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INDC International Nuclear Data Committee

21st Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

3-4 May 2018

Prepared by

C. Hill and K. Heinola

IAEA Nuclear Data Section

May 2018

IAEA Nuclear Data Section

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Abstract

The 21st meeting of the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) was held on 3-4 May 2018 at IAEA Headquarters in Vienna, Austria. Activities of the Atomic and Molecular Data Unit for the period 2016–2018 were reviewed and recommendations were made for continuing activities in 2018–2020 and for possible new projects in the 2020–2021 budget cycle. The proceedings, conclusions and recommendations of the Sub-committee meeting are briefly described in this report.

May 2018

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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 3-4 May 2018 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 since the last meeting in April 2016 and discussed priorities for database development and evaluation, Coordinated Research Projects and Workshops, as well as the Unit's web presence and other planned activities.

The IFRC Subcommittee offers the following specific recommendations.

1. The Subcommittee was pleased to welcome the new professional staff of the unit: Dr Christian Hill as Unit Head, and Dr Kalle Heinola as the Unit's Atomic Physicist. The committee also acknowledged the contributions of the previous professional staff, Dr Bas Braams and Dr Hyun-Kyung Chung. It regrets that a long delay occurred between the former Unit head's retirement and the recruitment of the new one. This was compounded by the difficulty in recruiting the Atomic Physicist in the same period. The Subcommittee recommends that the recruitment procedure be adapted to avoid such a gap in the future.
2. The Subcommittee noted that only two CRPs are currently running, while it has always been around three in the past years. Whether this is due to the Unit understaffing is difficult to ascertain. Nevertheless, it should be expected that the preparation and operation of ITER together with nuclearisation of the field will increase the data needs. The Subcommittee thus recommends that the number of running CRPs at any given time be increased back to at least three to keep up with the issues raised as the fusion field goes forward.
3. The Subcommittee recommends that the pending publications concerning the closed CRPs be completed, even if it requires to involve new potential authors.
4. The AMD Unit should initiate a CRP on the topic of Vapour Shielding, focusing on the data needs for research into liquid metal walls. The CRP proposal should be based on the outcome of the Consultancy Meeting held on the topic in March 2018.
5. The Unit should consider initiating an activity to promote the generation, compilation and evaluation of spectroscopic data on the middle charge-states of tungsten, W^{10+} – W^{25+}. The domain of applicability of these data goes beyond vapour shielding, and could be the subject of a CRP, although a Technical Meeting may be considered in the first instance.
6. The scope for a CRP on the topic of hydrogen permeation in fusion-relevant materials should be investigated through a Consultancy Meeting. Such a CRP may not be initiated until Q1 2020, and would be a suitable follow-up to the currently ongoing Steel Surfaces CRP.
7. The AMD Unit's online presence should be updated to make it more accessible, attractive and useable. This should involve an improvement to its website and modernisation of its database services.
8. A database of classified images of dust generated in fusion devices, first planned in relation to the CRP on *Characterization of Size, Composition and Origins of Dust in Fusion Devices* should be completed and made available online.
9. The AMD Unit's cooperative Workshops with the ICTP, Mod-PMI and SLSP should continue.

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 unique position of the Unit to strengthen community ties, through CRPs, DCNs and CCNs among

others, between researchers from basic atomic, molecular and materials science, and researchers from fusion energy science is strongly acknowledged by the Subcommittee. Its members can only recommend that the Unit keeps its efforts and involvement at the level of or above the past few years and that the Agency provide the Unit with the means necessary to fulfil its missions.

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.

2. Meeting Proceedings: Summary of the last two years

Opening

Nuclear Data Section Head Dr Arjan Koning 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), the Ion Beam Analysis Nuclear Data Library (IBANDL), and the Experimental Nuclear Reaction Database (EXFOR).

Participants briefly introduced themselves. The Subcommittee member Dr Haishan Zhou represented the Chinese Academy of Sciences for Dr Guang-Nan Luo, who sent his apologies. The Secretary Christian Hill asked Dr James Davis to act as Chair for the present meeting and this was accepted by Dr Davis and by the Subcommittee.

C. Hill: General Report on Unit Activities

The Unit Head, Christian Hill, presented an overview of Unit activities and actions in the context of advice given by the IFRC Subcommittee at their 20th meeting, 25 – 26 April 2016. The following topics are covered.

- Staffing situation of the Unit
- Completed Coordinated Research Projects (CRPs) since 2016
- Currently active CRPs
- Databases and Data Services
    - ALADDIN (numerical database)
    - AMBDAS (bibliographical database)
    - Knowledge Base
    - GENIE Search Engine
    - Other data services: HEAVY, AAEXCITE, RATES, FLYCHK, LANL, GRASP2K
- Analytics for the AMD Unit's Website
- Data Centre Network
- Data Evaluation Activities
- Code Centre Network
- Crowdsourcing "Challenge" on molecular dynamics simulations
- Experimentalists Network
- Other meetings and workshops

Staffing situation of the Unit

An account was given of the staffing status of the Atomic and Molecular Data Unit. The current Unit Head, Christian Hill, was appointed in October 2017, with an Atomic Physicist, Kalle Heinola, joining the Unit in May 2018. The IAEA policy of rotating personnel was discussed: this policy means that there is usually a hard limit of seven years as a maximum duration of appointment. The present Scientific

Data Manager, Andras Vasaros, reached this limit in March 2018 but was granted an exceptional extension of 6 months to bridge the gap before the appointment of his successor. In connection with this, an advertisement for the position will run on the IAEA's Taleo system from 26 April to 10 June 2018. The appointed person will have experience in scientific programming and the skills and experience to effectively manage the Section's databases and server infrastructure.

The Unit also seeks to hire a Junior Professional Officer (JPO), consultant under a Special Service Agreement (SSA) or Personnel Service Agreement arrangement, or intern for the development an application for network distributed computing within its CascadesDB project (Molecular Dynamics simulations of radiation damage in materials). This appointment is subject to approval and funding from the Agency and is the subject of ongoing negotiation.

The Subcommittee is pleased to see that the Unit staff is back at its nominal level, after several months of understaffing due to regrettable delays in the recruitment of the Unit Head and of the associated Atomic Physicist. The Subcommittee stresses that the appropriate staffing of the Unit is necessary to ensure the progress of all the Unit's missions and the continuity of its work. It recommends that the preparation of the next recruitment campaign takes the past situation into account. The Subcommitttee acknowledges the need for a consultant or Junior Professional Officer (JPO) to work on the planned crowdsourcing activity on network-distributed computing and recommends that the Agency prepare actively the recruitment of this professional.

Completed Coordinated Research Projects (CRPs) since 2016

CRP F43019: Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma (2011 – 2016).

This CRP aimed to assemble, generate and evaluate derived data for collisional and radiative processes of H, H^+, H^-, He, He^+, He^{2+}, He^-, H_2, H_2^+, H_3^+, HeH^+, He_2^+ and their isotopic variants, resolved with respect to excited states, in a fusion plasma environment. As discussed at the previous IFRC Subcommittee meeting, the data evaluation component of the CRP was focused on state-resolved collisions of hydrogen alone. After the final RCM in March 2016, the final report was published in the form of the following four articles in the journal *Atoms*.

1. Celiberto, Roberto, Mario Capitelli, Gianpiero Colonna, Giuliano D'Ammando, Fabrizio Esposito, Ratko K. Janev, Vincenzo Laporta et al. "Elementary Processes and Kinetic Modeling for Hydrogen and Helium Plasmas." *Atoms* **5**, no. 2 (2017): 18. Online: https://doi.org/10.3390/atoms5020018.
2. Ayouz, Mehdi, and Viatcheslav Kokoouline. "Cross Sections and Rate Coefficients for Vibrational Excitation of HeH+ Molecule by Electron Impact." *Atoms* **4**, no. 4 (2016): 30. Online: https://doi.org/10.3390/atoms4040030.
3. Sawada, Keiji, and Motoshi Goto. "Rovibrationally Resolved Time-Dependent Collisional-Radiative Model of Molecular Hydrogen and Its Application to a Fusion Detached Plasma." *Atoms* **4**, no. 4 (2016): 29. Online: https://doi.org/10.3390/atoms4040029.
4. Wünderlich, Dirk, and Ursel Fantz. "Evaluation of State-Resolved Reaction Probabilities and Their Application in Population Models for He, H, and H_2." *Atoms* **4**, no. 4 (2016): 26. Online: https://doi.org/10.3390/atoms4040026.

Not all of the data produced and assessed in this CRP has been placed in ALADDIN yet: it would be desirable to complete this activity to make the evaluated data more accessible to users.

This CRP was evaluated in the Sixth Full Session of the Committee for Coordinated Research Activities – Nuclear Sciences and Applications (CCRA-NA) meeting of 19 October 2017.

CRP F43020: Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials (2011 – 2016).

The properties of beryllium as a first wall material exposed to plasma in a fusion reactor environment are of considerable interest: it will be used in the main chamber for ITER and has been installed and tested for the Joint European Torus (JET) experiment since 2011. This CRP was intended to enhance the knowledge base on fundamental particle-material interaction processes (in particular, sputtering by H, He and Be) involving beryllium in the fusion plasma environment.

The final RCM was held in June 2016, when it was agreed that the final report should take the form of a review article to be submitted to the journal *Nuclear Fusion*. Contributions to this article are still awaited from several participants and this is something the Unit continues to press for.

The Subcommittee stresses that although the CRP was a relatively small one, with seven institutions represented, the final report is a potentially important and useful document that should be published without further delay, even if at this point, alternative authors need to be found for parts of it.

CRP F43021: Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices (2013 – 2017).

Tungsten is foreseen as a plasma-facing material in a fusion reactor, which provides an intense neutron radiation environment. This large CRP was planned to enhance the knowledge base on effects of neutron and surrogate irradiation upon tungsten and tungsten alloy microstructure, and thereby upon surface erosion as well as trapping and transport of tritium in tungsten-based plasma-facing materials.

The Subcommittee confirmed the success of this CRP, which combined experimental and theoretical approaches to an important issue in fusion reactor design. A notable activity arranged as part of the CRP was a round robin exercise involving Thermal Desorption Spectrometry (TDS) studies of well-characterized, plasma-deposited tungsten specimens containing known concentrations of deuterium. 17 groups participated in the exercise (not all of them members of the CRP) and produced strikingly disparate result, which were discussed in some detail at the final RCM. A consultancy meeting was subsequently arranged in April 2018 and has led to the preparation of an article reviewing the exercise and outlining the best practices that should be applied to the TDS technique to ensure the highest accuracy.

A breakout meeting involving many of the participants in this CRP is planned to take place during the 23rd International Conference on Plasma Surface Interactions in Controlled Fusion Devices (PSI 2018) at Princeton University in June 2018. Future collaborations and other activities will be discussed, with a view to the possibility of a follow-up Technical Meeting being arranged at the IAEA in 2019. The Subcommittee noted that (especially for ITER) beryllium is equally important as a topic of study as tungsten, particularly as there is a paucity of high-quality data concerning this material.

The final report for this CRP is planned to take the form of a special edition of the IAEA-published journal *Atomic and Plasma-Material Interaction Data for Fusion* (APID). Regrettably, given the long lead-time for publication of editions of this journal series, only seven out of an anticipated 16 articles have been received from CRP participants, as of May 2018.

The Subcommittee recommends that the Unit keeps putting in effort on the publication of all anticipated articles as these will be a rich and timely knowledge basis particularly useful for the preparation of ITER and DEMO

Currently active CRPs

CRP F43022: Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices (2014 –).

Various kinds of reduced-activation steel are being considered as wall material for a fusion reactor, but not enough is known about plasma interaction, erosion and tritium retention in such steels. It is currently thought of as the preferred material for the first wall in the planned DEMO fusion reactor demonstration

experiment. This CRP is intended to enhance the knowledge base on erosion, tritium deposition and tritium migration processes involving different fusion-relevant (reduced activation) steels. The plasma-wall interaction processes include sputtering by H and He and plasma impurities, trapping of hydrogen (H, D, T) in surfaces exposed to plasma, transport of hydrogen in the steel and means to extract trapped tritium.

Since the second RCM, held in October 2017, two more groups have applied to join the CRP; subject to approval, it is anticipated that the final RCM will be held in Q1 or Q2 2019. A small breakout meeting at the 23rd International Conference on Plasma Surface Interactions in Controlled Fusion Devices (PSI 2018) in June 2018. As well as discussing plans and objectives for the final RCM, this will be an opportunity to monitor ongoing collaborative activities in steel sample exchange and comparisons.

CRP F43023: Data for Atomic Processes of Neutral Beams in Fusion Plasma (2017 –).

Neutral beam injection (NBI) is a standard method to heat the plasma in fusion experiments and it is intended to be used for power control in ITER and perhaps in a fusion reactor. NBI also has important diagnostic use, both via photon emission from the beam neutrals due to interaction with the plasma and via photon emission from plasma impurities after interaction with the beam. This new CRP is intended to provide evaluated and recommended data for the principal atomic processes relevant to heating and diagnostic neutral beams in fusion plasmas. The primary emphasis is on processes of hydrogen (H, D, T) neutral beams in the high temperature core plasma.

The first RCM was held in June 2017, at IAEA headquarters in Vienna, with thirteen participants from ten countries. Participants presented their current and future research plans, and discussed coordinated activities to produce and evaluate atomic data needed for neutral beam injection.

Two Code Comparison Workshops are planned to complement this CRP: one, on *Neutral Beam Penetration and Beam-based Photoemissions* is planned for the second half of 2018 and will bring together a relatively small (less than 10 or so) group of neutral beam modellers using a variety of atomic models, data and codes. A second, larger event is planned for 2019 on *Electron Dynamics in Atomic Collisions* to compare methods and implementations for computation of electronic transition rates for the electronic Schrödinger equation with a time-varying potential, with test cases drawn from the application domain of ion-atom and ion-molecule collisions. The Unit will seek to attach this Workshop to a conference or similar meeting in Europe in 2019, possibly the 25th International Symposium on Ion-Atom Collisions (ISIAC 2019) in Paris.

Databases and Data Services

The Unit Head reported on the status and usage of the various databases that the Unit maintains. A general observation by the Subcommittee was made that the Unit's website is not as useable, accessible or widely-known as it could be. In general, the user interfaces of the databases and public-facing informational content are poorly-presented, outdated, and require updating.

ALADDIN

ALADDIN (A Labelled Atomic Data INterface) is the Unit's principal numerical database. It stores and maintains *only* recommended and critically assessed (evaluated) numerical databases of atomic and molecular (A+M) collisional and radiative properties (cross sections, spectroscopic data), plasma-surface interactions (PSI) processes (such as physical sputtering, erosion, etc.) and bulk material properties (e.g. thermomechanical properties, particle diffusion, retention, etc.) for nuclear fusion research.

Data are mostly compiled from the IAEA APID series, published results of Coordinated Research Projects (CRP) and from consultancies arranged by the Unit. There are 25 952 entries in the database.

AMBDAS

AMBDAS (Atomic and Molecular Bibliographic Data System) is a bibliographic database of peer-reviewed articles presenting data on atomic, molecular and plasma-surface interactions for nuclear fusion research. Publications are searchable by reactant species (or surface), data category (collisional process, electronic structure property, plasma modelling application, spectral parameters, etc). Updates to the database occur at least twice a year, in particular with regular contributions from colleagues at NIST (atomic spectroscopy), NFRI and NIFS (collisional processes). There are 50 162 entries in AMBDAS as of May 2018.

The Unit Head raised the question of the usefulness of the International Bulletin, a PDF file listing new entries to AMBDAS that has, historically, been periodically published by the Unit.

The Subcommittee acknowledged that the number of users of the International Bulletin is probably small. Since its production is not overly onerous, the Subcommittee recommends that it continue for now, but this issue should be revisited in the future to ensure that the Bulletin serves some purpose.

Knowledge Base

The AMD Unit's wiki-style Knowledge Base is found at https://www-amdis.iaea.org/w/. Although originally intended to be a community effort with contributions from invited researchers and even members of the public, in practice since its inception in 2010 all content has been generated by the AMD Unit itself from INDC reports, APID editions, and presentations at our meetings. For security reasons, this remains the only way to edit and add to the Knowledge Base. It was noted that the list of conferences, workshops and other meetings in the area of atomic and molecular data for fusion research remains the most popular page on the site.

The Subcommittee regrets that direct contributions to the knowledge base by the public is not permitted by the Agency rules. Given the popularity of the conference and workshop page, it recommends that a more convenient way to maintain this list be developed. It is anticipated that this activity could form part of a more general overhaul of the Unit's website.

GENIE Search Engine

The GENIE (GENeral Internet search Engine [for Atomic Data]) is a web application providing access to 15 databases in the area of atomic data through a common search interface. Over time, this interface has not been maintained to reflect changes in the APIs of the databases it accesses and seems at present only to reliably query the ALADDIN database. The suggestion of previous IFRC meetings that GENIE be retired in favour of the VAMDC Portal infrastructure (https://portal.vamdc.eu/) was reaffirmed, and it is unlikely that further effort will be expended on this search engine when the Unit's website is updated.

Other Data Services

The Unit's website contains a further set of links to atomic and molecular data resources:

- HEAVY: cross sections for heavy particle collisions;
- AAEXCITE: electron impact cross section calculations using the "average approximation";
- RATES: effective ionization and recombination rate coefficients calculated with atomic physics and plasma modeling codes from Los Alamos National Laboratory, published in APID Vol. 11;
- FLYCHK: a simple and general modeling capability to generate atomic level populations and charge state distributions for low-Z to mid-Z elements under NLTE conditions;
- LANL: an interface to the Los Alamos atomic physics codes for calculation of atomic structure, electron impact excitation, as well as ionization processes. *This service has been unavailable for the first half of 2018 whilst the LANL servers it resides on undergo maintenance*;
- GRASP2K: a package of programs implements the fully relativistic multiconfiguration Dirac-Hartree-Fock method.

Analytics for the AMD Unit's Website

Statistics were presented on the number of sessions, page views and visitors' geographic locations for the AMD Unit's website over the period January 2014 – April 2018. The number of page views is typically 1 000 – 2 000 per week with an average number of page views per session of 2.11; these numbers have not changed appreciably over the last four years. It was speculated that many regular users may have bookmarked the page(s) they use most often. The Subcommittee agrees that the number of sessions, and their duration should be higher. One reason for the relatively low number of "hits" was thought to be the poor usability and "busy-ness" of the user interface. The largest number of sessions was assessed to be due to the registry of all the fusion-relevant conferences, workshops, and meetings (part of the Knowledge Base).

The Subcommittee supports the idea of updating the Unit's webpages making them more usable and attractive for the end users, and recommends that this should be a priority in the coming months.

Data Centre Network

The Data Centre Network (DCN) includes about ten national data centres for collection, critical assessment (evaluation) and partly for generation of atomic and molecular (A+M), particle surface interaction (PSI) and bulk material properties (plasma-material interaction - PMI) data for fusion and other applications.

The participating centres are ADAS (UK), CRAAMD (China), FZJ (Germany), QST (Japan), KAERI (Korea), Kurchatov (Russia), NFRI (Korea), NIFS (Japan) and NIST (USA).

The heads of the national A+M/PMI data centres, members of the A+M/PMI DCN, constitute a standing Advisory Group for advising the Agency on the technical aspects of A+M/PMI data exchange and processing. This Advisory Group holds regular meetings every two years for analysis, coordination and planning of all DCN activities.

The 24th meeting of the DCN Advisory Group was held from 4 – 6 September 2017 at IAEA Headquarters in Vienna. Priorities in data compilation and evaluation were discussed, these being considered to be:

- Sn^{q+} for liquid metal divertors, vapour shielding
- Transition probabilities for BeH, H_2, HD, etc. → H* + D, Be^{q+} etc.
- Runaway electron mitigation
- (With particular relevance to the potential use of nitrogen in plasmas at ITER): molecular data relating to NH_3, in particular high-temperature, high-resolution spectroscopy

The first of these relates closely to the proposed new CRP endorsed by the Subcommittee and discussed below. It was noted that, principally with respect to the modelling of plasma-material interactions for ITER, there continues to be a need for data on all properties of beryllium hydride. The spectroscopy of ammonia and other nitrogen-containing molecules was assigned a rather lower priority by the Subcommittee, since it is by no means certain that nitrogen will be a component of "killer pellets" in any tokamak and the data required lack broader applicability to fusion applications. This observation informs the ranking of potential future CRPs given below.

Two new research institutions were recommended as members of the DCN: the Comisión Nacional de Energía Atómica (CNEA) in Argentina, represented by Raúl Barrachina and Queen's University Belfast (QUB) in the UK, represented by Connor Ballance. Both are highly-respected institutions with ongoing research programmes in the production and evaluation of atomic and molecular data of relevance to plasma applications. The Subcommittee endorsed this expansion of the network.

Data Evaluation Activities

The AMD Unit remains committed to the promotion of uncertainty quantification and has arranged several consultancies and Technical Meetings on this topic over the last few years. Since the last IRFC Subcommittee meeting, the Unit has published an article, "Uncertainty estimates for theoretical atomic and molecular data" (H.-K. Chung et al., *J. Phys. D* **49**, 363002, 2016; doi: 10.1088/0022-3727/49/36/363002), providing a review and guide to best practices in Uncertainty Quantification. A large Technical Meeting on the topic was held at IAEA Headquarters in December 2016.

Smaller, ad hoc consultancies are also arranged on a regular basis to evaluate and recommend specific data sets, often those relating to ongoing or recently-completed CRPs.

Code Centre Network

The Code Centre Network (CCN) is a collaborative effort to gather and provide access to any information relevant for modelers in fusion plasma science. CCN participants meet to review the current status and research activities in computational tools related to atomic, molecular and plasma surface interaction (AM/PSI) data generation, and to co-ordinate these research activities in the form of a network accessible by the fusion research community.

The most recent CCN meeting was held at IAEA Headquarters from 16 – 17 November 2017 on the topic of molecular dynamics modelling of collisional cascades due to high-energy particle impact in materials of relevance to fusion reactor design. It was convened by Dr Andrea Sand (University of Helsinki) and Dr Sergei Dudarev (Culham Centre for Fusion Energy, UK) to discuss the format, data model and implementation of CascadesDB, a database of such molecular dynamics simulation results.

Work on implementing the software infrastructure for this database is ongoing in the Unit, and forms the basis of the initial crowdsourcing "challenge" described below.

Crowdsourcing "Challenge" on molecular dynamics simulations

On 26 April 2018 the AMD Unit opened a crowdsourcing "challenge" inviting interested members of the public (who need not be material scientists) to analyse and classify features of interest in a set of molecular dynamics simulations of the collisional cascade following the impact of a high-energy particle in either iron or tungsten. Both materials are of interest in the construction of the plasma-facing components of a future fusion reactor (tungsten will be used in the divertor design for ITER; steel is considered to be a likely candidate for the first wall of DEMO). Details of the challenge, which runs for eight weeks and will be judged in July 2018 are available at:

https://challenge.iaea.org/challenges/2018-NA-Mat-Fusion.

The precise nature of the software solution to the challenge is deliberately left open to invite as many novel approaches as possible, but may involve one or more of the following:

- Novel software for visualizing the material damage represented by the data files in a way that aids its qualitative and quantitative assessment.
- New software tools to rapidly and reliably identify, classify and quantify new patterns and structures of particular kinds in the data sets.
- Efficient algorithms to depict and summarise the statistical distribution of atom displacements and to analyse the effect of impact energy on this distribution.

It is envisaged that analysis techniques applied in the domains of tomography, medical imaging, protein crystallography, or computer vision may be applied in a modified form to address the Challenge.

Experimentalists Network

An account was given of plans for the establishment of an "Experimentalists Network" in the domain of atomic and molecular spectroscopic and collisional processes in plasmas for energies in the range 10 – 100 eV. A scientific committee is being established to coordinate an inaugural meeting, probably to be held at IAEA Headquarters in November 2018. The initial goal was to allow a focus on overlooked molecular processes at energies relevant to edge plasmas; this is a field in which many groups have moved on from fusion-relevant processes to those involving larger, bio-molecules, and it was deemed desirable to help coordinate the experimental work of researchers whose output can help benchmark theoretical studies for fusion plasma modelling.

The Subcommittee expressed some concern that the energy range being considered was unduly restrictive, and it was agreed that this assumption would be revisited by the scientific committee, with a view to increasing the upper energy limit to 10 keV.

Other meetings and workshops

The Unit Head gave a brief account of other meetings and workshops organized by the AMD Unit since the Subcommittee last met:

- 2016 Joint ICTP-CAS-IAEA School and Workshop on PMI in Fusion Devices (18 – 22 July 2017, Hefei)
- 2017 Joint ICTP-IAEA School on Atomic Processes in Plasmas (27 February – 3 March 2017, ICTP Trieste)
- 2017 Spectral Line Shapes in Plasmas (SLSP) Workshop (20 – 24 March 2017, Baden)
- 2018 Joint ICTP-IAEA School on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments (16 – 20 April 2018, ICTP Trieste)

The Unit is also in the process of renewing the Practical Arrangement between the IAEA and NFRI, Republic of Korea in the area of atomic and molecular data for fusion physics. This arrangement has proved mutually beneficial in the past and NFRI is a valuable contributor of data to the Unit's ALADDIN and AMBDAS databases.

Planning and Priorities for the Next Biennium

Discussions were held over the second day of the IFRC Subcommittee's meeting to recommend activities for the AMD Unit over the coming two years. This section describes the outcome of these discussions. A Gantt chart of the planned timetable for these events is given in Appendix B.

Coordinated Research Projects

The Subcommittee affirmed the importance of CRPs amongst the AMD Unit's activities and made several suggestions for future projects, which are described in decreasing order of priority below. It was commented that a target of 2 – 3 active CRPs running concurrently should be set (we currently have two active CRPs).

Vapour shielding

The AMD Unit held a consultancy meeting from 19 – 20 March 2018 to prepare a proposal for a CRP on Atomic Data for Vapour Shielding in Fusion Devices. This meeting identified two broad areas of interest: one relating to the data needs of liquid metal wall researchers and one focused on the collisional-radiative properties of tungsten plasmas in the vicinity of the divertor region of tokamaks such as ITER. Whilst there are some commonalities in the physics of these two areas, there is insufficient intersection between them that sufficient collaboration and cooperation could be sustained within a single CRP.

The recommendation was made by the Subcommittee that the originally-proposed Vapour Shielding CRP should be initiated with a focus on the data needs of the liquid metal walls community: this includes

- *Collision cross section data for neutral – H^+ systems;*
- *Collisional-radiative data for Sn;*
- *Data on the interactions of LiH and SnH_4 with plasma species;*
- *An assessment of surface chemistry effects on evaporation and sputtering of relevant materials.*

Data for medium charge-states of tungsten

In the context of plasma-tungsten interaction, the Vapour Shielding Consultancy Meeting identified a lack of radiative data on medium charge-states of tungsten, considered to be in the range W^{10+} - W^{25+}. In addition (as ever) dielectronic recombination (DR) rates are relevant to the modelling of tungsten plasmas but are hard to calculate and are frequently provided without reliable uncertainty estimations.

The impact of tungsten vapour opacity in transient shielding is unknown and should also be assessed in the validation of models of plasma-surface interaction.

The Subcommittee took the view that filling the gaps in these data for tungsten could form the basis of a CRP, but that it need not be restricted to the consideration of vapour shielding alone. In general, the transport of heavy elements in tokamaks is important, and the consideration of relevant atomic data, which includes spectroscopic properties of the medium charge-states of tungsten, is of relevance. Facilities such as low-energy EBITs could be requested to provide experimental data and benchmarking and validation of theoretical calculations. Although a CRP proposal could be written on the basis of the information provided by the Vapour Shielding Consultancy Meeting held in March 2018, there is also scope for an initial Technical Meeting, to be held in 2019 to explore the issue.

The timing of this proposed activity is timely, taking into account the intense activity focussed on the role of W as wall material in tokamak operation and performances at a number of fusion research facilities, including JET, ASDEX and WEST, in preparation of ITER.

Hydrogen permeation

The evaluation of the permeability and solubility of hydrogen and its isotopes in the range of materials considered for plasma-facing components of a fusion reactor is a key issue concerning safety, fuelling and reliability. The Subcommittee proposed that a CRP focusing on this issue would be a suitable, timely and relevant activity for the Unit to initiate over the next 12 months or so. Such a CRP has an obvious connection to present, active projects such as the Steel Surfaces CRP described above, and the AMD Unit is well-placed to assist in the coordination of the necessary experimental and theoretical studies in a way that is difficult to otherwise achieve on an international scale.

Molecular spectroscopy of nitrogen-containing species

The behaviour of nitrogen-containing molecules in the subdivertor and pump regions of ITER is currently the subject of great interest. The production of ammonia, in particular, potentially creates a major hazard with respect to the tritium inventory of the device, to the extent that nitrogen may need to be entirely excluded from the ITER vacuum chamber.

An AMD Unit activity relating to filling the gaps in molecular spectroscopy relevant to experimental fusion reactors could be considered, but would need to focus on a subset of the possible species to be manageable. Consideration of nitrogen-containing species only runs the risk that the CRPs findings become irrelevant if nitrogen is simply never used in fusion experiments. However, it is noted, that an accidental air leak into the ITER vacuum vessel could lead to the production of nitrogen-containing compounds, resulting in some safety concerns. Further consultation on the issue with relevant researchers is encouraged with a view to assessing the scope for a future Unit activity in this area.

Website and online databases

The Subcommittee strongly recommends that the Unit's website be updated and its usability and accessibility improved. It was acknowledged that there are security implications to the implementation of online databases, but it is hoped that the Unit can work constructively with the relevant IAEA Division to facilitate these improvements.

ICTP Workshops

Over the last few years, the AMD Unit has co-organised, with the International Centre for Theoretical Physics (ICTP), Trieste, an annual week-long event intended to provide training and information exchange for computational scientists working on models and data for atomic, molecular and materials processes relevant to fusion energy research, industrial plasmas, laser-produced plasmas, and warm and hot dense matter. The training is aimed at advanced Ph.D. students, post-doctoral students and other early-career researchers, and the information exchange has spanned several disciplines: from

molecules to materials and from method developments to data treatments. Topics related to energetic events and electronic excited states are emphasized throughout the programme. The schedule typically features lectures by international experts, invited and contributed research talks, posters and discussion sessions, with good time available for personal interaction.

The Subcommittee reviewed the topics of the last two ICTP Workshops and endorsed plans for the two proposed for 2019 (atomic spectroscopy in plasmas) and 2020 (on the topic of plasma-material interaction).

Dust Database

Past experience with tokamaks such as TFTR and JET has shown that significant amounts of dust are formed in these machines. Accumulation of dust can become a significant safety hazard due to flammability, toxicity, potential respiratory problems and radiation concerns with tritium. Furthermore, a significant uptake of hydrogen isotopes occurs in dust, making the transport behaviour of this material a significant factor in tritium inventory studies of next generation machines such as ITER and DEMO.

The Unit came close to implementing a database of analysed images of dust as an outcome of its CRP *Characterization of Size, Composition and Origins of Dust in Fusion Devices* (2008 - 2011), but it was never completed because of the promotion of one of the key developers.

The Subcommittee noted that this CRP was carried out at a time when JET had a graphite wall, leading to a large amount (~ 450 g) of dust over its campaigns, and that the newer ITER-like Wall (ILW) has generated much less dust (~ 1 g). However, there is continuing interest in the analysis of dust within the ITER organization and the Subcommittee encourages the AMD Unit to complete the deployment of this database.

Other Activities

Distributed Computing

A longer-term crowdsourcing project, to develop a downloadable app allowing members of the public to carry out molecular dynamics simulations of radiation damage in fusion reactor materials on their own devices has been proposed. The app would allow the harnessing of a distributed network of volunteer computing capacity to carry out large-scale modelling of fusion-relevant processes in parallel and at low cost.

At the Code Centre Network meeting on Collisional Cascades in November 2017, a presentation was given by an invited consultant, David Wallom, about the feasibility of this project: the conclusion was that it would require 12-18 months of development time for a full-time researcher at post-doc level, and that this development would need to take place at a suitable institution such as the Oxford University e-Research Centre. There are major issues of online security and database integrity to be resolved with the IAEA's MT-IT division before such an app can be deployed, and funding needs to be obtained to second a consultant or Junior Professional Officer (JPO) for its development, but the Unit will continue to explore avenues to advance this project.

ICAMDATA

It was noted that the Unit Head had been invited to join the International Advisory Board of the International Conference on Atomic and Molecular Data and Their Applications (ICAMDATA) conference in 2018, to be held in Cambridge MA, USA this year, which he will attend as an invited speaker.

Assigning DOIs to IAEA publications

The Unit has taken a long-standing interest in the attempts being made by the IAEA's Publishing Section to allow Document Object Identifiers (DOIs) to be assigned to IAEA publications. This would greatly increase the accessibility and relevance of the Agency's grey literature, but implementation of an agreement with the International DOI Foundation (IDF), the governance body of the DOI system, has been snarled up due to objections from the IAEA's Office of Legal Affairs (OLA).

The Unit will continue working with the Publishing Section on this issue, where possible.

Appendix A: 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, electron-atom (ion) and atom-atom ("heavy particle") 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 **data dissemination** (database maintenance). 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 fusion 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 the construction of ITER. However, other experimental fusion devices are also being developed by national agencies, multinational collaborations and commercial entities, all of whom have data needs that can be met by the work of the Agency.

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 contribute to 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, and a wiki-style **Knowledge base**.

Active and recently-completed CRPs

Beryllium surfaces: Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials (2012-2016).

Irradiated tungsten: Plasma-wall interaction for irradiated tungsten and tungsten alloys in fusion devices (2013-2017).

Steel surfaces: Plasma-wall interaction with reduced-activation steel surfaces (initiated 2015).

Neutral beams: Data for Atomic Processes of Neutral Beams in Fusion Plasma (initiated 2017).

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.

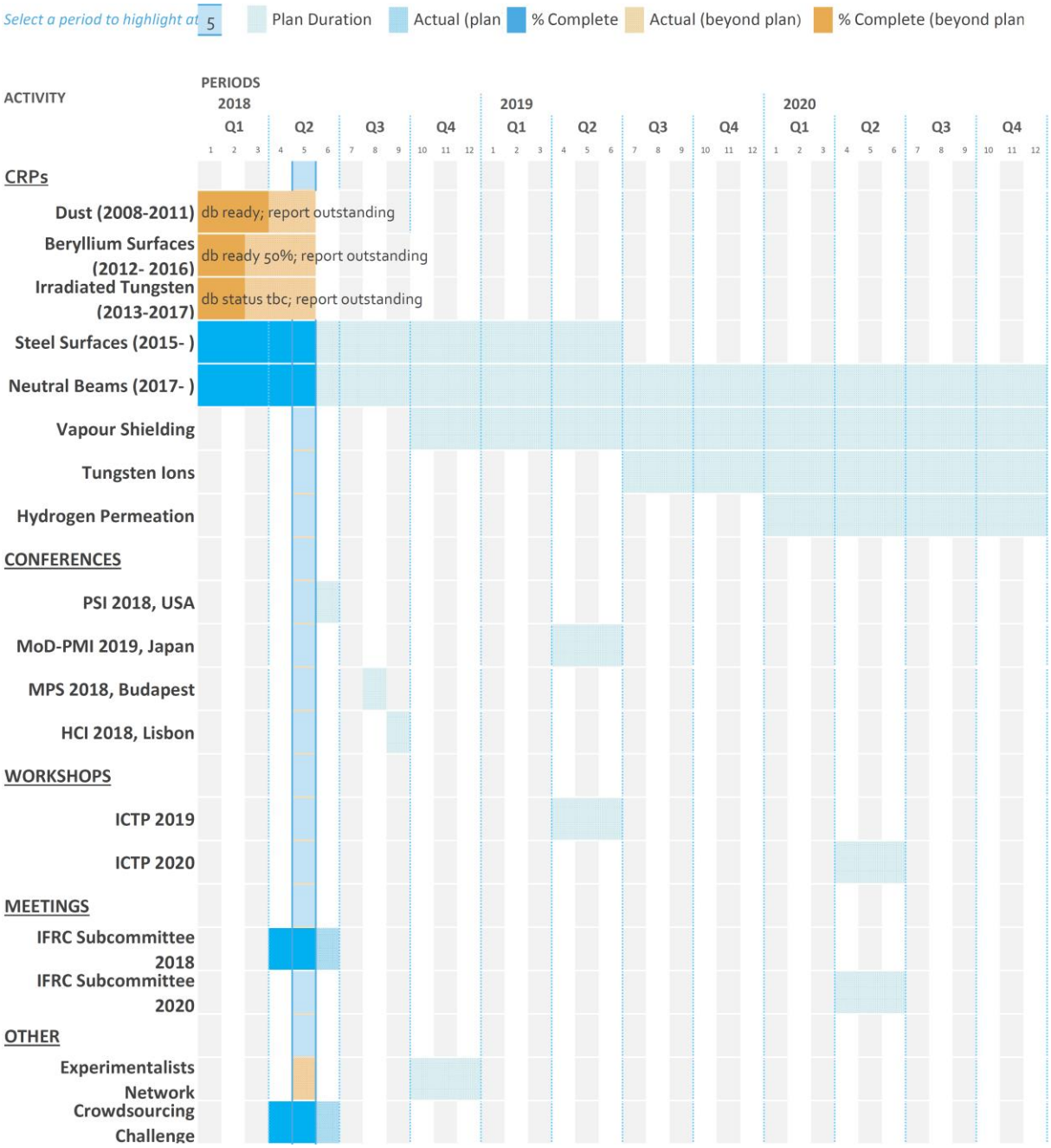
The new **A+M Code Centre Network** meets approximately every two years to review issues related to codes that are shared between the A+M+PMI and the fusion communities. Meetings have a focus topic and involve a subset of the network. In 2017 the meeting focussed on molecular dynamics modelling of collisional cascades.

The Unit has cooperated in several code comparison workshops: it continues to assist in the organisation of the **Mod-PMI** and **Spectral Line Shapes in Plasmas (SLSP) code comparison workshops**, which are held outside Vienna on an approximately biennial timetable.

The Unit organised a large Technical Meeting on **Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications** at IAEA Headquarters in December 2016.

An inaugural meeting of the **Experimentalists Network**, focusing on atomic and molecular spectroscopic and collisional processes in plasmas is planned for November 2018.

Appendix B: Timeline of future AMD Unit Activities



Appendix C: List of Participants of the 21st IFRC Subcommittee meeting

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

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IAEA

Mr Christian HILL

Mr Kalle HEINOLA

Appendix D: Meeting Agenda

Thursday 3 May 2018

10:00 – 10:15: Welcome, introduction of participants, election of a Chair. A. J. Koning and C. Hill.

10:15 - 11:15: General report on activities; discussion.

11:30 - 12:30: Review of Data Centre Network (DCN), databases and data evaluation; discussion.

12:30 – 14:00: ***Lunch***

14:00 - 15:30: Review of Coordinated Research Projects (CRPs); discussion.

16:00 - 17:15: Code Centre Network (CCN) and Code Comparison Workshops (CCW); discussion.

19:00: ***Social dinner***

Friday 4 May 2018

09:00 - 10:30: Other activities (ICTP workshop, Collisional Cascades "Challenge", other meetings); discussion.

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

12:30 – 14:00: ***Lunch***

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

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

17:00: ***Close of meeting***

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