develop a worldwide network devoted to an internationally agreed and recommended data library for fusion and other plasma applications.

The meeting in Cambridge, USA, in July 2014 is expected to bring together about 30 experts in computational A+M science to discuss the critical issue of uncertainty estimates for calculated scattering data.

#### B. J. Braams: Review of Coordinated Research Projects

The following recent and potential future CRPs were briefly described.

- 2008-2012: Characterization of Size, Composition and Origins of Dust in Fusion Devices
- 2009-2013: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions
- 2010-2014: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV
- 2011-2015: Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma
- 2012-2016: Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials

- 2013-2017: Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices
- Proposed to start in 2015: Plasma-Material Interaction With Reduced-Activation Steel Surfaces
- To be considered: Data for Beam-Plasma Interactions in Fusion Experiments

Please see the CRP web page, <u>https://www-amdis.iaea.org/CRP/</u>, for more detailed information about each CRP, including participants, meeting dates, links to meeting presentations and links to meeting reports. Here are some notes on each recent project.

#### 2008-2012: Characterization of Size, Composition and Origins of Dust in Fusion Devices

At the time that the Dust CRP was initiated and when its meetings were held tritiated dust was considered the most important safety issue for nuclear licensing of ITER. (S. Ciattaglia at the 2RCM.) Urgent interest in properties of dust in fusion devices declined towards the end of the CRP for several reasons: carbon was completely removed from the ITER divertor design, a submission by ITER to the French Nuclear Authority towards licensing was accepted in 2012, and the JET-ILW experiments since the Fall of 2011 showed little dust production. However, dust and characterization of dust remains a critical issue for ITER. It does not suffice for ITER to be persuaded that dust will probably not pose a major problem. Instead, operation of ITER requires ways to measure at any time (without need to shut down the machine) the dust inventory and the inventory of tritium in dust and to affirm positively that these quantities are within licensing limits.

The CRP was devoted to providing support for ITER's need to quantify dust and tritium in dust. The project sought to support the acquisition of data for properties of dust: distribution of particle size and composition, hydrogen content, origins in fusion machines. Contributors to the CRP came from major fusion experiments, laboratory experiments and modelling. There was very good cooperation, for example on video analysis of dust images, dust collection, and dust database development. Meetings were held in Dec 2008, Jun 2010 and Dec 2011.

This was a rather unusual project by our standards; most of our work before this Dust CRP has been concerned with cross sections for atomic and molecular processes or with directly quantifiable properties (reflection, sputtering, etc.) of particle-surface interactions. The characterization of dust production as a function of discharge conditions is a rather more challenging problem from the database perspective. In fact, this challenge was met and the most interesting output of the CRP is the infrastructure for a Dust database that is to be hosted at IAEA. The database was first developed at IPP Garching and development continues at NFRI (Korea) for proper standardization of database procedures (standard image analysis) and then international access through IAEA.

## 2009-2013: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions

The objective of this CRP was to generate data for processes including excitation, ionization, recombination and heavy particle collisions for atoms and molecules (hydrides) and their ions of Li, Be, B, C, N, O. Meetings were held in Nov 2009, May 2011 and Mar 2013. The participants are a diverse group with backgrounds in spectroscopy, electron-atom and electron-molecule collisions, charge transfer in atomic collisions, and some atom-molecule collisions. As reflects the situation with data for light element processes most participants come from theory, but there are two experimental teams as well.

The final output of this CRP will be special issue of the IOP open access Journal of Physics: Conference Series. At this time the refereeing is all done, the manuscript has been approved by the Publications Committee, and a final agreement with JPCS is expected soon. The agreement leaves copyright with IAEA and provides us the option to produce hardcopy in the style of the previous APID Greenbooks and we will deal with that once the on-line publication is done. Data will go into ALADDIN alongside the publication in JPCS.

#### 2010-2014: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV

This CRP is expected to support interpretation of spectroscopic measurements and modelling of tungsten in fusion plasma by providing fundamental experimental and calculated data for radiative and collisional atomic processes involving tungsten ions. Tungsten is the wall material for the regions of highest heat load in ITER and it is also used extensively on present experiments, with a view towards ITER and a reactor. This makes tungsten the most important heavy impurity ion in fusion energy research.

The CRP combines experiment and modelling and it covers all ionization stages. Participants include representatives of EBIT experiments, ablating plasma experiments, merged beam collision experiments and computations. This is a large CRP due to the strong interest world-wide in atomic processes for tungsten.

The first RCM was held in December 2010 and the second RCM was held in August 2012 in Heidelberg, Germany, back-to-back with the important biennial Highly Charged Ions (HCI) conference there. The third RCM is planned for October 2014.

Similar to the Light Elements CRP this CRP should lead to an open access journal publication and a hardcopy Greenbook. However, after the experience with JPCS for the Light Elements CRP we are now leaning towards use of the "Atoms" journal rather than JPCS. Reasons for this preference are that Atoms offers more service from the journal, they have probably a higher reputation, and they use a rotating publication schedule within a single special issue.

## 2011-2015: Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma

The objective of this CRP is to evaluate existing data for the relevant atomic and molecular processes of hydrogen and helium, generate new fundamental atomic and molecular data where this is needed, and assemble the information into a knowledge base and numerical databases for use by the fusion community. (Update of the "Janev-Reiter" database.) The primary application domain is edge plasma modelling, but there is also interest in negative ion processes that are relevant in connection with negative hydrogen ion beam production. The database should be isotopically complete and consistent with respect to hydrogen isotopes H, D and T, and the data should be resolved with respect to vibrational excited states, and ro-vibrational states where this is feasible. The relevant species include H,  $H^+$ ,  $H^-$ ,  $He^+$ ,  $He^-$ ,  $He^-$ ,  $H_2^+$ ,  $H_3^+$ ,  $HeH^+$ ,  $He_2^+$  and their (H, D, T) isotopic variants.

The participants are fusion plasma modellers and atomic physicists. Most come from theory and modelling, but there are also two experimental groups. The first and second RCM were held in August 2011 and July 2013 and the final RCM is to be held in 2015.

#### 2012-2016: Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials

This CRP had been recommended by the IFRC Subcommittee at their meeting in April 2010 as the highest priority in the area of plasma-material interaction, because of the need to support the JET IT-ER-Like Wall experiments and to prepare for operation of ITER. The detailed proposal for this CRP had been accepted by the Committee on Coordinated Research Activities (CCRA) in August 2011.

Processes of interest include physical and chemical sputtering and trapping and transport of hydrogen (H,D,T) for beryllium-based surfaces. The CRP will emphasize data for the relevant mixed materials, especially Be-(H,D,T,He), Be-C, Be-N, Be-O. (Stable binary phases: Be<sub>2</sub>C, Be<sub>2</sub>W, Be<sub>12</sub>W, BeO and Be<sub>3</sub>N<sub>2</sub>.) The most important projectiles are H, D, T, He, Be, C, N, O, Ne and Ar.

The First RCM of this CRP was held in September 2012 and the second RCM is expected to be held in August 2014. It is a small CRP, with only 6 Research Agreements at the time of the First RCM. On the side of experiment it is easy to understand why the CRP is small; it is very difficult to do experiments. At the 1RCM PISCES was the unique facility for well resolved experimental data, but we wish to add Troitsk (QSPA-Be at Bochvar) as a 7th participant in the CRP ahead of the 2RCM. On the side of theory it is perhaps surprising that the CRP is so small; one would think that beryllium, with only 4 electrons per nucleus, should be very attractive for computational materials scientists. We made a serious effort to find researchers that do fundamental modelling of beryllium, but it was difficult. The major issue at the 1RCM was differences between PISCES data and beam exposure data, presumed mainly due to hydrogen concentration (also morphology, oxygen layer). It is important to understand the effect of fluence via its effect on hydrogen concentration. There is also much experimental uncertainty still for hydrogen (tritium) retention in beryllium.

## 2013-2017: Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices

This CRP had been recommended by the IFRC Subcommittee at their meeting in April 2010 as the next one to start after the CRP on beryllium plasma-facing materials, and the subcommittee affirmed that recommendation in 2012. The CRP looks beyond ITER with the objective to support assessment of the prospects for tungsten-based plasma-facing materials in a fusion reactor environment.

The overall objective of the CRP is to support fusion plasma and fusion materials modelling and planning and design efforts towards DEMO and a Fusion Power Plant through the enhancement of the knowledge base on properties of tungsten as a plasma-facing material in a fusion nuclear environment, and thereby to contribute to the development of fusion energy generation. More specific objectives are:

- To inventorise knowledge about effects of neutron irradiation and charged particle surrogate irradiation on the microstructure of tungsten-based plasma-facing materials.
- To inventorise knowledge about the relation between tungsten microstructure after irradiation and plasma-material interaction properties for erosion, tritium retention and tritium migration.
- To perform coordinated experiments and computations (based on quantum theory and molecular dynamics) to improve the knowledge base on effects of irradiation upon tungsten microstructure.
- To perform coordinated experiments and computations to improve the knowledge base on the influence of tungsten microstructure on tritium retention and tritium transport properties.
- To synthesize new information, extrapolate to relevant fusion neutron fluence, and provide best expert estimates and uncertainties for plasma-material interaction properties (especially tritium retention and tritium transport) for tungsten-based materials in a fusion reactor environment.

In order to achieve these objectives the CRP relies on experiment and computation. It is understood that experiments cannot use the relevant neutron fluence, hence the interest in surrogate irradiation, and it is understood that many experiments will work with hydrogen or deuterium instead of tritium. Computations will help to bridge the gaps.

The CRP proposal was reviewed and approved by the Committee on Coordinated Research Activities in June 2013 and 19 Research Agreements were approved at the end of August. The participating projects are primarily experimental, but the CRP has good theory contributions too. Neutron irradiation is done in Japan and the USA and otherwise there is surrogate irradiation and computation. The CRP has a very substantial Chinese contribution; 3 participating projects and it could have been more if we didn't adhere to 3 projects as the maximum for one country. The first RCM of the CRP was held on 26-28 Nov 2013 and a second meeting is due in Q3 2015.

## For consideration to start in 2015: Plasma-Material Interaction With Reduced-Activation Steel Surfaces

At the meeting in April 2012 the IFRC Subcommittee on A+M Data had discussed candidate topics for a CRP or CRPs to start in the 2014-2015 biennium and had highlighted two projects for special consideration: one on plasma material interaction properties of steel and one on charge exchange in relation to diagnostic and heating neutral beams. When preliminary proposals were requested for the 2014-2015 plan the Unit put the Steel CRP in first place. However, a detailed plan for such a CRP has not yet been submitted and it is appropriate to review the plans and priorities at the present meeting of the subcommittee.

The objective of the proposed CRP on steel surfaces is to support an assessment as to where and to what extent steel can replace beryllium or tungsten for the first wall in DEMO/FNSF or a reactor. Beryllium is probably not useful beyond ITER because the erosion is too high, so the primary use of steel would be to replace beryllium on the main first wall. The CRP would focus on the erosion and tritium retention properties of low- or reduced-activation steels such as oxide dispersion strengthened (ODS) and reduced activation ferritic/martensitic (RAFM) steel.

In order to assess the breadth of interest in such a CRP we looked at activities at recent relevant meetings: the International Conference on Plasma-Facing Materials and Components (PFMC) in 2013, the International Conference on Fusion Reactor Materials (ICFRM) in 2013, the International Conference on Plasma-Surface Interactions in Fusion Devices (PSI) in 2014 and the Hydrogen Workshop satellite to PSI in 2014. The list of contributions given in Appendix 3 shows that there is plenty of interest in properties of steel as a plasma-facing material. Note that for this CRP we do not consider properties of steel as a structural material, and the list in Appendix 3 does not include such contributions; it is all plasma-material interaction.

If we pursue a CRP on plasma interaction with steel surfaces to start in 2015 then an appropriate schedule would involve a Consultancy Meeting before the end of 2014 to help prepare the detailed proposal, which is then submitted to the Committee on Coordinated Research Activities (CCRA) for their consideration. The first meeting could be held any time in 2015.

#### For consideration: Data for Beam-Plasma Interactions in Fusion Experiments

The second new CRP topic highlighted by the A+M Subcommittee in 2012 is that of charge exchange processes including cross sections and spectroscopic features related to diagnostic and heating neutral beams. The subcommittee said in 2012 that it needs further thought if this topic is perhaps more suitable for an incidental Technical Meeting or perhaps a Trieste Workshop.

Certainly there is broad interest in heating and diagnostic neutral beams and there are relevant atomic and molecular data issues to be studied. Such a CRP would consider processes on beams of the lightest elements H/D/T, He, and Li for sure; maybe also heavier beams such as Na. The key issues would be related to collisions in the core plasma: multistep processes, metastable excited states, level splitting, motional Stark effect. The CRP would have the task to produce and evaluate cross sections and spectra for beam interaction with plasma, and perhaps also data for processes in the production of the beam, e.g. in the negative ion beam box. The CRP would assemble people from fusion plasma diagnostics, diagnostic modelling and atomic physics. To the Unit this looks like an attractive CRP topic, but it needs the review of this committee. (As reviewed below, in the discussions the subcommittee recommended data for charge exchange processes in connection with neutral beams as the topic for the next CRP on atomic and molecular processes.)

## H.-K. Chung: Review of Code Centre Network and Code Comparison Workshops

#### **Code Centre Network**

The Code Centre Network (CCN; <u>https://www-amdis.iaea.org/CCN/</u>) is a joint effort to gather and provide access to codes and related information relevant for modellers in fusion plasma science. Members of the CCN are interested in online codes and downloadable codes. Besides, the CCN web pages provide contact information and information about expertise of the members and the group provides the (little used) Data For Fusion (DAFF) mailing list. From the start the CCN was foreseen as a rather loosely organized group of code developers.

At the 2nd meeting of the network, in 2010, it was agreed that the CCN would be developed into a larger and more diverse network. It implies that meetings of the network would each time assemble only a subset, for example focused on a particular area of A+M+PMI codes relevant for fusion. It was also agreed then that the CCN did not view the provision of codes as the key activity. For many codes considerable expertise is required to use them effectively and it is more important to provide data generated by expert users of the codes rather than to share the codes. This applies, for example, to many codes for scattering calculations, for which the output (cross sections) can be tabulated in a sensible way. One is really looking for an integrated database of recommended data and code capabilities, with description of data quality. The CCN activities should be formulated to benefit code developers directly and these activities may include code comparison workshops (as discussed below).

The present codes and participants in the Code Centre Network are:

• CCC & RCCC, Curtin University, Australia, I. Bray

- CR Model, Kitasato University, Japan, F. Koike
- MELDF\*-TCAM, QUAN, EIKON, CTMC, Universidad Autonoma de Madrid, Spain, I. Rabadan
- CDW and VPN, University P. & M. Curie, France, Alain Dubois; Centro Atomico Bariloche CNEA, Argentina, P.D. Fainstein
- Molecular cross Sections, SI calculations, University of Bari, Italy, M. Capitelli
- CR Models, Kurchatov Institute, Russian Federation, A. Kukushkin
- ATOM, ATOM-AKM, GKU, Lebedev Institute, Russian Federation, L. Vainshtein
- HYDKIN, Forschungszentrum Juelich, Germany, D. Reiter
- MCHF, GRASP2K, FLYCHK, NOMAD, National Institute for Standards and Technology, USA, Yuri Ralchenko
- DEGAS databases, Princeton Plasma Physics Laboratory, USA, D. Stotler
- LANL Codes, Los Alamos National Laboratory, USA, J. Abdallah, Jr.
- HULLAC code, ETHZ, Switzerland, M. Klapisch
- SDTRIM-SP, IPP Greifswald, Germany, R. Schneider
- Plasma formulary, Weizmann Institute of Science, Israel, E. Stambulchik
- AMD Services, International Atomic Energy Agency, H.-K. Chung

Some of the newer content in the domain of the CCN are results of FLYCHK calculations of charge state distributions and radiative cooling rates and FAC (Flexible Atomic Code) calculations of energy levels, transition rates and cross sections for elements He-Si. There is also a new database of results from the ATOM-AKM code (L. A. Vainshtein) for electron impact excitation and ionization cross sections and rate coefficients for the lightest elements.

The third Code Centre Network meeting was held in May 2013, bringing together A+M experts from the network to focus on guidelines for uncertainty assessment of calculated atomic and molecular data, especially for electron collision processes. Participants discussed propagation of uncertainties from structure data to scattering data, considered computational tools to facilitate uncertainty assessment and considered recommendations to code users for procedures to obtain an uncertainty estimate. This is a large complex of questions that are far from being solved, but the meeting had several significant outputs.

One output of the meeting was a joint session with a meeting of the eMOL project that is intended to perform evaluations for electron scattering data. (The CCN meeting was held Mon-Wed 6-8 May and the eMOL meeting was held 8-10 May, both in Vienna.) This particular eMOL meeting was devoted to evaluation of  $e-H_2O$  scattering data. In addition to synergy with the eMOL meeting the CCN meeting shared participants with a meeting on Auger electron emission in nuclear decay (see later).

The CCN meeting in May 2013 also stimulated a special issue of the journal Atoms on "Critical Assessment of Theoretical Calculations of Atomic Structure and Transition Probabilities" edited by Per Jönsson, Alexander Kramida and Hyun-Kyung Chung, which appeared in 2014 with 5 scientific contributions.

The CCN meeting recommended continuing follow-up by the A+M Data Unit to encourage community interest in uncertainty estimates, develop benchmark test cases, develop a network of theorists for code comparisons and coordinate further data evaluation group meetings.

#### Code comparison workshops

Since 2011 the A+M Data Unit has cooperated in a number of code comparison workshops:

- The 7th Non-Local Thermodynamic Equilibrium (NLTE) Code Comparison Workshop (2011); publication in High Energy Density Physics, 9, 645 (2013);
- The 1st Spectral Line Shapes in Plasmas Code Comparison Workshop (2012); publication in High Energy Density Physics, 9, 528 (2013);
- The 2nd Spectral Line Shapes in Plasmas Code Comparison Workshop (2013); publication as a special volume in Atoms journal (7 contributions).

We have also agreed to cooperate in the 3rd Spectral Line Shapes in Plasmas Code Comparison Workshop in March 2015.

The nature of the workshops, following the NLTE model, is that test cases are specified about 6 months before the meeting and participants are expected to do their best work on at least some of the cases. At the week-long meeting the results are then compared in fine detail. They are small, specialist meetings; for example 17 participants at SLSP2 representing 9 countries and 14 codes; 12 major cases were provided with a total of 134 subcases concerned with the topics of ion dynamics, broadening of Rydberg lines, plasma kinetics and lineshapes, Stark broadening, and stability and convergence of calculations.

#### Further activities on uncertainty assessment

In the area of uncertainty assessment the main focus is now on scattering calculations (more than on structure and spectra), and the main event is a workshop to be held in July 2014 at the Institute of Theoretical Atomic, Molecular and Optical Physics (ITAMP) at Harvard-Smithsonian Center for Astrophysics (CfA) in Cambridge, MA, USA. This meeting will bring together about 30 people who are working on electron collisions with atoms, ions, and molecules, heavy-particle collisions, and electronic structure of atoms and molecules. The objective is to come up with reasonable uncertainty estimates for calculations using the various methods of collision physics: perturbative, nonperturbative, time-independent, time-dependent, semi-classical, etc.. There will also be data users at the meeting, as well as some who manage databases. In addition to presentations (with good time for discussion) there will be topical sessions on electron-atom collisions (coordinated by K. Bartschat), electron-molecule collisions (coordinated by J. Tennyson) and heavy particle collisions (coordinated by D. Schultz). Further organizers are H. Sadeghpour and James F. Babb from ITAMP and H.-K. Chung and B. J. Braams from IAEA.

#### B. J. Braams: Review of Other Activities

#### Development of XML Schema for Atoms, Molecules and Solids (XSAMS)

XSAMS was developed by an international team with strong coordinating role by IAEA during 2003-2009 and version 0.1 of the Schema was released in Sep 2009. The project helped to inspire the creation of the Virtual Atomic and Molecular Data Centre (VAMDC): an EU Framework-7 infrastructure project with substantial funding that brought together ~20 partners and ~25 databases with the objective to create an interoperable database infrastructure. The interoperability refers to a common query language and a common format for transmission of query responses, all based on XSAMS. Besides, VAMDC provides automatic data discovery services (which databases can respond to a particular query) and keyword dictionaries. On top of the standards for the query language, data access protocols, dictionaries and registry VAMDC has developed a powerful web portal and desktop database access software to discover, download and visualize data. Further tools that rely on XSAMS and the VAMDC interfaces are being developed. Example: the SPECTCOL tool can be used to match spectroscopic and collisional data from different databases.

VAMDC has had the leadership role in development of XSAMS since 2010. There have been developments in all areas of the Schema since release 0.1, and especially the area of molecular spectroscopy has been thoroughly revised. The present stable XSAMS 1.0 agreed by the international XSAMS steering committee in February 2012 coincides with VAMDC XSAMS 1.0.

The Unit is very pleased with the success of VAMDC, which really grew out of activities coordinated by us in earlier years. At the present time Unit activities on XSAMS are rather low-key. We have the opportunity to provide a forum for further development of XSAMS outside the VAMDC domain; for example for particle-surface (plasma-material) interaction data. However, in practice we encourage adoption of XSAMS in fusion-oriented databases, including ALADDIN, and we are not looking now for expansion of XSAMS beyond the A+M domain.

#### **Events at International Centre for Theoretical Physics (ICTP)**

As was already reported at the IFRC Subcommittee meeting in 2012 the Unit organized the "Joint ICTP-IAEA Workshop on Fusion Plasma Modelling Using Atomic and Molecular Data", held at ICTP in Trieste, Italy, the week 23–27 January 2012. There were 4 main lecturers (D. Reiter, K. Nordlund, Yu. Ralchenko, H.-K. Chung), 6 further lecturers, and 20 participants, mainly at the level of advanced Ph.D. students or Post-Docs, but also some more senior researchers. Our perspective following that workshop is that the contact between plasma modellers, atomic and molecular physicists and materials modellers is valuable, but a future event at ICTP should be pitched at a more advanced level. It should also be advertised strongly to the fusion community.

We were successful with a proposal for a proper conference in 2014: The "Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices" is to be held 03-07 November 2014 at ICTP in Trieste. The conference will bring 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. So far we have had an excellent positive response; the ICTP name helps much and the conference announcement shows 34 well-known invited speakers. We expect 20-25 further participants by application.

For 2015 we have submitted a proposal to organize an "Advanced School on Modern Methods in Plasma Spectroscopy". The proposal is for a two-week event; the first week for advanced training in recent developments and results in the field and the second week for a conference that will stress application of advanced diagnostic methods to spectroscopy of fusion plasmas. Dr Yu. Ralchenko (NIST) is a co-Director of the proposed event. If the proposal is successful then the school and conference will bring together fusion and plasma scientists and experts in experimental and theoretical plasma spectroscopy. The meeting will allow for extensive discussions of practical application of advanced diagnostic methods to spectroscopy of fusion plasmas.

#### Meetings and duty travels in 2012-2014

For a list of meetings organized in 2012-2013 or planned in 2014 and a list of meetings attended and other duty travel please see Appendix 2. Here we just note some highlights.

The two Spectral Line Shapes in Plasmas (SLSP) code comparison workshops were described in the presentation on the Code Centres Network. The IAEA-NFRI Technical Meeting on Evaluation of Atomic, Molecular and Interaction Data for Fusion (4-7 Sep 2012, Daejeon, Korea) was described in the presentation on data evaluation. The past (2012) and planned (2014) ICTP events were described earlier in this section. Various RCMs were indicated in the presentation on Coordinated Research Projects.

An unusual meeting for the A+M Data Unit was the CM on "Auger Electron Emission Data Needs for Medical Applications" organized jointly with Nuclear Data Development Unit colleague R. Capote to explore work on data for Auger electron production in connection with internal radiotherapy applications. The meeting took place at IAEA on 9-10 May 2013 immediately after the Code Centres Network meeting and sharing some participants. The meeting was unusual because the topic is on the interface between atomic and nuclear physics.

The background to this meeting is the electron capture nuclear decay process,  $e+p \rightarrow n+v_e$ . An innershell electron is captured by the nucleus, leaving behind an inner-shell hole in the atomic structure. The nuclear process is followed by a cascade of emission of Auger electrons and photons. These low energy Auger electrons are of interest for precisely targeted radiation therapy and knowledge of the distribution of Auger electron energies is needed for simulations of damage. Meeting participants reviewed the status of data for this Auger emission process, made recommendations on data most needed and on worthwhile benchmark calculations, provided a compilation of references and experimental data, and motivation of new experiments especially on XFEL light sources.

The duty travel includes Unit participation in important A+M and PMI conferences and participation in ADAS and VAMDC events. There is also somewhat special twice-yearly travel by H.-K. Chung to

the USA in connection with her service on a proposal review panel for the Linac Coherent Light Source (LCLS) at Stanford, Palo Alto, California.

#### **Discussion on Priorities for Coordinated Research Projects**

The Subcommittee held extensive discussion about topics for future CRPs, leading to concrete recommendations for priorities in 2015 and the next (2016-2017) biennium. Recall the status at the time of the Subcommittee meeting in April 2012: the CRP on beryllium surfaces had been approved and the highest priority after that was agreed to be a CRP on irradiated tungsten. The Subcommittee had indicated 2 further CRP topics: plasma-material interaction with reduced-activation steel surfaces, and charge exchange processes involving neutral beams. In 2012 the Subcommittee had also considered a possible CRP on liquid metal surfaces, but had found the other mentioned CRP topics to be of higher priority.

The status in April 2014 is flexible and priorities are up for discussion. The irradiated tungsten CRP has started with a First RCM near the end of 2013. There is preliminary approval for a CRP on steel surfaces to start in 2015, but this is not yet a firm commitment.

The Subcommittee affirmed interest in CRPs on steel surfaces and on charge exchange processes, but before attempting a prioritization they reconsidered more closely a possible CRP on plasma interaction with liquid metal surfaces in view of the importance of the topic for possible fusion reactor application.

It was noted that there is plenty of diverse experimental work on liquid metals. Liquid lithium is the most important in present devices, but liquid tin, gallium and aluminum are also under consideration and are probably more relevant for a fusion reactor. Major experiments with liquid lithium have been done on T-11M, CDX-U, HT-7, FTU, NSTX and EAST among others.

Much of the research is on technological aspects of achieving a flowing liquid surface. There is not a good database of plasma-material interaction properties; certainly not for gallium and tin. On the one hand, therefore, there is a need for data on erosion (impurity production) at liquid surfaces and for tritium retention in those surfaces. On the other hand, at this time the technological issues are in the forefront, there is not yet much work on the precise plasma-material interaction properties, and it would probably be difficult to assemble a good CRP on the topic of plasma-material interaction properties for liquid metal surfaces, especially for the more reactor relevant materials of Ga, Sn, Al and some salts.

The Unit had assembled a list of recent conference contributions on plasma interaction with steel surfaces (Appendix 3) and it shows that there is much interest. Following the meeting a similar list was assembled for plasma interaction with liquid metal surfaces (Appendix 4). This list was therefore not directly discussed during the meeting, but it substantiates the sense that was obtained by the Subcommittee during the discussions: really the present interest in liquid metal surfaces is focused on technology. For plasma-material interaction properties there is much more interest in steel surfaces than in liquid metal surfaces.

Following this discussion the Subcommittee affirmed that at this time the topic of plasma interaction with steels has higher priority than that of plasma interaction with liquid surfaces. The Subcommittee also affirmed that plasma interaction with steels is a proper topic for a CRP: it will be possible to assemble a diverse group for a series of meetings devoted to quantification of erosion and tritium retention properties of reduced-activation steels that could be used as fusion wall material. Critical issues are erosion, tritium retention and tritium migration. The broad objective of a CRP on plasma interaction with steel surfaces would be to support an expert assessment of the extent to which steel could be used as plasma-facing material in a fusion nuclear environment. It is not expected that steel could be used in the regions of highest heat load, but the question is if steel can be suitable for the main wall.

The subcommittee recommends that the Unit looks at other ways, e.g. a Technical Meeting or Consultants' Meeting, to encourage coordinated work on data for plasma interaction with liquid metal surfaces. Such a meeting should emphasize reactor-relevant work on Ga and Sn and suitable compounds. The Subcommittee also discussed a possible future CRP in the area of atomic and molecular data. In that area the Subcommittee is convinced that a CRP on data for charge exchange processes in connection with heating and neutral beams is most appropriate. Primarily this CRP would be concerned with processes inside the fusion plasma. During the preparations for the CRP it needs to be reviewed if it makes sense to include also atomic and molecular processes relevant to production of the high-energy neutral beam; e.g. volume processes that produce or that neutralize a negative ion.

#### **Discussion on Other Meetings and Activities**

In the area of atomic and molecular processes the Unit has strongly emphasized the issue of data evaluation and uncertainty assessment. In the area of plasma-material interaction and related materials processes the emphasis continues to be the development of new data. The subcommittee agrees with this emphasis.

The subcommittee urges the Unit to proceed with the organization (presumably in cooperation with NFRI) of the large decadal (decennial) meeting on atomic, molecular and plasma-material interaction for fusion science and technology, following the earlier instances in Juelich (2002) and Cadarache (1992) and before that in Fontenay-aux-Roses (1980) and Culham (1976). The previous instances of this meeting have been very valuable in bringing together fusion energy researchers (modellers and diagnosticians) and researchers in atomic, molecular and materials science. The meeting should benefit both communities.

The subcommittee sees cooperation in the various code comparison workshops as an effective tool to build community that is interested in data. The subcommittee also appreciates the larger meetings organized by the Unit: one on data evaluation in Daejeon, Korea (2012), and one in preparation on uncertainty assessment in Cambridge, USA (2014).

In the area of plasma-material interaction the subcommittee has a special recommendation for an activity on plasma interaction with liquid metals with a view to reactor applications. As discussed, the subject is not the first priority for a CRP, but it is a good topic for a technical meeting. The focus at this meeting should be on plasma interaction with gallium and tin and relevant liquid salts in the context of future devices such as DEMO or an FNSF.

#### 3. Recommendations and Conclusions

The IFRC Subcommittee offers the following specific recommendations.

- 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.
- 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.
- 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.
- 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 scientists users of A+M+PMI data and atomic, molecular and materials scientists data producers.
- 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. 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.

- 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.
- 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.
- 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.

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. 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.

#### Appendix 1: Mission and General Activities of the Atomic and Molecular Data Unit

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 the end critical 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 and DEMO, and the fusion power plant.

#### Areas of emphasis

In our recent work and meetings we give new 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.

#### Active 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).

**Beryllium surfaces**: Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials (2012-2017).

**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 (planned for 2015-2020).

Please note the strong focus of our CRPs on topics connected to the problem of exhaust issues for fusion energy. 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.

#### Selected recent and planned 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.

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. We plan to cooperate again in the 3rd SLPS workshop in 2015.

In July 2014 the Unit works 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..

In November 2014 the Unit will organize the Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices at ICTP in Trieste. This conference will bring 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.

In December 2014 the Unit will organize in cooperation with National Fusion Research Institute (NFRI), Korea, the **Technical Meeting on Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology**, to be held in Daejeon, Korea. This approximately decennial meeting will bring 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, 2012-2013

(Much of the following was also presented in report INDC(NDS)-0662, "Report of the IAEA Nuclear Data Section to the International Nuclear Data Committee for the period January 2012 – December 2013", April 2014.)

#### **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 and meetings devoted to the development of XML standards for exchange of A+M and PMI data. Once every two to three years the Unit organizes a workshop addressed primarily to young researchers in the area of plasma modelling with use of A+M+PMI data, and at times the unit cooperates in more advanced workshops. In its work 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 Data Centre Network (DCN). The IFRC Subcommittee on Atomic and Molecular Data and the Data Centres Network 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 A+M Data Unit and are recommended data at the time of their compilation.

Several further numerical datasets that do not fit well into the ALADDIN framework are accessible through the A+M Data Unit 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).

In 2012-2013 a comprehensive collection of calculated data based on the Flexible Atomic Code (FAC) [Can. J. Phys. 86: 675-689 (2008)] was added 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). It is intended to integrate these FAC data with the FLYCHK code to support spectroscopic modelling of quasi-stationary multicomponent plasma.

#### **Bibliographic database**

AMBDAS, the Atomic and Molecular Bibliographic Data System, contains about 50,000 entries going back to the 1950s of articles and reports on atomic, molecular and particle-material or plasmasurface 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 2012-2013 the structure and spectra part of AMBDAS was updated with bibliographical data obtained from the NIST Atomic Spectra bibliographical databases.

#### 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 A+M 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 2012-2013.

#### **Coordinated Research Projects**

The A+M Data Unit has an active programme of CRPs. One CRP had its final Research Coordination Meeting (RCM) in 2012-2013, two CRPs had their second RCM in 2012-2013 and will meet again in the next biennium and two new CRPs had their first RCM in 2012-2013.

The CRP on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions held its third and final meeting in March 2013. This CRP is 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. Hydrogen isotopes constitute the fuel of fusion reactors, helium is the product of the fusion reaction, lithium is used for beam diagnostics and also as a wall material, beryllium is a wall material for JET and ITER, boron is used as a coating material in fusion vessels, carbon is often used in divertor target plates, nitrogen is used as a buffer gas and oxygen is a ubiquitous impurity. A final report is being prepared for publication in the IOP Journal of Physics: Conference Series.

The CRP on Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV had its second RCM in August 2012 and will meet again in 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 is to support the interpretation of spectroscopic measurements of tungsten in all regions of the plasma from the wall to the core.

The CRP on Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and their Isotopes in Fusion Plasma held its second RCM in July 2013. 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 first meeting in September 2012. 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 to be studied in the 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 will address 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 most recent CRP of the Unit is on Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices which had its first RCM in November 2013. 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 will be impacted the wrong way by the neutron fluence 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.

#### Data and Code Centre Networks and other meetings

The Data Centre Network (DCN) meets every two years to discuss data needs and coordinate activities. At their meeting in September 2013 at the IAEA in Vienna, participants discussed their activities on data development and data exchange, data evaluation and provision of recommended data, data exchange formats, bibliographical database maintenance, and priorities for new data development, evaluation and information exchange. These are all topics in which the data centres have a shared interest. Especially in the area of data evaluation there has been much new activity since the previous meeting of the DCN. The DCN meeting participants share a strong interest in systematic group evaluations of A+M collision data such as have been done recently in connection with the EU-funded EMOL project for electron scattering on several molecular targets and in meetings organized by NFRI specifically for electron-methane collisions.

The Code Centre Network (CCN) had its third meeting in May 2013 at the IAEA in Vienna. This meeting was coordinated with a meeting of the EMOL project, which met back-to-back with our CCN for their first evaluation, which was on electron-water molecule collision data. On one day participants of the EMOL group joined the CCN meeting to share the recommendations of the CCN meeting on uncertainty estimates of theoretical data and discuss data evaluation activities. The CCN meeting also benefited from interaction with nuclear data colleagues on the Unified Monte Carlo procedure for uncertainty assessment of nuclear cross section data. This CCN meeting made an inventory of many issues for provision of uncertainty estimates for calculated data, which vary between the type of target (atomic or molecular), the nature of the calculation (variety of computational methods) and the type of output that is considered (differential or integrated). The meeting is a part of an A+M Data Unit effort to develop community consensus on guidelines for uncertainty estimates for calculated scattering data. The CCN meeting also shared participants with the adjoining Consultancy Meeting on "Auger electron emission from nuclear decay: Data needs for medical applications", which is reported in Section 6.1.9.

Several other meetings were held on topics connected to data evaluation and uncertainty estimates. In February 2012 there was a Consultants' Meeting held at the National Institute for Fusion Science (NIFS) in Japan on procedures for evaluation of atomic, molecular and plasma-material interaction data for fusion. This CM was organized at NIFS because of strong evaluation activities in Korea and Japan. Five scientists from Korea attended, one from China and five from Japan. A related consultancy meeting was held in Vienna in June 2012 with 7 participants from fusion research, A+M data centres and A+M physics.

The "Joint IAEA-NFRI Technical Meeting on Data Evaluation for Atomic, Molecular and Plasma-Material Interaction Processes in Fusion" was held in September 2012 in Daejeon, Korea in conjunction with the one-day "8th International Symposium on Standard Reference Data" organized by the Korean Research Institute of Standards and Science (KRISS). This Technical Meeting attracted 27 participants from 11 countries. In addition to the presentations there were extended discussion sessions on 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. Invited papers from this TM have been published as a special issue of the journal Fusion Science and Technology. The Unit cooperated with the Weizmann Institute of Science in the organization of the First Spectral Line Shapes in Plasmas (SLSP) code comparison workshop in April 2012 and, due to its success, the Second SLSP code comparison workshop in August 2013, both meetings held in Vienna. These workshops followed the model of the well-established Non-local Thermodynamic Equilibrium code comparison workshops. The nature of the workshop is that 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. Line shapes are used in plasma diagnostics, hence our interest. Each of these meetings attracted about 20 participants.

#### **Development of XSAMS**

The "XML Schema for Atoms, Molecules and Solids" (XSAMS), developed under coordination by the A+M Data Unit, was adopted by the EU Framework-7 Virtual Atomic and Molecular Data Centre (VAMDC) project in 2010 and in the following years it became established for about 25 databases that participate in VAMDC. A Consultants Meeting on XSAMS was held in conjunction with a VAMDC project meeting on the Campus of the University of Vienna in February 2012. This meeting reviewed developments of XSAMS and agreed on a joint standard for the International and the VAMDC XSAMS version 1.0. At present, activities around XSAMS are concentrated on user tools and broader implementation. Further development of the Schema, for instance with respect to particle-surface interaction data, is not a priority.

#### ICTP workshop

The "ICTP-IAEA Joint Workshop on Fusion Plasma Modelling Using Atomic and Molecular Data" was held the week 23–27 January 2012 at the International Centre for Theoretical Physics (ICTP) in Miramare, Trieste, Italy. Earlier similar workshops were held in 2003 (1 week), 2006 (2 weeks) and 2009 (2 weeks). The 2012 workshop had 10 invited lecturers, 21 other participants, plus the director and the local organizer. The following countries and international organizations were represented (in brackets the total number if more than one): Algeria, Burundi, Cameroon, China (2), Finland, France (2), Germany (6), India (6), Italy (2), Japan, Kazakhstan, Pakistan, Tunisia (3), USA (2); IAEA (2), ICTP.

The aim of the workshop was to bring together plasma modellers that use atomic, molecular and plasma-material interaction (A+M+PMI) data in their work with researchers in the field of atomic, molecular or plasma-material interaction physics that produce relevant data. The workshop was addressed to early-career researchers, generally beyond the level of a Ph.D. that wanted to broaden their outlook with respect to plasma modelling and relevant A+ M+ PMI processes.

In principle four broad topics are in the domain of the workshop: plasma modelling, atomic processes and spectroscopy, molecular processes, and plasma-material interaction. Within the one-week slot it was not possible to do justice to all four topics and molecular processes received less coverage.

Lecturers D. Reiter, K. Ohya and B. Ziaja-Motyka presented plasma modelling, Yu. Ralchenko and H.-K. Chung presented computational procedures for atomic processes and spectroscopy, Yaming Zou/R. Hutton and J. Clementson described EBIT atomic data experiments, M. Telmini spoke on electron-molecule collisions and K. Nordlund, A. Allouche and P. Giannozzi presented plasma-material interaction processes. A poster session provided all participants the opportunity to present their research. The poster session was preceded by a session of 3-minute mini-talks for each participant to introduce his or her poster.

#### Meetings organized by us in 2012-2013

Joint ICTP-IAEA Workshop on Fusion Plasma Modelling using Atomic and Molecular Data (23-27 Jan 2012)

CM: Procedures for Evaluation of Atomic, Molecular and Plasma Material Interaction Data (7-9 Feb 2012, NIFS, Japan)

CM: XML Schema for Atoms, Molecules and Solids (20-22 Feb 2012)

Cooperation: First Spectral Line Shapes in Plasmas code comparison workshop (2-5 Apr 2012)

TM of IFRC Subcommittee on Atomic and Molecular Data for Fusion (26-27 Apr 2012)

CM: Development of a Recommended Library for Atomic, Molecular and Plasma-material Interaction Processes in Fusion (20-22 Jun 2012)

2RCM: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV (29-31 Aug 2012, Heidelberg)

Joint IAEA-NFRI Technical Meeting on Evaluation of Atomic, Molecular and Interaction Data for Fusion (4-7 Sep 2012, Daejeon, Korea)

1RCM: Erosion and Tritium Retention for Beryllium Plasma Facing Materials (26-28 Sep 2012)

3RCM: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions (20-22 Mar 2013)

TM of International Code Centre Network (6-8 May 2013)

CM: Auger Electron Emission from Nuclear Decay (9-10 May 2013, with Nuclear Data colleagues)

2RCM: Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium (3-5 Jul 2013)

Cooperation: Second Spectral Line Shapes in Plasmas code comparison workshop (5-9 Aug 2013)

TM of International Data Centre Network (4-6 Sep 2013)

1RCM: Plasma-wall Interaction of Irradiated Tungsten and Tungsten Alloys in Fusion Devices (26-28 Nov 2013)

#### Meetings planned for 2014

(Status of June 2014)

TM of IFRC Subcommittee on Atomic and Molecular Data for Fusion (28-29 Apr 2014)

Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data (7-9 Jul 2014)

2RCM: Erosion and Tritium Retention for Beryllium Plasma Facing Materials (18-19 Aug 2014)

CM: Plasma Interaction With Steel Surfaces (prepare CRP proposal) (20 Aug 2014)

Cooperation: 16th International Workshop on Radiative Properties of Hot Dense Matter (29 Sep - 03 Oct 2014)

3RCM: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV (planned for 6-8 Oct 2014)

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

Technical Meeting on Atomic and Plasma-Material Interaction Data for Fusion Science and Technology (15-19 Dec 2014, Daejeon, Korea)

#### Meetings attended and other duty travel in 2012-2013

Duty travels are sometimes at no cost or limited cost to the Agency. This applies in particular to the twice-yearly travel by H.-K. Chung to the USA in connection with her service on a proposal review panel for the Linac Coherent Light Source (LCLS) at Stanford, Palo Alto, California.

20th PSI, 21-25 May 2012, Aachen, Germany (HKC)

Workshop on Hydrogen Isotopes in Fusion Reactor Materials, 29-31 May 2012, Schloss Ringberg (BJB) (+ visit to IPP)

LCLS Proposal Review Panel, 1-2 Oct 2012, Palo Alto (HKC)

ICAMDATA Meeting, 1-4 Oct 2012, NIST (BJB)

ICAMDATA Meeting, 3-5 Oct 2012, NIST (HKC) (+ visit to NIST)

IFRC Meeting and start of FEC, 7-9 Oct 2012 San Diego (BJB)

Final annual meeting of VAMDC and Strategic Advisory Board meeting, 14-16 Nov 2012, Paris (BJB)

Workshop on Theory of Electron-Molecule Collisions for Astrophysics, Biophysics and Low Temperature Plasmas, 3-6 Dec 2012, Cambridge, USA (HKC)

Code Camp Workshop on Boundary Plasma Modelling, 6-8 Mar 2013, IPP Garching (BJB)

Seminar at ITAMP/CfA, 11-12 Mar 2013, Cambridge, USA (HKC)

LCLS Proposal Review Panel, 11-12 Mar 2013, Palo Alto (HKC)

14th International Conference on PFMC, 13-17 May 2013, Aachen (BJB)

7th International Workshop on Warm Dense Matter and 4th International Conference on High Energy Density Physics, 23-28 Jun 2013, Saint-Malo, France (HKC)

Data Evaluation for Electron Collisions with Methane, 24-28 Jun 2013, Daejeon (BJB) (+ visit to NFRI)

9th International Conference on Dissociative Recombination, 8-11 Jul 2013, Paris (BJB)

First Annual Meeting and Board Meeting of Sup@VAMDC, 23-25 Sep 2013, Milton Keynes, UK (BJB)

LCLS Proposal Review Panel, 23-24 Sep 2013, Palo Alto (HKC)

66th Annual Gaseous Electronics Conference, 30 Sep – 04 Oct 2013, Princeton (BJB)

18th International Conference on Atomic Processes in Plasmas, 7-10 Oct 2013, Auburn (BJB)

8th NLTE Code Comparison Workshop, 4-8 Nov 2013, Santa Fe (HKC)

Seminar at Center for Free-electron Laser Science (CFEL), 3-4 Dec 2013, Hamburg (HKC)

Seminar and discussions at Seoul National University, 16-17 Dec 2013 and 3-6 Jan 2014, Seoul (HKC)

#### Duty travel in early 2014

Flyfac cooperation at Weizmann Institute of Science (WIS) and Seminars at WIS, Soreq Institute and Hebrew University, 9-21 Mar 2014, Rehovot, Israel (HKC)

## Appendix 3: Recent Conference Activity on Plasma Interaction With Steel Surfaces

This information was assembled in connection with an intended proposal for a CRP on plasma interaction with reduced-activation steel surfaces in fusion devices. The intent is that the list includes presentations in which the emphasis is on plasma-material interaction or on tritium retention properties and excludes presentations on steel as a structural material.

## 14th International Conference on Plasma Facing Materials and Components for Fusion Applications (PFMC 2013), Jülich, 13-17 May 2013

Papers are in Physica Scripta: http://iopscience.iop.org/1402-4896/2014/T159.

#### Invited and oral contributions

C9 A. V. Spitsyn, A. V. Golubeva, M. Mayer, D. I. Cherkez, N. P. Bobyr, N. S. Klimov, Yu. M. Gasparyan, O. V. Ogorodnikova, V. Kh. Alimov, V. S. Efimov, A. Putrik, V. M. Chernov: Retention and Permeation of Deuterium in Low-activation Steels by Gas and Plasma Exposure

#### **Poster contributions**

A042 S. Korica, A. Manhard, T. Schwarz-Selinger, M. Siljegovic, A. Kalijadis and W. Jacob: Fe and Cr as Model Systems for Deuterium Retention Studies in EUROFER

A048 O. V. Ogorodnikova, K. Sugiyama, Yu. Gasparyan, V. Efimov: Deuterium retention in displacement damage produced by fast heavy ions in tungsten and Eurofer

A062 S. Lindig, A. Houben and T. Schwarz-Selinger: The Native Hydrogen Content in EUROFER97

A068 V. Kh. Alimov, Y. Hatano, K. Sugiyama, T. Höschen, M. Oyaidzu, J. Dorner, M. Fußeder, T. Yamanishi: Surface Modification and Deuterium Retention in Reduced Activation Ferritic Martensitic Steels Exposed to Low-Energy, High Flux D plasmas and D2 Gas

A120 A. Houben, F. Koch, and Ch. Linsmeier: Ceramic Coatings as Tritium Permeation Barriers on Eurofer97

## 16th International Conference on Fusion Reactor Materials (ICFRM 2013), Beijing, 20-26 Oct 2013

#### Plenary, invited and other talks

Farhad Tavassoli, CEA, France: Current status and recent research achievements in ferrit-ic/martensitic steels

Natalia Luzginova, NRG, Netherlands: An overview of 10 years of irradiation experiments on EU-ROFER 97 steel at high flux reactor in Petten

Takuya Yamamoto, UCSB, USA: In situ He injection and dual ion irradiation studies of reduced activation tempered martensitic steels and nanostructured ferritic alloys

Zhongwen Yao, QueensU, Canada: Radiation induced microstructures in austenitic ODS steels under dual-beam ions

Viacheslav Kuksenko, PSI, Switzerland: Nano-sized clusters formation in ferritic-martensitic steels under mixed proton-neutron irradiation

Jean-Louis Boutard, CEA, France: Oxide dispersion strengthened ferritic steels, a basic research joint program in France

Xu Wang, UM, USA: Microstructure analysis of ion beam irradiated CNSI and CNSII steels

Alexander V. Spitsyn, NRC KI, Russia: Retention of deuterium in damaged low-activation steel RUSFER (EK-181) after gas and plasma exposure

#### **Poster contributions**

16-110 Hui Zheng: The inhibition effect of low-temperature pre-irradiation of helium ions on the growth of helium bubble in 316L stainless steel: A Monte Carlo simulation

16-140 Dmitry Terentyev: Interaction of minor alloying elements with lattice defects in ferritic high-Cr steels: Ab initio study

16-162 Hongen Ge: Microstructure investigation on clam steel under H+/He+ dual-beam irradiation

16-234 Haishan Zhou: Plasma- and gas-driven hydrogen permeation through a reduced activation ferritic steel alloy F82H

16-248 Olga V. Ogorodnikova: Deuterium retention in reduced-activation ODS steels irradiated by 20 MeV W ions

16-281 Christiane Vieh: Pressure analysis of He-bubbles in He-implanted bcc and fcc steel

16-475 Naoko Ashikawa: Effects of helium bombardment on hydrogen retention in F82H steel

16-530 Chenyang Lu: Effects of helium ion implantation on the microstructure of two 9Cr ODS steels

16-537 Takuya Yamamoto: Modeling of helium effects on microstructural evolution in reduced activation tempered martensitic steels and nanostructured ferritic alloys: the effects of He/dpa, temperature, dose and dose rate

16-158 Chi Zhang: Microstructural evolution of nanocrystalline RAFM steel irradiated with helium ion

16-049 Djamel Kaoumi: Irradiation induced defect structures in two model F/M steels

16-116 Jihong Chen: Microstructure of reduced-activation martensitic steels irradiated by sequential He and Fe ions

16-211 Jinsung Jang: Irradiation induced microstructure evolution in ferritic and austenitic oxide dispersion strengthened steels

16-398 Qian Zhan: Effects of ion irradiation on microstructure of precipitates in China low activation martensitic steel

16-419 Weiwei Zhao: Research progress of tritium permeation barrier coatings on CLAM steel for CN DFLL-TBM

16-163 Yanhong Chang: Comparison between hydrogen and helium irradiation effects on both surface and bulk mechanical properties of 12Cr-ODS steel

16-255 Hui Zheng: The inhibition effect of low-temperature pre-irradiation of helium ions on the growth of helium bubble in 316L stainless steel: A Monte Carlo simulation

16-277 Inês Carvalho: Characterization of He implanted and neutron irradiated Eurofer97 steel

16-467 V.I. Zhurba: Step character of deuterium retention coefficient in austenitic stainless steel implanted at temperature~295K

#### 21st International Conference on Plasma Surface Interactions in Controlled Fusion Devices (PSI 2014)

Kanazawa, Japan, 26-30 May 2014.

#### Invited and oral contributions

O9 K. Sugiyama, J. Roth, V. Kh. Alimov, K. Schmid, M. Balden, S. Elgeti, F. Koch, T. Höschen, M. J. Baldwin, R. P. Doerner, H. Maier, W. Jacob: Erosion study of Fe-W mixed layer towards assessment of RAFM steel as plasma-facing material

#### Poster contributions (first author only)

P1-023 A. Hakola: Erosion of tungsten and steel in the main chamber of ASDEX Upgrade

P1-096 N. Yoshida: Retention and Desorption of Hydrogen and Helium from Stainless Steel Exposed to Plasmas of LHD

P2-005 N. Ashikawa: Effects of helium bombardment on hydrogen retention properties in F82H steel

P2-016 R. A. Pitts: Final case for a stainless steel Diagnostic First Wall on ITER

P2-026 T. Takizuka: Combination of helical ferritic-steel inserts and flux-tube-expansion divertor for the heat control in tokamak DEMO reactor

P3-020 M. Balden: Surface modifications of RAFM steels by deuterium exposure: Variation from coral-like/fuzz-like to blister-like features

P3-048 H. Zhou: Effects of surface conditions on the plasma-driven permeation behavior through a ferritic steel alloy observed in VEHICLE-1 and QUEST

## 12th International Workshop on Hydrogen Isotopes in Fusion Reactor Materials, Toyama, 2-6 June 2014

Yu. M. Gasparyan, I. M. Timofeev, V. S. Efimov, M. S. Zibrov, A. A. Pisarev: Effect of Surface Conditions on Deuterium Retention and Desorption in Ferritic-Martensitic Steels

Y. Hatano, V. Kh. Alimov, N. Yoshida, H. Watanabe, M. Oyaidzu, T. Hayashi: Surface Morphology of F82H Reduced Activation Ferritic/Martensitic Steel Exposed to High Flux Deuterium Plasma

V. Kh. Alimov, Y. Hatano, J. Roth, K. Sugiyama, M. Oyaidzu, M. Baldwin, R. Doerner, M. H. J. 't Hoen, H. T. Lee, Y. Ueda, M. Matsuyama, T. Hayashi: Deuterium Retention in Reduced Activation Ferritic Martensitic Steels Exposed to D Plasmas and Irradiated with D Ions

## Appendix 4: Recent Conference Activity on Plasma Interaction With Liquid Surfaces

This information was assembled subsequent to the IFRC Subcommittee meeting in order to clarify the breadth of activity that is relevant for a possible CRP on plasma interaction with liquid metal surfaces in fusion devices. The list includes any contribution in which the emphasis is on impurity production or hydrogen (tritium) retention, but also includes more general contributions on experience with liquid surfaces in fusion devices.

## 14th International Conference on Plasma Facing Materials and Components for Fusion Applications (PFMC 2013), Jülich, 13-17 May 2013

Papers are in Physica Scripta: http://iopscience.iop.org/1402-4896/2014/T159.

#### **Poster contributions**

A011 J.Ren et al.: First experiment of flowing Liquid Lithium Limiter in HT-7

A028 F. L. Tabarés et al.: Studies of H retention and LiH formation in liquid lithium in TJ-II and laboratory experiments

A133: J. W. Coenen et al.: Liquid Metals as alternative solutions for the Power Exhaust of Future Fusion Devices: Status and Perspective

A208 M. A. Jaworski et al.: Plasma-Facing Component Research on the National Spherical Torus Experiment–Upgrade (NSTX-U)

## 16th International Conference on Fusion Reactor Materials (ICFRM 2013), Beijing, 20-26 Oct 2013

#### **Poster contributions**

16-498 Irina Tazhibayeva: Effects of reactor irradiation on tritium and helium interaction with lithium-containing materials of fusion reactors

#### 21st International Conference on Plasma Surface Interactions in Controlled Fusion Devices (PSI 2014)

Kanazawa, Japan, 26-30 May 2014.

#### Invited and oral contributions

O12 I. Lyublinski, S. Mirnov, A. Vertkov: Lithium capillary-pore systems as solution of plasma facing materials problem for fusion reactors

#### Poster contributions (first author only)

P1-075 R. Majeski: Recent results from the Lithium Tokamak eXperiment (LTX)

P2-108 G.L. Jackson: Effect of lithium in the DIII-D SOL and plasma-facing surfaces

P2-109 J. Ren: Investigations on interactions between the flowing liquid lithium limiter and plasmas

P2-111 B. Unterberg: Plasma exposure of liquid tin targets in PSI-2 and TEXTOR

P3-014 M.A. Jaworski: High-temperature liquid lithium divertor targets: analysis and experiments in support of NSTX-U and next-step devices

P3-015 Y. Hirooka: The Present Status and Future Perspective of the Application of Liquid Metals as Plasma-Facing Materials in Magnetic Fusion Devices

P3-087 G. Mazzitelli: Experiments on FTU with an actively water cooled liquid lithium limiter

P3-106 F. L. Tabarés: Liquid Lithium Limiter biasing experiments in the TJ-II stellarator

## 12th International Workshop on Hydrogen Isotopes in Fusion Reactor Materials, Toyama, 2-6 June 2014

2-PM-1 S. Fukada, S. Sugie, K. Esaki, K. Hiyane, Y. Edao, E. Wakai, H. Kondo, Y. Itoh: Recovery of Hydrogen Isotopes from Liquid Li under Forced Convection Flow

2-PM-2 M. Shimada, R. J. Pawelko, K. Katayama, S. Fukada, T. Terai: Low Partial Pressure Tritium Permeation in Lead Lithium Eutectic

2-PM-3 B. Unterberg, J. W. Coenen, M. Freisinger, A. Kreter, V. Philipps, M. Reinhart, G. Sergienko, A. Terra, T. Wegener: Deuterium Retention in Liquid Tin after Exposure in the Linear Plasma Device PSI-2

2-PM-4 A. Nakamura, S. Fukada: Hydrogen Isotope Behavior in a Molten Salt

## Appendix 5: List of Participants of the 19th IFRC Subcommittee meeting

**Mr James W. DAVIS**, Institute for Aerospace Studies, University of Toronto, 4925 Dufferin Street, Toronto M3H ST6 Ontario, CANADA

**Mr Guang-Nan LUO**, Institute of Plasma Physics, Chinese Academy of Sciences, P.O. Box 1126, Hefei 230031, CHINA

**Mr Remy GUIRLET**, Association EURATOM-CEA, Centre d'Etudes Nucleaires de Cadarache, Saint-Paul-lez-Durance F-13108, FRANCE

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**Mr Alexander KUKUSHKIN**, National Research Centre "Kurchatov Institute", Kurchatov square 1, 123182 Moscow, RUSSIAN FEDERATION

**Ms Inga TOLSTIKHINA**, P.N. Lebedev Physical Institute, Leninskii pr. 53, 119991 Moscow, RUSSIAN FEDERATION

**Mr Klaus-Dieter ZASTROW**, Culham Centre for Fusion Energy (CCFE), Abingdon, OX14 3DB, UNITED KINGDOM

**Mr Joseph READER**, National Institute of Standards and Technology (NIST), 100 Bureau Drive, Gaithersburg, MD 20899-0001, UNITED STATES OF AMERICA

IAEA

Mr Bastiaan J. BRAAMS

Ms Hyun-Kyung CHUNG

#### **Appendix 6: Meeting Agenda**

#### Monday 28 April 2014

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

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

11:15 - 12:30: Review of Data Centre Network, databases and data evaluation; discussion. H.-K. Chung.

12:30 – 14:00: *Lunch* 

14:00 - 15:30: Review of Coordinated Research Projects; discussion. B. J. Braams.

16:00 - 17:15: Code Centre Network and Code Comparison Workshops; discussion. H.-K. Chung.

19:00 - ...: Social dinner

#### Tuesday 29 April 2014

09:00 - 10:30: Other activities (XSAMS, ICTP workshop, possible large A+M+PMI meeting); discussion. B. J. Braams.

11:00 - 12:30: Broad review and discussion. Activities on atomic, molecular and plasma-material interaction data activities worldwide. What is most needed? All.

12:30 – 14:00: *Lunch* 

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

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

17:00: Close of meeting

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