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IFRC Subcommittee on Atomic and Molecular Data for Fusion: Report on the Activities of the Atomic and Molecular Data Unit, May 2018 – June 2021

Prepared by

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February 2022

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ABSTRACT

This report details the activities of the Atomic and Molecular Data Unit in the Nuclear Data Section of the IAEA during the period May 2018 – June 2021. The COVID-19 pandemic prohibited the usual biennial meeting of the International Fusion Research Council (IFRC) Subcommittee on Atomic and Molecular Data and an interim report covering the period May 2018 – April 2020 was distributed to committee members and discussed at an online meeting in May 2020. The present report incorporates the material from that interim report and describes the further Virtual Meeting of the IFRC Subcommittee which was held from 14 – 15 June 2021.

February 2022

Table of Contents

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 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.

The 22nd Meeting of the Subcommittee was scheduled to be held from 7 – 8 May 2020. However, travel restrictions imposed in response to the global COVID-19 pandemic prohibited an in-person meeting. Therefore, an interim report was prepared and discussed at an online meeting held on 9 July 2020.

It was hoped that a full, in person meeting of the Subcommittee could be held in 2021, but continuing pandemic conditions prevented this and a virtual meeting was arranged for 14 – 15 June 2021 to discuss activities since July 2020 and to set priorities for the coming biennium. This report documents both that meeting and the earlier interim meeting, and provides a record of the projects and activities of the Atomic and Molecular Data (AMD) Unit since May 2018. A regular, in-cycle meeting of the Subcommittee is planned for spring or early-summer 2022.

This report is divided into sections describing:

- Staffing and other administrative matters concerning the AMD Unit;
- The status of completed and ongoing Coordinated Research Projects (CRPs);
- Activities relating to data evaluation, data provision and standards recommendations in the Unit;
- Reports of discussions concerning the Data Centres Network (DCN), Code Centres Network (CCN), Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP) and other Technical Meetings;
- Training workshops planned at the Abdus Salam International Centre for Theoretical Physics (ICTP) – two confirmed workshops for 2021 will be held as virtual events;
- An account of the crowdsourcing activity on radiation damage in nuclear materials;
- The new AMD Unit website and related data services;
- Duty travel undertaken by Unit staff;
- A list of publications produced by the Unit staff members;
- Cooperations and other activities;
- A summary of planned activities for the current biennium, 2020–21.

2. Staffing and Administrative Issues

Since the previous meeting, the AMD Unit has continued to operate with its full complement of staff. The roles of the Unit members are as follows:

Christian Hill	Unit Head
Kalle Heinola	Atomic Physicist
Ludmila Marian	Scientific Data Manager*
Marco Verpelli	Nuclear Data Analyst/Programmer*

* The duties and responsibilities of these roles are shared with other Units in the Nuclear Data Section.

The Unit was granted a significant proportion of its unspent funds from 2020 in the form of a budget carry-over to 2021, and at the time of writing is engaged in appointing a one-year Special Service Agreement (SSA) consultant at the P3-level to work in the area of atomic and molecular data evaluation with a focus on providing improved data services. It is anticipated that the appointed individual will be in post from the summer of 2021.

Two further home-based consultancies have been granted to work on:

(a) extending the functionality of the DefectDB database of DFT calculations of radiation-induced defects in nuclear materials (10 days until 31 July); and
(b) on improving the data model behind the ALADDIN database of evaluated collisional cross sections for plasma processes (63 days until 31 October).

Further home-based consultancies are planned for the future as the AMD Unit aims to meet its programmatic objectives in the absence of its regular, in-person technical and consultancy meetings and Duty Travel-related activities.

3. Coordinated Research Projects

F43020: Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials

Beryllium is an attractive candidate for the first wall of an experimental magnetic confinement nuclear fusion device because of its high conductivity, low activation and favourable properties as a plasma impurity. Although it is not envisioned for extensive use in the plasma-facing components of future commercial power reactors, it is the material used in the ITER experimental device and has been deployed and tested in the JET ITER-Like Wall (ILW) project [1].

The CRP F43020: *Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials* aimed to enhance the global knowledge base on fundamental particle–material interaction processes involving beryllium in the fusion plasma environment, in particular physical and chemical sputtering by H, He and Be; the transport of hydrogen in beryllium; and the means to extract trapped tritium. It ran from 2012 – 2016 and involved six fusion research laboratories and university departments from five Member States. Three Research Coordination Meetings (RCMs) were held over the course of the project; details and links to the meeting reports are available on the AMD Unit's website (https://amdis.iaea.org/CRP/beryllium-surfaces).

A final report of the CRP in the form of a review article has now been published in the journal *Nuclear Materials and Energy* [1]. The project will be formally closed through the IAEA's CRP evaluation procedures at the earliest opportunity.

[1] G. De Temmerman, K. Heinola, D. Borodin, S. Brezinsek, R. P. Doerner, M. Rubel, E. Fortuna-Zaleśna, C. Linsmeier, D. Nishijima, K. Nordlund, M. Probst, J. Romazanov, E. Safi, T. Schwarz-Selinger, A. Widdowson, B. J. Braams, H.-K. Chung, C. Hill, "Data on erosion and hydrogen fuel retention in Beryllium plasma-facing materials", *Nuclear Materials and Energy* **27**, 100994 (2021).

F43022: Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices

Various kinds of reduced-activation steel are being considered as wall material for a fusion reactor, such as the planned DEMO demonstration power plant. However, not enough is known about plasma interaction, erosion and tritium retention in such steels. This CRP aims to enhance the knowledge base and develop new databases on the interaction of fusion plasma with the reduced-activation steel alloys that are being considered for constructing the plasma-facing components of a fusion reactor. It seeks to quantify the erosion due to exposure to plasma and to determine the retention and transport properties of tritium in the surface.

At the third RCM, a further activity, Comparison Experiment for the Sputtering of Steel (CESS), was initiated, which is being coordinated by Dr. habil. Wolfgang Jacob at the Max Planck Institute for Plasma Physics, Garching, Germany. Its aim is to compare sputtering yields in different experimental devices: as far as possible, identical samples (with comparable histories) will be exposed to deuterium plasma or ion irradiation under comparable exposure conditions and analysed by a range of techniques including (but not limited to) Mass loss, Scanning Electron Microscopy (SEM), and Thermal Desorption Spectroscopy (TDS). More details, including a list of participants, the distribution of steel samples and sample preparation techniques are available on the AMD Unit website at https://amdis.iaea.org/workshops/cess.

It is anticipated that the results of this CRP will be presented in a final report, possibly in the form of a review article or "special topic", to be submitted to the journal *Nuclear Fusion*.

Preparation of this article will begin after the conclusion of the CESS exercise, which has been delayed by the ongoing COVID-19 pandemic. The scope remains for a small Consultancy Meeting to be arranged in Vienna in late 2021 or early 2022 to plan and coordinate the preparation of this report and dissemination of the CRP results.

F43023: Data for Atomic Processes of Neutral Beams in Fusion Plasma

Neutral beam injection is a standard method to heat the plasma in fusion experiments also has important diagnostic uses. Modelling of beam penetration into the plasma and of photoemission signals relies on detailed data for atomic processes. There are quite significant gaps in these data and the data that are available are often of uncertain quality. This CRP aims 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 and second RCMs were held in Vienna in 2017 and 2019, respectively; the third meeting was due to be held in late 2020 but was postponed to November 2021 by the COVID pandemic, which prevented the completion of calculations for its two code comparison exercises (described below). There are 11 participants from 10 Member States engaged in both the calculation of fundamental atomic collisional data and its application in neutral beam modelling codes.

Two code comparison exercises are associated with the Neutral Beams CRP. The first took the form of a workshop, held at the Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI) in Debrecen, Hungary from 26 – 28 August 2019. It was conceived in order to assess the sensitivity of predictions of hydrogen beam penetration and of beam emissions in relevant fusion plasma conditions to different modelling codes and uncertainties in atomic data. Test cases were shared in advance with the eight participating research groups, which involved H, D, He, and (optionally) Li and Na, at beam energies of 30, 100 and 1000 keV and plasma conditions representative of those present in fusion devices. The results were compared at the August workshop, with most participants presenting remotely. Although it was felt that more time would be needed to fully analyse the results of the simulations carried out, some useful comparisons were made. Work continues with a view to revisit the topic in a session at the third RCM at the end of 2021. More details are available at https://amdis.iaea.org/workshops/neutral-beam-penetration-and-photoemission.

The second code comparison activity was initiated at the second RCM in February 2019; over the course of the year, participants have been producing calculated, state-resolved cross sections for the process $Be^{4+} + H(nl)$ using the following computational methods:

- Semi-classical Molecular Orbital (SC MO) close-coupling
- Classical Trajectory Monte Carlo (CTMC)
- Semi-classical Basis Generator Method (BGM) close-coupling
- Convergent Close-Coupling (CCC)
- Semi-classical Atomic Orbital (SC AO) close-coupling

Three projectile energies: 20, 100 and 500 keV/u are to be considered; these are chosen to be of relevance to fusion plasmas and overlap the typical validity range of the selected theoretical methods. The hydrogen target is considered in the ground state (1s) and excited states 2s, $2p_m$ ($m = 0, \pm 1$). The aim is to produce and compare data for a collision system in order to evaluate and assess these methods and to estimate the typical accuracy of the calculated cross sections for:

- Total electron capture
- Total ionization
- Total excitation
- State-selective processes (for the dominant channels).

Comparison of the results of these calculations will occur throughout 2021 for discussion at the third RCM, planned as an in-person meeting from 24 – 26 November 2021. More details are available at https://amdis.iaea.org/workshops/atomic-collisions-ccw.

F43024: Atomic Data for Vapour Shielding in Fusion Devices

In the course of a fusion device or reactor operation, energy is deposited onto the walls through small or large bursts known as plasma edge-localized modes (ELMs) and plasma disruptions. Depending on plasma conditions and on the wall material these ELMs and disruptions can lead to evaporation or ablation, potentially causing significant damage to plasma-facing components.

When wall material is rapidly evaporated or ablated a dense expanding plasma cloud may be formed in front of the surface. In this dense plasma the incoming energy may largely be converted from fast particle kinetic energy into radiation energy, and gradient effects may cause this radiation to be directed away from the wall back into the plasma. This conversion of energy into radiation largely directed away from the material wall is referred to as vapour shielding. The reduction in energy to the surface can be very large; much larger than a simple factor of two that would be expected for isotropic emission of radiation. Continuous vapour shielding has been demonstrated to reduce the heat flux to surfaces coated with liquid metals, such as lithium (Li) and tin (Sn), and their mixtures. Atomic data is needed to simulate the vapour shielding processes as well as to interpret spectroscopic measurements when vapour shielding is happening, either in transient or steady-state plasma conditions of a fusion device.

The participants in this CRP are engaged in the theory and modelling of plasma and vapour particle collisional processes, and of experiments of spectral line properties, vapour formation and spectral analyses. The CRP is organized to provide evaluated and recommended data for the principal atomic and molecular processes relevant to vapour formation, and data related to the elemental processes affecting the vapour shielding phenomenon. The primary emphasis is on interactions of hydrogen (H, D, T) with the liquid metal particles being ejected from Li and Sn targets.

Nine research institutions from nine Member States were awarded Research Agreements or Research Contracts at the start of the project. Unfortunately, the Macedonian Academy of Sciences and Arts (MASA) withdrew from the CRP after the death of the Chief Scientific Investigator, Dr Ratko Janev. Dr Janev was an eminent atomic physicist and served as Head of the Atomic and Molecular Data Unit for more than a decade from 1986.

The second RCM took place as a virtual event from 7 – 9 Oct 2020 and was attended by 10 participants from 8 Member States. In addition to a review of past and ongoing research activities, priorities for future work were agreed and work plans for the next 18 months outlined. Data produced as part of this CRP that have already been deposited in the AMD Unit's data libraries include:

- Heavy particle collisional processes:
  - p + $Be^{1,3+}$ and p + Li (AOCC, MOCC)
  - p + H (CCC)
- Electron-molecule collisional processes:
  - e + LiH, e + Li_2

Ten peer-reviewed articles in direct connection with this CRP have been published in the scientific literature[1-10].
More details and a meeting report[11] are available at https://amdis.iaea.org/meetings/vapour-shielding-rcm2/.

[1] I. B. Abdurakhmanov, C. Plowman, A. S. Kadyrov, I. Brayand A. M. Mukhamedzhanov, "One-center close-coupling approximation to two-center rearrangement collisions", *J. Phys. B: At. Mol. Opt. Phys.* **53**, 145201 (2020).

[2] R. Celiberto, R. K. Janev, A. Laricchiuta, "Electron-impact state-to-state cross sections and rate coefficients for X(v)→A(v') excitation of LiH molecule", *Plasma Sources Sci. Technol.* **29**, 035008 (2020).

[3] Z. Bouza, J. Scheers, A. Ryabtsev, R. Schupp, L. Behnke, C. Schah, J. Sheil, M. Bayraktar, J. R. Crespo López-Urrutia, W. Ubachs, R. Hoekstra, O. O. Versolato, "EUV spectroscopy of Sn^{5+} - Sn^{10+} ions in an electron beam ion trap and laser-produced plasmas", *J. Phys. B: At. Mol. Opt. Phys.* **53**, 195001 (2020).

[4] J. Scheers, C. Shah, A. Ryabtsev, H. Bekker, F. Torretti, J. Sheil, D. A. Czapski, J. C. Berengut, W. Ubachs, J. R. Crespo López-Urrutia, R. Hoekstra, O. O. Versolato, "EUV spectroscopy of highly charged Sn^{13+} - Sn^{15+} ions in an electron-beam ion trap", *Phys. Rev. A* **101**, 062511 (2020).

[5] L. Liu, C. H. Liu, J. G. Wang, R. K. Janev, "Electron capture and 2s-2p excitation in Be^{3+} - Li collisions", *Journal of Quantitative Spectroscopy and Radiative Transfer* **242**, 106804 (2020).

[6] L. Liu, C. H. Liu, J. G. Wang, R. K. Janev, "Electron capture, excitation and ionization in H^+ - Be^+ collisions", *Eur. Phys. J. D* **73**, 200 (2019).

[7] M. X. Ma, B. H. Kou, L. Liu, Y. Wu, J. G. Wang, "Electron capture in collisions of Li^{3+} ions with ground and excited states of Li atoms", *Chinese Physics* **B29**, 013401 (2020).

[8] N. Singh, A.Goyal, "Energy levels, transition data and collisional excitation cross-section of Sn^{3+} and Sn^{4+} ions", *J. Electron Spectros. Relat. Phenomena* **244**,146982 (2020).

[9] N. Singh, S. Aggarwal, M. Mohan, "Extended atomic structure calculations for W^{11+} and W^{13+}", *Atoms* **8**, 92 (2020).

[10] A. Devitre E. Oyarzabal, I. Fernandez-Berceruelo, D. Tafalla, F.L. Tabares, "Boron synergies in lithium-film performance", *Nucl. Fusion* **60**, 106001 (2020).

[11] K. Heinola, *Atomic Data for Vapour Shielding in Fusion Devices Summary Report of the Second Research Coordination Meeting,* IAEA Virtual Meeting, 7 – 9 October 2020, INDC(NDS)-0826 [https://www-nds.iaea.org/publications/indc/indc-nds-0826/].

F43025: Hydrogen Permeation in Nuclear Materials

The AMD Unit's most recent CRP focuses on research topics on experiments, modelling and theory related to hydrogen permeation in fusion reactor first wall materials and components. It is important to know as much as possible about the behaviour of these materials with respect to permeation of hydrogen isotopes in order to assess their suitability for containing and isolating the T fuel of a fusion reactor from the surrounding components. Of particular concern is the trapping and retention of T inside the reactor wall materials, and the possibility of T diffusing through the material finding its way into the coolant water of the reactor components, where it would pose a potentially serious environmental hazard.

The main topics of this CRP are as follows:

- To inventorize knowledge of parameters affecting hydrogen permeation in fusion-related materials (e.g. W, Be, ferritic/martensitic steels, coolant materials Cu, cladding materials, CuCrZr), including temperature, microstructure and irradiation-induced defects (elastic effects: lattice defects and collisional cascades; inelastic effects: neutron-induced transmutations and gas formation). As a novel feature, there will be a limited availability to perform research with neutron-irradiated tungsten samples as provided within the CRP.
- To assemble, evaluate and recommend data needed for hydrogen permeation in fusion materials, particularly diffusivity, retention, solubility, recombination and dissociation coefficients of hydrogen on unirradiated and irradiated materials.
- To increase the knowledge of the isotope effect on hydrogen diffusion.
- To decrease the uncertainties related to diffusion parameters affecting permeation.
- To expand the knowledge base concerning the influence of material defects and microstructure on permeation, including the evolution of defects and microstructure during permeation experiments.
- To assess and, as far as possible quantify, the effect of surface and sub-surface conditions on permeation.

- To perform coordinated experiments and simulations (DFT, KMC, Rate Theories, etc.) to improve the knowledge-base on hydrogen permeation processes with non-irradiated and irradiated material.
- to compare experimental facilities and techniques in hydrogen permeation.

At the time of writing, there are 16 participating research institutions from 13 Member States, with six more awaiting an exchange of signatures to formalise their participation. Two Research Contracts were initially awarded, followed by two more in 2021. The first RCM of this CRP was held virtually from 23 – 27 November 2020 and attracted 51 participants from 15 Member States (including observers and co-workers of the CRP Principal Investigators). After presentations from participants on their research and workplans for the CRP, the final day was devoted to the determination of data needs as described above and the planning of collaborative activities.

Two major experimental round-robin activities are planned as part of this CRP:

Hydrogen Gas-Driven Permeation in Fusion Materials (GDPFM)

This round-robin exercise focuses on gas-driven permeation (GDP) of deuterium in reduced-activation ferritic materials (RAFM). The activity aims to cross-compare permeation results obtained in different GDP facilities by using identical RAFM samples. The RAFM studied is EUROFER97 provided by IPP Garching (Germany), and samples have been polished, annealed and pre-characterised at Forschungszentrum Jülich (Germany) prior to distribution to participating laboratories at CEA (France), Forschungszentrum Jülich, NRC "Kurchatov Institute" (Russia), ASIPP (China) and CNEA (Argentina). The samples will be used for GDP studies between 30 ºC and 550 ºC in the upstream pressure range between 1 – 1000 mbar.

Defect Evolution and Hydrogen Permeation in Neutron-Irradiated Samples

Neutron-irradiated samples can be provided by SCK•CEN from two campaigns, covering a variety of dpa (up to 1 dpa) and temperatures (50 – 1200 °C). Tungsten samples have already been produced in a campaign from 2017 – 2019; the campaign in 2021 will use various grades of tungsten, CuCrZr, Mo, Fe, and (to be confirmed) EUROFER 97.

Permeation studies and the effect of the evolution of neutron-induced defects will be studied using (at least) the following experimental techniques: gas-driven permeation (GDP), plasma-driven permeation (PDP), Positron Anihilation Spectroscopy (PAS), thermal desorption spectroscopy (TDS) and nuclear reaction analysis (NRA).

The participants in this exercise, to whom irradiated samples will be distributed in the second half of 2021 are: Idaho National Lab (INL, USA) [subject to approval from the US Department of Energy to join the CRP], MEPhI (Russia), UKAEA (UK) and the University of Helsinki (Finland).

More information is available on the AMD Unit website at https://amdis.iaea.org/CRP/hydrogen-permeation.

A second, in-person Technical Meeting of participants in this CRP along with colleagues from other interested organisations is planned for 4 – 6 October 2021 (*Technical Meeting on Nuclear Fusion Fuel Permeation in Reactor First Wall Components*, see below).

[1] https://amdis.iaea.org/meetings/hydrogen-permeation-cm/

4. Data Services

The AMD Unit maintains several databases of fundamental atomic and molecular data of relevance to nuclear fusion. They are updated by Unit staff, and through projects, ad hoc consultancies and arrangements with research institutes in several Member States, particularly NIST (USA), KFE (formerly NFRI, Republic of Korea) and NIFS (Japan).

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. This database and its online interface is currently being improved to integrate better with other resources and to improve the validation and provenance of its data.

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).

A new online interface for AMBDAS, available at https://amdis.iaea.org/db/ambdas has been developed over the last year and was deployed in May 2021. As well as improving the search functionality, the references were reclassified according to the plasma processes identified in the Technical Meeting *Standards and Software Tools for Atomic and Molecular Databases* held at IAEA Headquarters in November 2019. These processes and the abbreviations used for them in AMBDAS are described at https://amdis.iaea.org/databases/processes.

CascadesDB

The CascadesDB database project, which was initiated by the 5th Code Centres Network Meeting held in November 2017, is a repository of molecular dynamics simulations of collision cascades in materials of relevance to nuclear fusion energy research. At the time of writing it contains 14382 simulations for eight different elemental materials in 814 GB of data, a significant increase on the 1532 simulations / 132 GB of data over the course of one year. The data are described by a flexible and comprehensive metadata schema; the online, searchable interface can be queried by author, material, temperature and projectile or primary knock-on atom (PKA) energy, and returns links to compressed archives containing the simulation xyz files and the associated metadata in HTML, XML, JSON and plain text formats. Further details are available at the URL https://cascadesdb.iaea.org/.

A short Home-Based Consultancy runs over July 2021 to implement a data upload functionality into the CascadesDB database: a Representational state transfer (RESTful) interface enabling data providers to upload JSON documents representing metadata for their simulations which are translated into the internal, searchable representations of those metadata in the relational database management system (RDBMS) used.

A further Consultancy is planned to implement the CSaransh software[1] developed by the Bhabha Atomic Research Centre (BARC) to post-process molecular dynamics simulations of collision cascades. CSaransh provides the following functionality:

- Defect statistics;
- Defect locations, classification, clustering;
- Metadata validation;
- Comparisons between cascade simulations;
- Subcascade identification.

[1] https://github.com/haptork/csaransh

DefectDB

The 6th Code Centres Network Meeting, held in October 2019, revisited the CascadesDB database with further recommendations for extending and improving it, and also proposed a new, related database of density functional theory (DFT) calculations of radiation-induced defect structures in materials of interest to nuclear fusion and fission applications. A subsequent Consultancy Meeting, held in January 2020 with experts from CEA Paris-Saclay, developed the relational database model for this repository and deployed a prototype interface at https://db-amdis.org/defectdb.

The COVID-19 pandemic has slowed development of this database, although progress has been made on the functionality for data providers to upload their calculations. It is hoped that the relaxing of European travel restrictions in the second half of 2021 will facilitate the population of this library with DFT data from, in particular EDF and CEA Paris-Saclay. The

software functionality being developed for upload to the CascadesDB database will help further improve the DefectDB for data providers.

Clerval

Clerval[1] is a database of institutions and events of relevance to the use, calculation and measurement of atomic, molecular and plasma-material interaction data in nuclear fusion research. In addition to being a resource for the fusion community, it serves as part of the backend of the new AMD Unit website to assist with the management of meetings, CRPs and other projects. Institutions, events and people are associated with keywords which help organize content and facilitate searching. At the time of writing, Clerval contains 318 institutions, 200 keyword classifications and 711 people. Parts of the Clerval resource, particularly the list of fusion-relevant conferences and meetings[2] replace the Knowledge Base wiki on the old website.

The AMD Unit also maintains a list of external databases in atomic and molecular physics at https://amdis.iaea.org/clerval/databases/ – at the time of writing 30 such resources are described and linked to on this page.

[1] https://amdis.iaea.org/clerval/
[2] https://amdis.iaea.org/clerval/events/

Data Standards

The Technical Meeting *Standards and Software Tools for Atomic and Molecular Databases* held in November 2019 updated and expanded the classification of collisional processes in plasmas maintained by the AMD Unit at https://amdis.iaea.org/databases/processes. In the last year there have been a few minor changes and corrections to this list, which is now at Version 2.1. The process codes were deployed in the AMBDAS database, as described above, and will be used in the forthcoming release of the latest version of the Unit's ALADDIN database.

The AMD Unit remains an active participant in the Virtual Atomic and Molecular Data Centre (VAMDC) consortium[1]: AMBDAS is deployed as a node for its "portal" of searchable databases, and work within the Unit on the PyValem Python package[2] is carried out in consultation and cooperation with the VAMDC. This software package enables the manipulation and validation of chemical formulas and species states for analysis and storage in databases.

[1] http://www.vamdc.org/
[2] https://github.com/xnx/pyvalem

5. Technical Meetings

Data Centres Network

The Technical Meeting of the International Atomic and Molecular Data Centres Network (DCN) is a biennial meeting of the Advisory Group of the DCN on atomic and molecular data relevant for nuclear fusion research. The Data Centres represented in the meeting were:

- Atomic Data and Analysis Suite consortium (ADAS), United Kingdom
- China Research Association of Atomic and Molecular Data (CRAAMD), China
- Forschungszentrum Jülich (FZJ), Germany
- National Institutes for Quantum and Radiological Science and Technology (QST), Japan
- National Institute for Fusion Science (NIFS), Japan
- Korea Atomic Energy Research Institute (KAERI), Korea
- Korea Institute of Fusion Energy (KFE), Korea
- Kurchatov Institute, Russia
- National Institute of Standards and Technology (NIST), USA
- Bariloche Atomic Centre (BAC), Argentina
- Queen's University Belfast (QUB), United Kingdom

The DCN meeting has taken place since 1977 and has been coordinated and hosted by the AMD Unit of the IAEA. The objectives of the DCN meeting are to exchange information regarding the activities of the data centres and to review their progress; to coordinate the work in the data centres by assessing priorities in data evaluation and production, and to make plans for specific evaluations; to evaluate and revise procedures for collection and exchange of bibliographical and numerical data; and to review atomic and molecular data needs for nuclear fusion research. It has been agreed within the DCN that IAEA should give priority to the collection and compilation of evaluated atomic collision data. This international atomic and molecular data programme provides information for the use of the global nuclear fusion research community on critically reviewed data on atomic and ionic collision processes as well as data on plasma-surface interactions important to fusion research, which could be used as a common database by fusion laboratories globally. The DCN plays an important role in setting priorities and recommending experts for data evaluation and validation.

The 25th meeting of the DCN took place at the IAEA Headquarters on 30 Sep – 2 Oct 2019. Representatives from the following national data centers were at the meeting: NIST, NIFS, NFRI, ADAS, KAERI, Kurchatov, CRAAMD, BAC, QUB and FZJ. In addition, a new national data center Consiglio Nazionale delle Ricerche (CNR), Italy, was presented. QST has not been involved in producing fusion A+M data since 2015 and hence did not participate in the meeting this time. An invited presentation was given by D. Brown from Brookhaven National Laboratory, USA. All the data centres provided an overview of their current status on AMD activities with special focus on fusion-related progress. All the details can be found on the meeting web page and in the meeting summary report [1, 2]. The presentations were

followed by data centre search engine and software demonstrations. Issues related to data exchange formats were reviewed; especially highlighted was the status of GENIE Atomic Data Search Engine, which was concluded to be useful, but outdated in terms of operational reliability. Discussions focusing to A+M data for fusion and on coordinated activities on data evaluation highlighted the importance of uncertainty quantification and error propagation in fusion A+M systems. It was especially noted the importance of well-established A+M fusion data as the data is employed in analysing full plasma conditions, which in turn will be used further in large-scale evaluations of processes taking place in the edge regions of the fusion plasma or in the surfaces or bulk of the fusion reactor components during plasma-wall interactions. Hence, it was concluded to organize a workshop, or a technical meeting, with a focus on a well-defined and pre-determined computational problem in fusion plasma processes. The problem to be placed under close scrutiny should act as a benchmarking case for laboratory or plasma device experiments. It was soon concluded to leave out test cases involving beryllium due to its toxicity and the resulting difficulties with experimental handling. Nitrogen was chosen as the topic of the computational workshop because it is complicated enough from the A+M point of view, but also extremely relevant to fusion reactor operation as potential impurity gas to be used for power exhausting at the divertor. The project leaders for this workshop were chosen to be ADAS and QUB. Due to the COVID-19 outbreak, the planned Nitrogen Workshop is unlikely to take place before 2022.

[1] https://amdis.iaea.org/meetings/dcn-25/
[2] K. Heinola, *Technical Aspects of Atomic and Molecular Data Processing and Exchange, 25th Meeting of the A+M Data Centres Network: Summary Report of an IAEA Technical Meeting*, IAEA Headquarters, Vienna, Austria , 30 Sep – 2 Oct 2019: https://nds.iaea.org/publications/indc/indc-nds-0801/.

Code Centres Network

The Code Centres Network (CCN), coordinated by the AMD Unit, is a joint effort to gather and provide access to any information relevant for modellers in fusion plasma science. Its focus is on the modelling and calculation of data that are difficult to measure experimentally. The CCN was initiated as the "A+M Computer Code Network" in a Technical Meeting held at IAEA Headquarters in 2005, with 11 participating research groups; since then the Network has become a Technical Meeting Series on computational aspects of fundamental data for fusion energy research, with no fixed membership or Advisory Committee. Every two years, AMD Unit staff identify an area with data needs within the scope of the the Network and invite qualified participants to contribute to addressing these needs.

The 6th meeting of the CCN was held from 16 – 18 October 2019 and continued the theme of the previous meeting in considering the ongoing development and promotion of data resources for radiation-induced damage in nuclear materials. Since the previous meeting, a database of collisional cascades simulations, CascadesDB, which is described above, has been developed by the AMD Unit and deployed on the IAEA website at https://cascadesdb.iaea.org/. The most recent meeting discussed further improvements to this resource, including analysis and visualization tools, and the need to acquire more data.

The crowdsourcing challenge, held over the summer of 2018, on the development of machine learning algorithms to analyse data in CascadesDB, was reviewed by the meeting: a summary of this activity is provided in Section 7 of this report.

A further database, DefectDB, of Density Functional Theory (DFT) calculations of radiation-induced defect structures was also proposed. Building on work of meeting participant M. C. Marinica and colleagues, this will serve as a repository for theoretical calculations of the structure and dynamics of point and extended defects in materials of relevance to fission and fusion applications. A Consultancy Meeting, held in January 2020, focused on the development of a suitable data schema and backend software for the database, which is currently available as a prototype browser-based service at https://db-amdis.org/defectdb.

The two databases, CascadesDB and DefectDB, are intended as part of a more broad-ranging suite of databases for fusion and fission material science with the following goals:

- To include experimental measurements and observations, particularly on steel (microscopy, XRD, positron emission, etc.)
- A fully-described set of DFT simulations and predictions of defect formation and behaviour, particularly in Fe.
- To expose an API so that data can be retrieved automatically from the database and included in computational workflows. This would allow, for example, cascade simulations to be input into hybrid models which use additional data and modelling to predict embrittlement of reactor structural components.
- To facilitate machine learning on large data sets, where available.
- To assess uncertainty propagation and estimation.

Further details, including the report of the 2019 CCN meeting and participant presentations, is available from the AMD website at https://amdis.iaea.org/meetings/ccn-6/.

The next meeting of the CCN is planned for 18 – 20 October 2021, in person or virtually as the prevailing COVID restrictions and Agency policies dictate: https://amdis.iaea.org/meetings/ccn-7/.

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

The Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP) is a consortium of research groups working in the area of fundamental atomic and molecular physics relevant to plasma processes. Its focus is on promoting collaboration and communication between experimentalists and theoreticians to improve the quality and completeness of data used in modelling and interpreting fusion plasmas. The Network provides a forum for the evaluation, validation and dissemination of data, the benchmarking of relevant modelling codes and the formulation of research guidelines and priorities.

The first GNAMPP meeting was held in November 2018 at IAEA Headquarters. 18 participants from 11 Member States attended and made recommendations about the scope, practices and membership of the Network. The convening Scientific Committee was:

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

The goals of the project were identified to be:

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

To ensure the effective operation of GNAMPP the research activities of its members must involve the production, evaluation or use of fundamental atomic and molecular data in one or more of the following categories:

- Tokamak diagnostics;
- Fundamental theory in the atomic and molecular physics of plasmas: the modelling of collisional and spectroscopic processes;
- Edge-plasma physics;
- Neutral beam modelling;
- Experimental collisional and spectroscopic physics, particularly research groups with ion beams and EBIT devices;
- Heavy ion reactions;
- Small molecular species in the divertor region.

Specifically excluded is research related to industrial plasma processing, medical plasmas, plasma-material interactions and modelling of plasma dynamics.

The GNAMPP website is https://amdis.iaea.org/GNAMPP/, which provides profiles and contact details of research groups in the Network. Details of the first meeting, including the meeting report[1] are available from https://amdis.iaea.org/meetings/gnampp-1/.

At the time of writing there are two collaborations within GNAMPP, also described on the website: a collaboration between the ITER Technology and Diagnostics Division (ITED) of

the Max Planck Institute for Plasma Physics in Garching, Germany and the Faculty of Science and Engineering at Curtin University, Australia to provide more reliable data on electron-H_2 collisions for use in the collisional-radiative modelling of tokamaks[2]; and a multi-group collaboration on the provision of evaluated fundamental data for modelling beryllium species in edge plasmas[3].

The second GNAMPP meeting was scheduled to be held in Vienna in November 2020; because of the COVID-19 pandemic and the impact it has had on research (and meeting room capacity at IAEA Headquarters), this meeting will now be held as a large virtual meeting, on the topic of tungsten and hydrogen ions in the edge plasmas of magnetic confinement fusion devices, from 6 - 9 December 2021: https://amdis.iaea.org/meetings/gnampp-2/.

[1] C. Hill, Atomic, Molecular and Plasma-Material Interaction Data Evaluation and Development: Summary Report of a Technical Meeting, *INDC(NDS) Report* 779 (2019) [https://www-nds.iaea.org/publications/indc/indc-nds-0779].

[2] https://amdis.iaea.org/GNAMPP/collaborations/1.

[3] https://amdis.iaea.org/GNAMPP/collaborations/2.

Technical Meeting on the Fundamental Data for Edge Plasma Modelling

A Technical Meeting on the Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasma of Fusion Devices was held online from 29 March – 1 April 2021. Originally to have been held in 2020 at Forschungszentrum Jülich, Germany, the venue was changed to IAEA Headquarters in late 2019, before the COVID-19 pandemic led to it being postponed. 39 participants from 14 Member States attended.

The meeting was held to evaluate and recommend fundamental data concerning tungsten, hydrogen, their ions and molecules in the edge plasma region of experimental nuclear fusion devices with a view to quantifying and reducing the uncertainties in the modelling of its collisional, radiative and plasma-material interaction properties. The organizing committee is:

- Ursel Fantz (University of Augsburg, Germany)
- Kalle Heinola (IAEA; *Scientific Secretary*)
- Christian Hill (IAEA)
- Sebastiján Brezinsek (Forschungszentrum Jülich, Germany)

Working Groups on the relevant aspects of CR modelling were established, and plans for a follow-up Virtual Technical Meeting, possibly to be held in late 2021 where made.

Sessions

The meeting was divided into the following sessions focussing on various modelling and experiments relevant to the properties and behaviour of tungsten and hydrogen ions in edge plasmas.

A. Experiments: Tokamaks, Linear Plasmas, Stellarators

Experimental devices: JET (attached/detached), AUG, DIII-D, MAGNUM, PSI-2, ITER , JT60-SA, T10

- Metallic vs. graphite surfaces
- Isotope experiments
- Reflection and recycling
- Surface conditions and processes
- Spectroscopy and other methods

B. Modelling: Tokamaks, Linear Plasmas, Stellarators

Codes: SOLPS-ITER, EMC3-EIRENE, SONIC NEUT2D, EDGE2D-EIRENE, TOKAM3-X, SOLEDGE-EIRENE

- Issues with benchmarks
- Attached and detached conditions
- Isotope effects
- Spectroscopy
- Neutral pressure benchmarks

C. Experiments: Atomic and Molecular Data, Cross Sections, Processes

- Isotope effects
- Rotationally and vibrationally-resolved spectroscopy
- Highly-excited species
- Mixed molecules
- Other hydrogen-containing molecules
- Spectroscopy tools

D. Modelling: Atomic and Molecular Data calculations

- Convergent-close coupling methods
- High-temperature molecular spectroscopic line lists

E. Collisional Radiative Models

Codes: YACORA, EIRENE, EUMONIA, NEUT2D

- Outcome of EU-ADAS for molecules
- Vibrationally resolved CR
- Time dependent methods
- Application to detached conditions

F. Needs and Conclusions

- Publications

- Potential CRP

Topics

Recombination rate coefficients for W^{q+}: experiments and theory

Existing experimental recombination rate coefficients and cross sections are known for electron energies up to several hundred eV (*i.e.* for $W^{18+-21+}$). However, at low energies the total recombination cross sections are orders of magnitude above those for radiative recombination. EBITs can be used for obtaining recombination cross sections, but energies below about 20 eV are not accessible experimentally, and this is the region with largest theoretical uncertainty.

The role of external electromagnetic fields on dielectronic recombination: high fields may have a large effect on plasma rate coefficients. For example, in Fe^{15+} the dielectronic recombination can change by a factor of 3 at temperatures of 10^5 to 10^6 K and at an electric field strength of kV/cm.

Electron-impact ionization of W^{q+}

The effect of long-lived states: experimental electron-impact ionization cross sections for W^{q+} (q = 1 – 19) with energies up to 1 keV exist. However, in the experiments even if the multiply-charged ions are stored for some time, the effect of long-lived excited states (in the parent ion beam) will be present in the cross section measurements. Fine energy scans and good statistics can reveal these metastable ions. Theoretical modelling of the resulting cross sections can provide information on the long-lived beam components. Fusion plasma will contain such species in long-lived excited states whose cross sections are needed.

Resonant processes in high charge states and their contribution to net ionization: it is necessary to explore which charge states of W might have resonant contributions and to assess the related cross sections (modelling with, for example, R-matrix methods may be necessary as experiments are challenging).

Electron-impact excitation of W^{q+}

There is a lack of experimental data for electron-impact excitations in W.

Charge-transfer collisions of W^{q+} with plasma species

Particular species of interest are: H/D/T, He and He+. The cross sections are well known in general, but at very low energies their uncertainties are unquantified. As with electron-collision experiments involving multiply charged W, the role of metastable states is largely unknown.

Spectroscopic issues in the divertor region

Non-LTE modelling: near the divertor the electron density is higher and the temperature lower than in main plasma, but due to divertor conditions non-LTE modelling may be required: emission data are needed for W erosion assessments (maximum charge states anticipated are W^{6+-8+}; excluding transient events, are higher charge states expected?) No reliable NLTE modelling exists for W^{0-5+}.

Re-assessment of the role of MAR in tungsten machines: Molecular Assisted Recombination (MAR) can play an important role in assisting the volume recombination (by three-body and radiative recombination of atomic ions) in detached divertor plasma. Detailed investigations of MAR were done almost two decades ago, but on machines using carbon as a plasma-

facing material. The properties of carbon and tungsten with respect to their interaction with hydrogen (*i.e.* the probability of H_2 formation at their surfaces) are very different; therefore, the role of MAR in modern fusion devices may differ from that determined for carbon machines.

Tungsten charge state distributions: plasma transport may shape the W charge state distribution (CSD): transport effects may change the averaged charge density <*Z*> and broaden the spatial range. The CSD deviates from transport-free, equilibrium values and offers information on plasma transport, *provided that adequate ionization balance calculations are available*. This is crucial for ITER: plasma transport measurements focus on the ionization balance of W. In ITER there will be no low-*Z* neutral beams employed, which are used in other fusion devices to monitor and observe plasma transport.

Atomic and molecular data: theory and modelling

Collisional-Radiative (CR) modelling: the relation of CR modelling to plasma transport simulations; non-LTE code activities on testing CR codes for W; CR model implementations: configurational average (*i.e.* <*Z*>) vs. detailed models (up to thousands of charge states).

Molecular radiation of hydrogen and deuterium (OES and UV/VUV ranges): Detecting and interpreting molecular radiation gives access to molecular fluxes as well as vibrational and rotational populations: parameters that are of relevance to assessing the effectiveness of MAR (see above), The accuracy of modelling molecular radiation by collisional-radiative models is directly correlated with the accuracy and completeness of the set of input data used, including the cross sections for electron-impact excitation of molecular states. Up to now, two strongly-diverging sets of cross sections were available; the first steps towards establishing a more reliable and accurate alternative set are currently in progress.

The effect of opacity

Self-absorption caused by optical thickness of the atomic Lyman emission lines can result in significant radiation trapping, influencing the energy balance and the ionization / recombination rates in the divertor plasma. If the radiation trapping is high, this may make the transition to a detached divertor more difficult. A second effect of opacity is that it strongly affects the intensity of emission lines and has to be taken into account in population models used for interpreting such emission. To do so, profiles of the opacity along the line-of-sight used are needed; this information is not presently available.

Middle-charge states of W ($W^{10+-25+}$)

In ITER medium charge states of W are expected to be responsible for the majority of re-radiation from transient pulses. Key processes for which data is needed are: ion line data and ionization, recombination and excitation rates.

More details are available on the meeting webpage, at https://amdis.iaea.org/meetings/tm-tungsten-hydrogen/.

6. ICTP Schools and Workshops

The IAEA organizes several Workshops in conjunction with the Abdus Salam International Centre for Theoretical Physics (ICTP) in Trieste, Italy; in recent years the AMD Unit has participated in this by running an annual event 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.

6.1 ICTP Workshop 2019: Atomic and Molecular Spectroscopy in Plasmas

This joint IAEA–ICTP Workshop, which was held at the ICTP from 6 – 10 May 2019, was a 5-day series of lectures and computing practical exercises to help early-career plasma physicists develop an understanding of the techniques used to model and simulate radiative processes in plasmas. The focus was on plasmas of relevance to fusion, astrophysics and other high-energy environments, and the aim is to facilitate knowledge-transfer between researchers from developed and developing countries.

The course directors were:

- Hyun-Kyung Chung (National Fusion Research Institute, Republic of Korea)
- Kalle Heinola (IAEA)
- Christian Hill (IAEA)
- Yuri Ralchenko (NIST, USA)

44 participants from 20 Member States joined 10 lecturers and directors for a combination of lectures, posters and practical sessions covering the following topics:

- Experimental plasma spectroscopy
- Atomic structure and radiation
- Collisional physics in plasmas
- Spectral line broadening
- Line intensities and collisional-radiative modelling
- Astrophysical spectroscopy
- Plasma opacity
- Radiative transfer in plasmas
- Spectroscopy of magnetic confinement fusion (MCF) plasmas
- Molecular structure and spectroscopy
- Experimental plasma spectroscopy

More details are available at https://amdis.iaea.org/workshops/ictp-2019. The Workshop was well-received, as interpreted through the anonymous, online questionnaire that participants were invited to complete (Appendix C). 30 responses were received; the mean overall rating given was 8.63/10 (σ = 1.08) and 90% of participants attended more than three-quarters of the lectures.

6.2 ICTP Workshop 2020: Radiation Damage in Nuclear Systems: from Bohr to Young (CANCELLED)

The AMD Unit received funding from the ICTP to organise a two-week Joint IAEA–ICTP Workshop, titled *Radiation Damage in Nuclear Systems: from Bohr to Young*, which was due to be held at the ICTP from 11 – 22 May 2020.

The Workshop aims to assist Ph.D. students and early-career researchers in developing a quantitative understanding of the impact of radiation damage on materials, both for existing fission and proposed fusion reactors. There is an emphasis on the conceptual progression of theoretical and experimental techniques across spatial scales from atomistic descriptions to the macroscopic behaviour of bulk material.

The event is organised by the AMD Unit, which is responsible for the fusion-related content of the course, in cooperation with the Nuclear Data Services Unit, represented by the Unit Head, Jean-Christophe Sublet, which covers fission-related parts of the syllabus. The topics covered are as follows:

- Irradiated material: defect production and damage metrics
- Dose-rate, damage energies, atomic displacement
    - Transmutation, activation, depletion
- Neutron-induced material defect simulation
- Nuclear Kinematics
- Void swelling, post-short-term cascades
- Correlation and prediction of material behaviour under irradiation
- Paradigms for irradiation testing: accelerator simulation
- Using ion irradiation as a proxy for neutrons
    - Ion accelerators, standardised testing, interstitials
- Theoretical modelling of radiation effects
- Micro-structure and microchemistry
- Ion versus neutron irradiation within a steady state microstructure
- Multiscale modelling of structural materials for nuclear systems
- From Bohr model to Young modulus
    - Physics – Chemistry – Material science – Engineering
    - Femtometres to metres; attoseconds to days
- Plasma-material interaction
    - Erosion and surface-evolution studies
    - Surface chemistry, codeposition
- The effect of neutron and surrogate radiation on the properties of fusion-relevant materials
    - Molecular Dynamics and Kinetic Monte Carlo studies (esp. W and Fe)
    - Quantum transition state theory, path integral approaches to hydrogen and defect migration
    - Experimental techniques
    - Prospects for “advanced materials” development such as high-entropy alloys
- Hydrogen isotope deposition, trapping and permeation in fusion-relevant materials
    - Experimental studies
    - *Ab initio* and semi-empirical quantum mechanical approaches
    - Prospects for uncertainty quantification (UQ)

The course directors are:

- Céline Cabet (CEA, France)
- Kalle Heinola (IAEA)
- Christian Hill (IAEA)
- Wolfgang Jacob (Max Planck Institute for Plasma Physics (IPP), Garching, Germany)
- Sabina Markelj (Jožef Stefan Institute, Slovenia)
- Jean-Christophe Sublet (IAEA)
- Gary Was (University of Michigan, USA)
- Steven Zinkle (University of Tennessee, USA)

Sponsorship for poster prize to a total value of €500 was secured from the *Journal of Nuclear Materials*, and a Memorandum of Understanding between the Physics and Nuclear Data Sections and the Conference and Document Services Division of the Department of MT-CD Publishing Section, which is responsible for publishing the journal *Nuclear Fusion*. Subject to their funding priorities, the journal may sponsor the travel and accommodation expenses of a suitable lecturer to an ICTP Workshop arranged in cooperation with the Physics or Nuclear Data Sections. Priority would likely be given to individuals with an existing relationship with the journal (for example, current or former members of the editorial board).

Before the COVID-19 pandemic, 54 participants had been selected from 175 applicants. The travel restrictions and closure of the ICTP for external activities imposed by the pandemic in 2020, led to this event being postponed and then eventually cancelled. It will be re-proposed for the 2022 calendar, and a Virtual Workshop on "Atomistic Modelling of Radiation Damage in Nuclear Systems" held from 4 – 8 October 2021 instead: https://amdis.iaea.org/workshops/ictp-2021.

6.3 ICTP Workshop 2021: Atomic Processes in Plasmas: Data-Driven Research

A further Joint ICTP-IAEA Workshop, on the topic of "Atomic Processes in Plasmas: Data-Driven Research" was approved for the 2021 calendar, and will take place as a virtual event from 13 – 17 December 2021. Its goal is to assist Ph.D. students and other early-stage career researchers to develop their quantitative understanding of the fundamental processes that produce the observed behaviour and properties of plasmas; through lectures and practical computing sessions they will also gain skills in the application of modern data science techniques to the calculation and evaluation of data on these processes. The course directors are:

- Christian Hill (IAEA)
- Ludmila Marian (IAEA)
- Hyun-Kyung Chung (Korea Institute of Fusion Energy, Republic of Korea)
- Claudio Mendoza (Western Michigan University, USA)
- Yuri Ralchenko (National Institute of Standards and Technology, USA)
- Udo von Toussaint (Max Planck Institute for Plasma Physics, Garching, Germany)

The topics to be covered include:

- Plasma emission modelling
- Practical exercises using the NIST ADS and LIBS databases
- The principles of Molecular Dynamics modelling
- Bayesian Inference for the determination of plasma-material interaction parameters
- Demonstration and practical exercises using LAMMPS
- Accessing, assessing and exploiting online data resources
- Managing atomic and molecular data
- Linux command line usage; Using Python and the JupyterLab environment for research

More details are available on the AMD Unit's website at https://amdis.iaea.org/workshops/ictp-2021b and the ICTP's website at http://indico.ictp.it/event/9657/.

7. Crowdsourcing Challenge

7.1 Introduction

The IAEA Challenge on Materials for Fusion presented participants with a set of data files from a simulation of neutron damage in two materials of interest for use in a controlled nuclear fusion reactor, iron and tungsten. The data files consisted of the locations of the atoms after the collisional cascade of displacements caused by the primary knock-on atom (PKA): the first atom to interact with the neutron.

Participants were invited to come up with innovative ways to visualise, analyse and explore the provided data. The precise nature of the software solution to the challenge was deliberately left open to invite as many novel approaches as possible, but it was suggested that one or more of the following might be involved:

- 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.

Details, registration and administration of the Challenge was handled through the IAEA's website; the data files (3.8 GB, compressed) were hosted on the Atomic and Molecular Data Unit's server. Participants were required to "subscribe" to the challenge before being given access to complete details and provided with the URL for data download.

The Challenge was opened on 26 April 2018 with an initial closing date of 23 June 2018, which was extended to 14 July 2018.

The website for the Challenge allowed participants to communicate with the organisers to ask questions: several such queries were received, three of which were of general enough interest to be placed on the site's "Frequently Asked Questions" (FAQ) page. Challenge "solutions" were submitted through the website as a PDF file describing the solution and as a compressed archive of software to a dedicated Dropbox location.

7.2 Promotion

The Challenge was promoted through the following channels.

- Google Ads campaign (€700)
    - 420,000 Impressions, 5000 clicks leading to 13 registrations ("subscriptions")
    - Targeted regions: Africa, Americans, Asia, Europe, Oceania
- Facebook and Instagram Ad campaign (€800):
    - 12,000,000 Impressions, 6,000,000 Reach, 20,000 clicks
- Posts on the IAEA's Facebook page
- Tweets on the IAEA's Twitter feed
- Posts on the IAEA's Instagram and LinkedIn pages
- An announcement on the UN General Marketplace (UNGM)
- Direct contact with senior individuals in national laboratories and universities, followed by posts in local institutional mailing lists and newsletters
- An article on the IAEA's website, issued by the NAPC Communications unit, describing the Challenge: https://www.iaea.org/newscenter/news/iaea-issues-crowdsourcing-challenge-for-materials-for-fusion-technology
- A separate direct-mailing campaign to senior figures in the Chinese fusion community, with a brief statement of the Challenge in Mandarin, inviting them to publicise the activity within their own institutions

Visitors from non-paid promotion (posts on Twitter and LinkedIn) spent substantially longer on the website (average 1 min 30) than those from paid advertisements (on Facebook and Google) (average 25 secs).

The organisers contacted the subscribed participants once, on 30 May 2018, inviting feedback on the project and asking if an extension to the initial deadline would be desirable. Responses were received from 12 participants (of whom seven would go on to submit proposed "solutions" to the Challenge). It was on the basis of this feedback that the Challenge deadline was extended by three weeks. No problems were identified with the data or with the administration of the Challenge, and all participants who responded said they had a clear idea of what they hoped to achieve within the activity.

7.3 Response

There were 142 "subscriptions" to this Challenge, and data files were downloaded by 121 unique IP addresses in the locations given in the first table of Appendix D. Of these, 14 submitted solution description forms, and eight of those uploaded a compressed archive of their software.

A pre-filtering was applied to the 14 submissions to create a shortlist of proposals to be examined in detail. Those submissions rejected by this process are described in the table below.

User ID Number	Reason for Rejection
698	No novel analysis and no original software provided
722	Submission did not attempt to address the Challenge's theme or use the provided data
662	Submission did not attempt to address the Challenge's theme or use the provided data
609	No novel analysis
694	Submission did not attempt to address the Challenge's theme or use the provided data
726	No analysis of the provided data was attempted; no novel approach taken to the Challenge's theme

The remaining eight submissions were from five different countries, as summarized in Figure 1. One was submission was received from a company; three were from universities and the remaining four from national laboratories. Six of the eight submissions were from participants who heard about the Challenge by word-of-mouth or direct contact. Seven of the eight participants submitted their code under open source licences (GPL, MIT, BSD); the remaining submission was transferred under commercial terms and assessed under a trial licence

7.3 Demographics

Gender

Although participants were not invited to specify their gender in registering with the Challenge website, an approximate estimate of the gender proportions can be obtained from the required first name field. Disappointingly, it is estimated that only 10 % of participants were female. It is hard to be certain, but on the basis of their first names, it seems that none of the participants who submitted a solution to the Challenge was female.

By Country

Figure 2 illustrates the distribution of countries in which the Challenge subscribers are located. A full list of countries is given in the second table of Appendix D. No subscribers were identified as coming from Russia or South Korea, and only one participant came from Japan. The 11 participants from China all registered after a specific email campaign directly contacting senior figures at national laboratories and universities in that country. This was initiated after recognising that China was not being exposed to the existing advertising and outreach campaigns (via Facebook and Google, for example); it could be that future

Challenges would benefit from extending this type of by-country promotion to Russia, Japan and South Korea. It is also noted that only one subscriber was identified as coming from the whole of South America.

How did subscribers become aware the Challenge?

Subscribers were invited to specify how they found out about the Challenge. 97 participants did so, and their responses are summarised in Figure 3. It should be noted that these classifications are not necessarily orthogonal: in many cases, an announcement is made in a newsletter or passed on by word-of-mouth after being seen on a mailing list or online advertisement.

In some cases, subscribers specified which Social Media platform they became aware of the Challenge from. It was almost never clear whether they saw a paid advertisement or a post (tweet, etc.) by the IAEA or other organisation or individual. Figure 4 gives a breakdown of the different Social Media platforms specified by participants who found out about the Challenge via this medium.

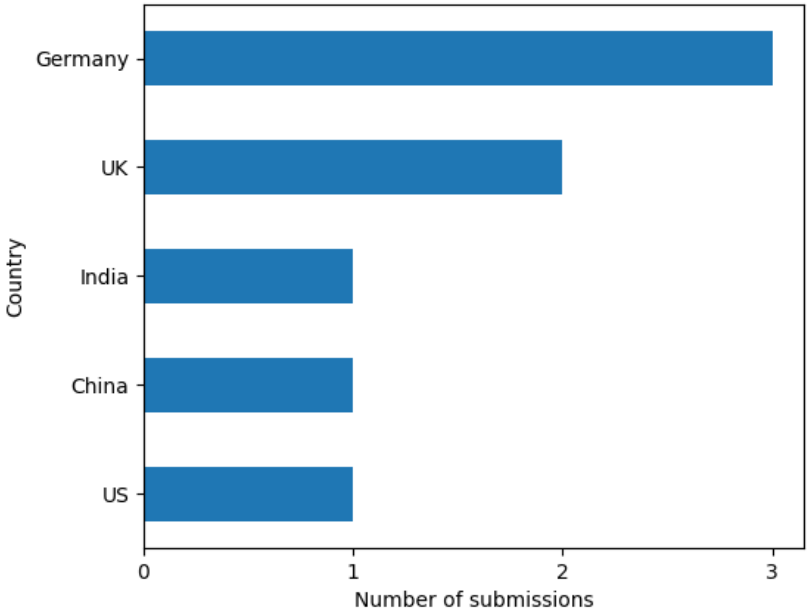

Figure 1. Number of Challenge submissions by country.

7.4 Submissions

The eight, pre-filtered submissions were judged by the Challenge organising committee (after one recused themselves because of a close association with one of the submissions): Andrea Sand (University of Helsinki), Christian Hill (IAEA) and Kalle Heinola (IAEA). The submitted software was compiled and installed on a Virtual Machine and executed against the supplied data and the required, descriptive report was assessed based on its novelty, utility and applicability to the stated problem domain.

Highlighted submissions included:

- An extension to the popular Ovito molecular dynamics (MD) visualization package, submitted by the authors of that application.
- A Python package for exploring interstitial and vacancy defects in a browser-based Jupyter Notebook environment.
- A suite of data-reduction, analysis and visualization tools to provide in-browser visualization and statistical information about each MD simulation.
- An implementation of an efficient algorithm to calculate and summarise the statistical distribution of atom displacements as a function of the PKA energy.

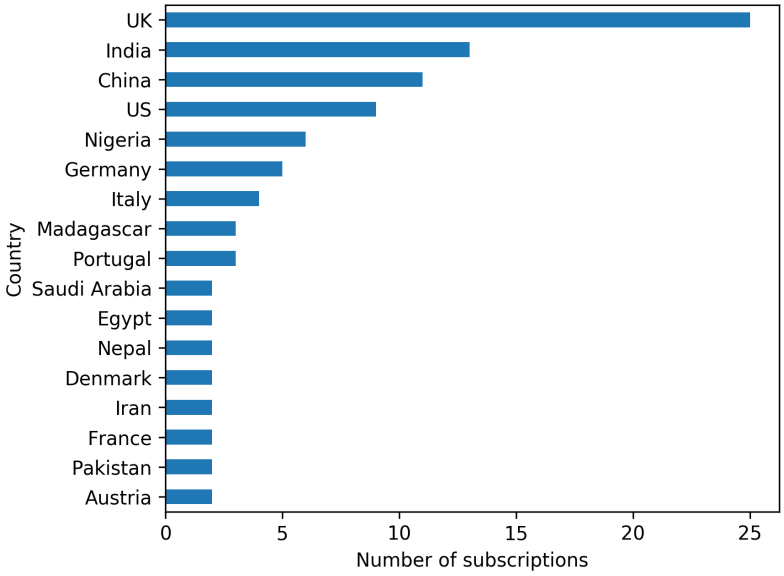

Figure 2. Number of Challenge subscribers by country, for

The winning submission was judged to be that of the research group of U. von Toussaint at the Max Planck Institute for Plasma Physics, Garching, Germany, which applied techniques from data science: the reduction of a Smooth Overlap of Atomic Positions (SOAP) descriptor vector by principal component analysis (PCA) to identify novel defect types in the simulated post-cascade atom positions. A previously-unknown defect cluster type, consisting of a triangular arrangement of vacancies was discovered by this process. The report of the

winning submission is provided in Appendix E. Work to integrate the functionality provided by the winning code with the CascadesDB database is planned.

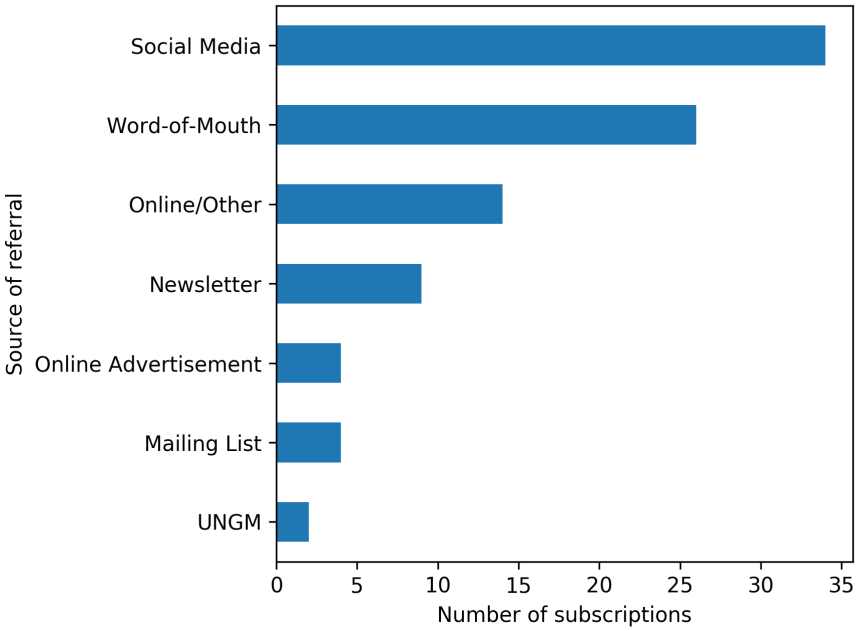

Figure 3. Numbers of subscribers by source of referral, where provided.

The highly-commended submission by U. Bharadwaj and M. Warrier at the Bhabha Atomic Research Centre, India, provides a very helpful way to visualize and statistically analyse the defects produced in a cascade simulation in a browser; their software, CSaransh is available online at https://github.com/haptork/csaransh and a Consultancy Meeting (originally planned for May 2020) will aim to incorporate its functionality into CascadesDB.

7.5 Recommendations

The following observations and recommendations were suggested by the experience of this Challenge.

- Despite the popularity of Google, Facebook and Twitter, bespoke promotional campaigns are necessary to reach certain regions including China, Russia, Japan, South Korea and South America.

- The Challenge website, although it provided secure and functional platform for managing the project, should be improved and made easier to maintain, modify and update. Current problems with it include difficulties in updating content consistently, slow responsiveness, and an unintuitive and frustrating administrative interface.

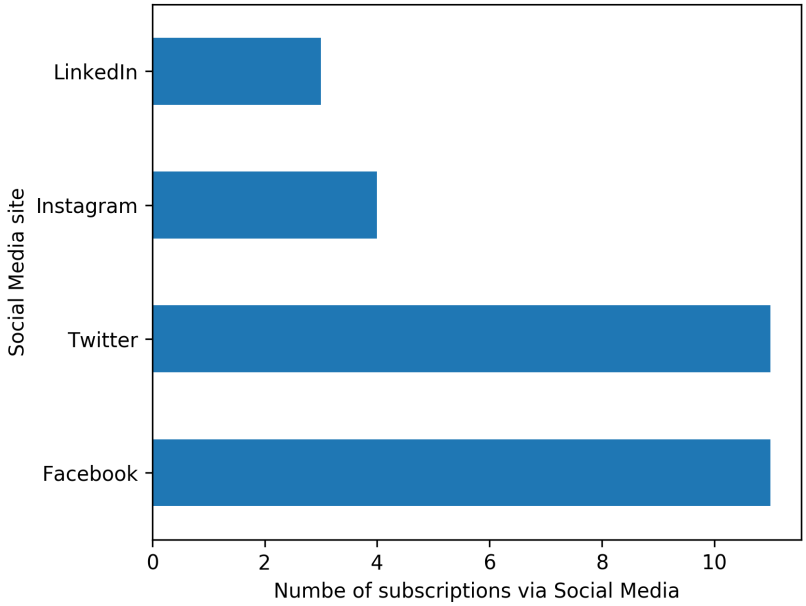

Figure 4. Numbers of subscribers referred by Social Media, by

8. Unit Website

Developments

The Atomic and Molecular Data Unit has developed a new website to communicate its work and provide details to meeting and project participants. Until the arrival of the new Scientific Data Manager, this website was deployed at the url https://www-amdis.org/ – in 2020 received an official IAEA domain and can be viewed at https://amdis.iaea.org/. Some resources, particularly the ALADDIN and legacy AMBDAS databases remain on the older website, https://www-amdis.iaea.org/, which is still available. ALADDIN will be migrated onto the new platform over the next year.

The new website, its relational database backend and administrative interface is easier to navigate and makes updating content easier and less error-prone. Its development, as an internal project, did not require external consultants or the procurement of professional services.

A further domain, https://cascadesdb.iaea.org/ serves the Unit's CascadesDB database, and another, https://amdis.iaea.org/db/ will host other data resources, including the new DefectDB database, currently in prototype form at https://db-amdis.org/defectdb.

Statistics

The original website, https://www-amdis.iaea.org/, received 93,650 page views by 24,083 users over the time period 1 May 2018 – 30 April 2020. The new website, https://amdis.iaea.org/ is attracting new users, with 1758 page views over March and April 2020; and the temporary domain, https://www-amdis.org/ served 708 pages over the same timeframe. As more content was migrated, the new, official URL has become the main point of contact for users of the AMD Unit's resources: in the 12 months from June 2020, it

received 35,000 page views by 12,000 users. It is noted that the top 10 countries visiting the site are all members of the ITER consortium.

9. Duty Travel

Christian Hill, 10 – 22 June 2018, Participation in the HITRAN/ASA meeting (Boston, MA, USA) and Plasma-Surface Interaction conference (PSI-23) (Princeton, NJ, USA). Poster presentation on CascadesDB and other AMD Unit activities; coordination meetings with participants involved in AMD Unit databases and CRPs, including a satellite meeting concerning the Irradiated Tungsten CRP at PSI-23.

Christian Hill, 21 – 24 August 2018, Participation in the biennial International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces (MPS-2018) in Budapest, Hungary. Meetings with the conference chair (Károly Tokési) and other participants concerning the Code Comparison Workshop on Neutral Beam Attenuation and Experimentalists' Network (now called GNAMPP).

Kalle Heinola, 3 – 7 September, 2018, Participation in the 19th International Conference Physics of Highly Charged Ions (HCI-2018), Lisbon, Portugal. Poster presentation on the A+M general activities of the AMD Unit. Focus on introducing the AMD Unit to the HCI community. Highlighting the Unit's new Vapour Shielding CRP resulted one conference participant (University of Groningen, Netherlands) joining the CRP. This participation provides valuable experimental fundamental data on Sn excitation states for the A+M fusion community.

Christian Hill, 11 – 15 November 2018, Invited oral presentation at the 11th International Conference on Atomic and Molecular Data and their Applications (ICAMDATA 2018) (Cambridge, MA, USA). Meetings with current, former and prospective participants in CRPs and the Data Centres Network. The AMD Unit Head is an ex officio member of this conference's International Programme Committee (IPC); during the conference a meeting was held to plan 2020's meeting, in Bari, Italy [now postponed to 2021 because of the COVID-19 pandemic].

Christian Hill, 9 – 12 April 2019, Invited oral presentation at the 20th Atomic Processes in Plasmas Conference (APiP) (NIST, Gaithersburg, MD, USA), and participation as member of the Organising Committee; the AMD Unit will host the next APiP meeting in 2021 in Vienna.

Christian Hill and Kalle Heinola, 6 – 10 May 2019, Participation as Course Directors and lecturers in the Joint IAEA–ICTP School on Atomic and Molecular Spectroscopy in Plasmas (ICTP, Trieste, Italy) – see Section 6.1.

Kalle Heinola, 20 – 24 May, 2019, Participation in the 17th International Conference on Plasma-Facing Materials and Components (PFMC-17), Eindhoven, The Netherlands. Poster presentation on AMD Unit activities on plasma-surface interactions and on CascadesDB.

Several monitoring and planning meetings with participants from CRPs “Data on Beryllium Erosion” and “Steel Surfaces.”

Christian Hill, 20 – 22 July 2019, Participation in the 26th International Symposium on Ion-Atom Collisions (ISIAC-2019), Sorbonne University, Paris, France. Meetings with six of the participants of the Unit’s Neutral Beams CRP to coordinate the Code Comparison Workshop Activities and receive updates on Workplan progress for this CRP.

Christian Hill, 26 – 28 October 2019, Invited oral presentation at the Open Libraries Workshop associated with the 2019 IEEE Nuclear Science Symposium (NSS) and Medical Imaging Conference (MIC) in Manchester, UK. Presentation given on behalf of the Nuclear Data Section on the IAEA’s atomic and molecular data services and the IAEA’s role in ensuring the availability, sustainability and quality of nuclear, atomic and molecular data discussed, particularly in the context of a planned review article on relevant databases.

Kalle Heinola, 27 Oct – 1 Nov, 2019, Participation in the The Nineteenth International Conference on Fusion Reactor Materials (ICFRM-19), La Jolla, California, USA. Poster presentation on AMD Unit’s activities on plasma-surface and plasma-material interactions including new databases CascadesDB and DefectDB. Focus on the Unit’s new CRP “Hydrogen permeation in fusion-relevant materials.” Several one-to-one and small-group meetings with current and future CRP participants.

Christian Hill, 13 – 23 November 2019, “Invited oral presentation at the Workshop on Rovibrational Molecular Spectroscopy: Setting Standards for Software Packages and Toolkits,” held at the Molecular Sciences Software Institute (MolSSI), Blacksburg, VA, USA; and collaborative work in implementing a new software tool (pyref) for managing bibliographic databases, at the Harvard-Smithsonian Center for Astrophysics (CfA), Cambridge, MA, USA.

Ludmila Marian, 25 – 27 November 2019, Participation in the European Women in Technology Conference (4000 participants from 48 countries), held in Amsterdam, The Netherlands. Presentation on “Modernizing Legacy Systems for Improved Security and Efficiency”; conducted one hour workshop on “Contributing to Open Source.”

Kalle Heinola, 28 – 31 January, 2020, EUROfusion’s Joint Working Session on SOL and PSI Modelling for Work Packages WPJET1/WPMST1/WPPFC, Tervaniemi, Finland. Invited key note lecture for session “Data production and model development for PSI codes”. Meetings with several Unit’s CRP participants on the current CRP activities. Information sharing on Unit’s current and future databases (Aladdin, CascadesDB, DefectDB), and on participation to the new CRP “Hydrogen permeation in fusion-relevant materials.”

10. Publications

Scientific Articles

F. M. Skinner, I. E. Gordon, C. Hill, R. J. Hargreaves, K. E. Lockhart, L. S. Rothman, *Referencing Sources of Molecular Spectroscopic Data in the Era of Data Science: Application to the HITRAN and AMBDAS Databases*, Atoms **8**(2), 16 (2020); doi:10.3390/atoms8020016

A. Widdowson, J. P. Coad, E. Alves, A. Baron-Wiechec, N. Catarino, V. Corregidor, K. Heinola, S. Krat, C. Makepeace, G. F. Matthews, M. Mayer, K. Mizohata, M. Sertoli, *Deposition of impurity metals during campaigns with the JET ITER-Like Wall*, Nucl. Mat. Energy **19**, 218 (2019); doi:10.1016/j.nme.2018.12.024

K. Heinola, T. Ahlgren, S. Brezinsek, T. Vuoriheimo, S. Wiesen, *Modelling of the effect of ELMs on fuel recycling at the bulk W divertor target of JET*, Nucl. Mat. Energy **19**, 397 (2019); doi:10.1016/j.nme.2019.03.013

S. Brezinsek, A. Kirschner, M. Mayer, A. Baron-Wiechec, I. Borodkina, D. Borodin, I. Coffey, J. W. Coenen, N. d. Harder, A. Eksaeva, C. Guillemaut, K. Heinola, A. Huber, V. Huber, M. Imrisek, S. Jachmich, E. Pawelec, S. Krat, G. Sergienko, G. Matthews, A. Meigs, S. Wiesen and A. Widdowson, *Erosion, screening, and migration of Tungsten in the JET divertor*, Nucl. Fusion **59**, 096035 (2019); doi:10.1088/1741-4326/ab2aef

M. Mayer, S. Moller, M. Rubel, A. Widdowson, S. Charisopoulos, T. Ahlgren, E. Alves, G. Apostolopoulos, N. Barradas, S. Donnelly, S. Fazinic, K. Heinola, O. Kakuee, H. Khodja, A. Kimura, A. Lagogiannis, M. Li, S. Markelj, M. Mudrinic, P. Petersson, I. Portnykh, D. Primetzhofer, P. Reichart, D. Ridikas, T. Silva, S. Gonzalez de Vicente and Y. Wang, *Ion beam analysis of fusion plasma-facing materials and components*, Nucl. Fusion **60**, 025001 (2019); doi:10.1088/1741-4326/ab5817

A. Hakola, K. Heinola, K. Mizohata, J. Likonen, C. Lungu, C. Porosnicu, E. Alves, R. Mateus, I. B. Radovic, Z. Siketic, V. Nemanic, M. Kumar, C. Pardanaud and P. Roubin, *Effect of composition and surface characteristics on fuel retention in beryllium-containing co-deposited layers*, Phys. Scripta **T171**, 014038 (2020); doi:10.1088/1402-4896/ab4be8

N. Catarino, A. Widdowson, A. Baron-Wiechec, J. P. Coad, K. Heinola, M. Rubel, N. P. Barradas and E. Alves, *Deposition in the tungsten divertor during the 2011-2016 campaigns in JET with ITER-Like Wall*, Phys. Scripta **T171**, 014044 (2020); doi:10.1088/1402-4896/ab4df7

A. Widdowson, S. Aleferis, E. Alves, L. Avotina, A. Baron-Wiechec, N. Catarino, J.P. Coad, V. Corregidor, K. Heinola, I. Jepu and C. Makepeace, *Fuel inventory and material migration of JET main chamber plasma facing components compared over three operational periods*, Phys. Scripta **T171**, 014051 (2020); doi:10.1088/1402-4896/ab5350

T. Vuoriheimo, P. Jalkanen, A. Liski, K. Mizohata, T. Ahlgren, K. Heinola and J. Raisanen, *Hydrogen isotope exchange mechanism in tungsten studied by ERDA*, Phys. Scripta **T171**, 014056 (2020); doi:10.1088/1402-4896/ab57ad

Tommy Ahlgren and Kalle Heinola, *Critical improvements to sink strengths used in multi-scale rate equation simulations of defects in solids*, Materials, submitted (2020)

G. De Temmerman, K. Heinola, D. Borodin, S. Brezinsek, R. P. Doerner, M. Rubel, E. Fortuna-Zalesna, C. Linsmeier, D. Nishijima, K. Nordlund, M. Probst, J. Romazanov, E. Safi, T. Schwarz-Selinger, A. Widdowson, B. J. Braams, H.-K. Chung, C. Hill, *Data on erosion and hydrogen fuel retention in Beryllium plasma-facing materials*; submitted (2020)

INDC Reports

C. Hill, Development of Software Programs and Database Tools for Modelling Edge Plasma Processes in Fusion Devices: Summary Report of a Technical Meeting, *INDC(NDS) Report* 805 (2020) [https://www-nds.iaea.org/publications/indc/indc-nds-0805/]

C. Hill, International Atomic and Molecular Code Centres Network: Database Services for Radiation Damage in Nuclear Materials: Summary Report of the 6th Biennial Technical Meeting, *INDC(NDS) Report* 803 (2020) [https://www-nds.iaea.org/publications/indc/indc-nds-0803/]

C. Hill, Atomic, Molecular and Plasma-Material Interaction Data Evaluation and Development: Summary Report of a Technical Meeting, *INDC(NDS) Report* 779 (2019) [https://www-nds.iaea.org/publications/indc/indc-nds-0779/]

C. Hill, Data for Atomic Processes of Neutral Beams in Fusion Plasma: Summary Report of the Second Research Coordination Meeting, *INDC(NDS) Report* 780 (2019) [https://www-nds.iaea.org/publications/indc/indc-nds-0780/]

C. Hill, Plasma-Wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices: Summary Report of the Third Research Coordination Meeting, IAEA Headquarters, Vienna, Austria, 25 – 27 March 2019, *INDC(NDS) Report* 782 (2019) [https://www-nds.iaea.org/publications/indc/indc-nds-0782/]

K. Heinola, Atomic Data for Vapour Shielding in Fusion Devices: Summary Report of the First Research Coordination Meeting, IAEA Headquarters, Vienna, Austria, 13 – 15 March 2019, *INDC(NDS) Report* 781 (2019) [https://www-nds.iaea.org/publications/indc/indc-nds-0781/]

C. Hill, Atomic Data for Vapour Shielding in Fusion Devices. Summary Report of a Consultancy Meeting, IAEA Headquarters, Vienna, Austria, 19–20 March 2018, *INDC(NDS) Report* 755 (2018) [https://www-nds.iaea.org/publications/indc/indc-nds-0755/]

C. Hill and K. Heinola, 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, *INDC(NDS) Report* 765 (2018) [https://www-nds.iaea.org/publications/indc/indc-nds-0765/]

Atomic and Plasma–Material Interaction Data for Fusion

Atomic and Plasma–Material Interaction Data for Fusion, Vol. **18**, STI/PUB/023/APID/18, 212pp., ed. C. Hill, (2019). Available at https://www.iaea.org/publications/13560/atomic-and-plasma-material-interaction-data.

11. Cooperations and Other Activities

- The Practical Arrangements between the IAEA and the Korea Institute of Fusion Energy (KFE), formerly named the National Fusion Research Institute (NFRI), for cooperation in the area of atomic, molecular and plasma-material interaction data relevant to fusion remain in place until 4 September 2021; the process of renewing them is underway, following the IAEA's current procedures.

- The AMD Unit entered into a cooperation agreement with the organisers of the 5th Spectral Lineshapes in Plasmas (SLSP) Workshop, which was held in Vrdnik, Serbia from 27 – 31 May 2019 [1, 2]. Christian Hill joined the Scientific Organising Committee for this event but, because of Departmental limitations on Duty Travel, did not attend in person.

- The AMD Unit entered into a cooperation agreement with the International Workshop on Models and Data for Plasma-Material Interaction in Fusion Devices (MoD-PMI), held in Toki, Japan from 18 – 20 June 2019 [3, 4]. Kalle Heinola joined the Scientific Organising Committee of the event but, because of Departmental limitations on Duty Travel, did not attend it in person.

- Kalle Heinola was a member of International Program Committee of "International Workshop on Hydrogen Isotopes in Fusion Reactor Materials (HWS)".

- Christian Hill was a member of the International Organizing Committee of the International Conference on Atomic and Molecular Data and their Applications (ICAMDATA) [5] and Atomic Processes in Plasmas Conference (APiP) [6] conferences.

[1] https://amdis.iaea.org/workshops/slsp-5

[2] https://plasma-gate.weizmann.ac.il/projects/slsp/slsp5/

[3] https://amdis.iaea.org/workshops/mod-pmi-2019

[4] http://dpc.nifs.ac.jp/dkato/MoD-PMI2019/

[5] https://projects.iq.harvard.edu/icamdata

[6] https://pml.nist.gov/apip2019/

12. Planned Future Meetings

The COVID-19 pandemic has caused a great deal of uncertainty about the timing of the following planned events, many of which have been postponed until 2021

Third RCM of the Neutral Beams CRP

The final RCM of CRP F43023: Data for Atomic Processes of Neutral Beams in Fusion Plasma is planned for December 2020. The CRP participants will meet at IAEA Headquarters to review the data produced during the project, which will be distributed through the AMD Unit's website services, and to plan the writing of a final report. A special issue of the journal *Atoms*, titled "Neutral Atoms in Controlled Fusion and Space Plasmas" is planned, to be guest-edited by AMD Unit staff, with P. Goncharov of Peter the Great St. Petersburg Polytechnic University; CRP participant groups are invited to submit articles for inclusion in this special issue in order to create a review of the project's results and outcomes.

The Third RCM will also review the Code Comparison Workshops on Electron Dynamics in Atomic Collisions and Neutral Beam Penetration and Photoemission, and consider prospects for future work on these topics.

Second Meeting of GNAMPP

The Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP) will hold its second meeting from 6 – 9 December 2021. This meeting will follow on from the Technical Meeting on aspects of the collisional-radiative properties of tungsten and hydrogen in the edge plasma of fusion devices held in March 2021. Sessions on each of the following Working Groups will be held:

- WG1: Atomic and Molecular Data Recommendation and Validation with CR Models
- WG2a: Plasma Experiments and Comparison Activities with CR Models: W and Hydrogen Experiments with Fusion Devices and Linear Plasma Devices
- WG2b: Plasma Experiments and Comparison Activities with CR Models: Photon Opacity Models of Hydrogenic Atomic and Molecular Species

Topics to be discussed include:

- Missing tungsten data in edge plasma models
    - Rates for ionization, recombination and excitation
    - Multi-step ionization and excitation
    - Non-resonant charge exchange

- Recommended tungsten and hydrogen data for edge plasma modelling
    - Large scatter in the various sets for W atomic data (in particular excitation rates)
    - Hydrogen molecular data: impact and need of vibrationally-, rotationally- and isotopically-resolved data; mixed molecules; limited data available for T, TH and TD
    - Metastable states of W

    - Uncertainties of W and hydrogen data: atomic data used in CRM dependent on the range of plasma parameters

- The inclusion of reduced photon opacity information in collisional-radiative models
    - Revised CRM with (semi)opaque lines
    - Full non-linear model or a reduced CRM
    - Isotope effects of collisional broadening in high plasma density
    - Wall reflection models for photons: on W and Be or deposited layers; surface roughness effects

- Data needs for ITER
    - Accuracy improvement for ionization, recombination, radiation and CX rates of W
    - CR: to obtain reliable charge distribution of W for modelling W upstream migration and penetration to core plasma
    - Spectral lines of interest W0 to at least W64+
    - Dielectronic recombination rates and photon opacity for W vapour shielding during fast transients

The meeting will be open to participations from anyone nominated through their Member State following the submission of a “Form A” (for attendance) and, optionally, a “Form B” (for presentation of a poster). More details are available from https://amdis.iaea.org/meetings/gnampp-2/.

Atomic Processes in Plasmas (APiP) (2023 Technical Meeting)

This biennial conference series originally planned to hold its 21st meeting in Vienna in the spring of 2021. The disruption caused by the COVID pandemic have led to its postponement, and it is intended that the event should be held as a Technical Meeting, jointly with the 27th meeting of the Data Centres Network from 15 – 19 May 2023. The organising committee is chaired by the AMD Unit Head.

The committee members are:

- Djamel Benredjem, Laboratoire Aimé-Cotton de l'université Paris-Sud, France
- Hyun-Kyung Chung, Korea Institute of Fusion Energy, Republic of Korea
- Christian Hill, International Atomic Energy Agency, Vienna, Austria
- Hae Ja Lee, Stanford Linear Accelerator, United States of America
- Oleksandr Marchuk, Forschungszentrum Jülich, Germany
- Taisuke Nagayama, Sandia National Laboratories, United States of America
- Nobuyuki Nakamura, University of Electro Communications, Japan
- Olivier Peyrusse, Lab. PIIM, Aix-Marseille Université, France
- Matthew Reinke, Oak Ridge National Laboratory, United States of America

The topics sessions proposed so far encompass a wide range of theoretical and experimental techniques relevant to the fundamental physics of plasmas:

- Magnetically-confined fusion plasmas
- Astrophysical and atmospheric plasmas
- Atomic and molecular data for plasma research
- Low-temperature plasmas
- X-ray sources
- Warm dense matter
- Medical applications of plasmas
- High energy-density plasmas
- Laser-plasma interactions
- Data resources for plasma modelling
- Plasma spectroscopy

23rd Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

It was agreed that the next IFRC Subcommittee meeting should be held according to the regular biennial cycle as an in-person meeting (if allowed by the COVID-related regulations at the time) in the spring of 2022.

Planned Future CRPs

Atomic Data for Injected Impurities in Fusion Plasmas (F43026)

Impurity ions are deliberately seeded into fusion plasmas for a variety of purposes. From the earliest days of magnetic-confinement fusion energy research, the spectra of light impurity ions, such as those of helium, lithium and carbon were used as a diagnostic tool to determine plasma properties. With the advent of very large scale experimental devices such as ITER, impurity injection is increasingly being used to redistribute the power transported from the plasma core to the reactor wall in order to reduce the heat load on, and hence damage to, the plasma-facing reactor wall components. Furthermore, impurities such as nitrogen, neon and argon and have been used in such devices to improve plasma control by diminishing the amplitude of edge-localized modes (ELMs), plasma disruptions and other transient events that inhibit confinement and have the potential to cause serious damage to wall components.

In order to interpret and predict the behaviour and properties of impurities in fusion plasma, a significant amount of modelling, involving data on the collisional-radiative characteristics of the impurities and their environment is required. For a few species, high-quality data is available, but in many cases the currently-available data is incomplete, missing, or of uncertain quality.

This planned CRP will provide fundamental data for modelling the behaviour of first-row and noble gas atoms in edge and divertor plasmas for ELM and disruption mitigation and for plasma diagnostics, and establish a trusted repository of data concerning the collisional–radiative properties of plasma–impurity interactions to facilitate modelling of plasmas in magnetic confinement fusion devices.

The CRP will be proposed to the relevant Committee for Coordinated Research Activities (CCRA) with a view to holding its first Research Coordination Meeting in 2022 after a Consultancy Meeting to address more specifically its scope, participation and expected outputs.

Formation and Properties of Molecules in Edge Plasmas (F43027)

This CRP, discussed in the interim IFRC Subcommittee meeting in 2020, will address fundamental data needs concerning the formation, spectroscopic properties and reactions of molecular species in the boundary plasmas of magnetic-confinement fusion devices. It will result in the establishment of a trusted repository of evaluated data concerning the molecular species, particularly metal and nitrogen hydrides, relevant to the diagnostics and safety assessment of fusion energy reactors.
The CRP will be initiated before the end of the 2022–23 biennium, through the IAEA's usual mechanisms (CCRA approval, and preliminary Consultancy Meeting).

Appendix A: Terms of Reference

The Terms of Reference guiding the scope, operation and membership of the IFRC Subcommittee on Atomic and Molecular Data for Fusion is given below, with the changes proposed by the current Chairman indicated. It is presented to the Subcommittee for discussion and review. Of particular concern is the need to formalize the procedures for membership of this subcommittee and the need to improve its gender representation, in line with the ongoing IAEA-wide drive towards gender parity in its professional staff, meetings and cooperation activities.

METHODS OF WORK

IFRC Subcommittee on Atomic and Molecular Data for Fusion

Under the Terms of Reference of the IFRC Subcommittee on Atomic and Molecular Data for Fusion (hereinafter referred to as the Subcommittee), as approved by the IAEA Administration on ……1993, the Subcommittee is authorized to determine its own Methods of Work.

I. Scope and Responsibilities

In addition to the general functions of the Subcommittee, stated in the Terms of Reference, the Subcommittee shall

- regularly review the IAEA programme on A + PMI for Fusion;
- review Atomic, Molecular and Plasma-Material Interaction data needs and recommend their priorities;
- assist in specifying and planning topical data meetings and coordinated research programmes;
- assist in maintaining contacts between the IAEA Atomic and Molecular Data Unit and the fusion community;
- assist in the coordination of data centres.

II. Organization

1. Chairman: the Chairman shall be a member of the Subcommittee and shall serve for two meetings. The Chairman may be renominated by the Subcommittee. The responsibility of the Chairman shall remain in effect between meetings, until the following meeting, and he shall be kept informed by the Subcommittee members and the Scientific Secretary of relevant activities and developments.

2. Vice-Chairman: a Vice-Chairman shall be a member of the Subcommittee and shall serve for two meetings.

3. Scientific Secretary: the Scientific Secretary shall be the Head of the A + PMI Data Unit of the IAEA Nuclear Data Section, and shall serve as a member of the Subcommittee.

4. Membership: the Subcommittee shall be composed of 12 – 14 scientists representing the diverse national (e.g., Universities, National Laboratories, etc.) and international (eg., EURATOM, ITER, etc.) organizations involved in related research activities. Should it become necessary for a Subcommittee member to be relieved of his or her membership, it shall be their responsibility to arrange for their replacement in collaboration with the Chairman and the Scientific Secretary of the Subcommittee, and the pertinent IFRC member.

III. Meetings

1. Preparation: the preparation of the meetings shall be done in a timely manner by the Scientific Secretary of the Subcommittee in collaboration with the Chairman.

2. Frequency: the Subcommittee shall nominally meet every two years at the IAEA headquarters.

3. Proceedings: the proceedings of the meetings shall be written by the Scientific Secretary, and shall be issued as an IAEA report after having been approved by all Subcommittee members. The proceedings of every meeting shall be distributed to the IFRC and INDC committees, the A + PMI data centres and to the directors of all major fusion laboratories in member states.

4. Observers: all meetings of the Subcommittee shall be open to observers.

Appendix B: Subcommittee Members

Robin BARNSLEY, ITER Organization Headquarters, Diagnostics Division, Bldg 72/377, Vinon-sur-Verdon, CS 90046, 13067 ST PAUL LEZ DURANCE, FRANCE

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Appendix C: 2019 Joint IAEA–ICTP Workshop on Spectroscopy in Plasma

The organisers of the 2019 Joint IAEA–ICTP Workshop on Atomic and Molecular Spectroscopy in Plasmas, which was held 6 – 10 May 2019, invited participants to complete an anonymous online questionnaire to gain feedback on the event; the results are given in this appendix.

2019 Joint ICTP-IAEA Workshop on Atomic and Molecular Spectroscopy in Plasmas

Summary of 30 responses.

What best describes your academic position?

Graduate Student	20
Post-doc	3
Career Scientist	6

Which describes your research best?

Theory	9
Experiment	21

Which *operating system* do you use most?

Windows	17
macOS	2
Linux / Unix	10
Other	1

How would you rate the School, overall?

mean = 8.63 (1.08)

1	0
2	0
3	0
4	0
5	0
6	2
7	1
8	10
9	10
10	7

How useful was the School to you, overall?

mean = 4.20 (0.70)

Not useful at all	0
A bit useful	0
Satisfactory	5
Good	14
Fantastic	11

How did you find out about this School?

wiki list of atomic meetings

Yuri spoke about that at RPHDM2018
supervisor
Supervisor
From colleagues in my research group
Via an Aalto University internal fusion group meeting.
Announcement of ICTP Scientific calendar.
From colleagues
My supervisor Prof. Pramod Goliath has participated in Winter school on plasmas at ICTP,Trieste exactly twenty years back. He provided me an opportunity to apply for this School .
Previous participants
advertised by a colleage (who visited a similar school some years ago)
A friend from my research group went to this school 2 years ago, and he recommended it to me.
from the advertisement in the conference
I came to know about it through my colleague.
Received an email with the flyer
A researcher, Dr. Yang Yang, in my group recommended me to participant this School.
Organizators told me about it
From ICTP webpage.
From my director.
My professor told me about the school.
I found out about this School from my doctoral supervisor.
Colleagues
My Ph.D. supervisor suggested me for ICTP school.
My advisor Lan Gao participated in the school in 2017.
By an announcement e-mail

What *percentage of the lectures* did you attend?

mean = 3.90 (0.30)

0 – 25%	0
26% – 50%	0
51% – 75%	□□□ 3
76% – 100%	□□□□□□□□□□□□□□□□□□□□□□□□□□ 27

How did you find the *level of difficulty* of the ATOMIC STRUCTURE lectures?

mean = 3.07 (0.52)

Far too easy	0
A bit too easy	□□□ 3
Just right	□□□□□□□□□□□□□□□□□□□□□ 21

A bit too hard	5
Impossible to follow!	0

How *useful* did you find the ATOMIC STRUCTURE lectures?

mean = 4.24 (0.62)

Not at all useful	0
Not very useful	0
Useful	3
Very useful	16
Exceptionally useful!	10

How did you find the *level of difficulty* of the MOLECULAR SPECTROSCOPY lectures?

mean = 3.37 (0.60)

Far too easy	0
A bit too easy	1
Just right	18
A bit too hard	10
Impossible to follow!	1

How *useful* did you find the MOLECULAR SPECTROSCOPY lectures?

mean = 3.50 (0.76)

Not at all useful	0
Not very useful	3
Useful	11
Very useful	14
Exceptionally useful!	2

How did you find the *level of difficulty* of the COLLISIONAL PHYSICS lectures?

mean = 3.24 (0.50)

Far too easy	0
A bit too easy	1
Just right	20
A bit too hard	8
Impossible to follow!	0

How *useful* did you find the COLLISIONAL PHYSICS lectures?

mean = 4.00 (0.74)

Not at all useful	0
Not very useful	1
Useful	5
Very useful	16

Exceptionally useful!	7

How did you find the *level of difficulty* of the LINE BROADENING lectures?

mean = 3.00 (0.37)

Far too easy	0
A bit too easy	2
Just right	25
A bit too hard	2
Impossible to follow!	0

How *useful* did you find the LINE BROADENING lectures?

mean = 3.76 (0.86)

Not at all useful	0
Not very useful	2
Useful	9
Very useful	12
Exceptionally useful!	6

How did you find the *level of difficulty* of the COLLISIONAL RADIATIVE MODELLING lectures?

mean = 3.18 (0.54)

Far too easy	0
A bit too easy	2
Just right	19
A bit too hard	7
Impossible to follow!	0

How *useful* did you find the COLLISIONAL RADIATIVE MODELLING lectures?

mean = 3.75 (0.95)

Not at all useful	0
Not very useful	3
Useful	8
Very useful	10
Exceptionally useful!	7

How did you find the *level of difficulty* of the OPACITIES lectures?

mean = 3.14 (0.43)

Far too easy	0
A bit too easy	1
Just right	23
A bit too hard	5
Impossible to follow!	0

How *useful* did you find the OPACITIES lectures?

mean = 3.66 (0.76)

Not at all useful	0
Not very useful	1
Useful	12
Very useful	12
Exceptionally useful!	4

How *useful* did you find the PRACTICAL SESSIONS?

mean = 3.52 (1.07)

Not useful at all	2
A bit useful	3
Satisfactory	6
Good	14
Fantastic	4

How did you find the *lecture facilities and resources* (room, projector, website, etc.)

mean = 3.76 (0.86)

Awful	0
Bad	4
Average	3
Good	18
Excellent	4

(If you stayed in an ICTP Guesthouse) How do you rate the *accommodation* offered for the School

mean = 3.92 (0.83)

Awful	0
Bad: worse than I would have expected	0
Neither better nor worse than expected	10
Better than I was expecting	8
Excellent	8

What did you NOT like about the School? Please be open and honest.

Too many classes on thursday.

The lecture room had stale air and was crowded with too many chairs.

I think the material should be available online in advance of the lectures, at the latest during the lecture - as is, any "as we saw on previous slides"-statements are more annoying than helpful when one cannot check yourself. The room was quite dark at times, and air could be really bad, which really hampers focusing on the lectures.

it would be much more better if the slides in addition to the references related to each lecture were published on the website a day before the lecture. now some of them are not available even after the lectures.

A bit hard to follow a pure présentation the whole day long. À bit more practical sessions (morning or after noon sessions) would have been even more appreciated.

The period of the school should be longer because the lectures of the school are great. However, it should have more time for discussion with experts and understanding the materials.

Too high temperature in the lecture room.

I expected we will be able to visit laboratories and facilities available for plasma experiments like Elettra facility. But the schedule of the programme was tight to provide us an opportunity to visit those facilities

I would like to have some real practise during the practical sessions. It would very nice for example to see how FAC or othe relative softwares are working.

the practical sessions were a bit too superficial; a "real" practical session, e.g. by providing a task to solve by means of e.g. FLYCHK (or any other resource) to have a meaningful exercise would have been very nice.

Some of the lecturers had just a lot of maths on the slides and were going through it too fast to follow it properly (especially line broadening and first lecture of molecular spectroscopy) . The mathematics weren't extremely complicated but some lecturers just didn't give enough time to follow the talk properly and appreciate the presentation. I enjoyed the school immensely and found it extremely useful and informative, however the practical sessions were a bit of a disappointment. I understand that we were very short on time, but if it was possible to extend the school for a little longer and have more practical sessions in which we would go through some calculations (by hand like Dr. Yuri Ralchenko had during one of his classes), and also some more modelling. I was also expecting to use more advanced modelling codes (Cowan or FAC) during the school, so I was a little disappointing about not learning about that. However I understand that we had time constraints and Flychk was a good introduction into atomic physics modelling. The fusion talks were a bit difficult to follow, once the lecturer went into greater detail, but I think it was simply because of different background and lack of knowledge in the area.

The school should prapare some materials before the beginning so we can flow the lectture

It would be great if there were also practical sessions related to each lecture topic.

More communication before the school started would've been very helpful, even a quick email with the basic information a week or two before would've helped. Otherwise, everything was fantastic!

I actually like every thing about the School, and find the lectures are really useful for me.

There is nothing that I really didn't like about this school.

I like all the activities.

Maybe students can make one presention to describe their present works, so that communication for each other could be much easier.

It was a good experience at ICTP and I like it.

The food is not very delicious.

The biggest issue on a daily basis was that the lecture room was so uncomfortable and hot. It was actually distracting. I think having more group events outside of the lectures would have been nice. Maybe a group trip to visit something in the city?

I found during the poster session, all the participants were presenting their poster together. I realized that when I was presenting my poster, I got less time for the discussion. It would be nice if organizers can organize two poster sessions for good discussion.

Some lectures (though not on topics mentioned above) were not very interesting or useful, in particular the ones that focused heavily on ITER engineering rather than spectroscopic considerations. These felt like long slogs with little benefit -- an opinion which I heard echoed by others who study magnetic confinement. There was also a lack of communication before the school that made some things surprising at the outset. I wish I had been explicitly told of the following before arrival: - The ICTP is in fact not in Trieste, but in Grignano, a bus ride away from the city (it is not really excusable that I didn't know this before arriving, but it would be nice to have stated this openly) - Posters were required and to be presented by all attendees on Monday (though we all promised this in the application, I heard no communication about a poster and remembered with not much time to prepare. Others seemed to be in a similar boat.) - There are two guest houses, which was not clear to me when I began searching for the Adriatico. I was lucky to have others on my bus to direct me.

Please write any further comments you would like to add below.

Good amount of lectures, breaks, and coffee/snacks. Some of the practical sessions could have been shorter or one swapped for social program. Great that affordable accommodation close to the venue was offered. I would love more information on molecular processes and spectroscopy. Accompanying manuscripts for the lectures would be great for future reference as they tend to be more comprehensive than the slides, and tend to contain references to important original papers.

i appreciate you for all your efforts for this exceptional useful workshop.
Very nice school. Many thanks for providing this opportunity to me.
Theory of plasma spectroscopy was covered in great detail. To my mind, it would be beneficial for students of this School to have a lecture or two on each of the following topics: Spectroscopic Equipment and Spectroscopic Techniques. This way students will get, in addition to theoretical background, basic information on how to measure important plasma parameter like Ne, Te, Zeff, E, B. Modern spectroscopic techniques could be discussed too: MSE, LIF, Doppler-free spectroscopy, etc.
The best summer school I have ever attended!
I thank
Its a really usefull school.
very nice school with nicely selected and balanced topics. Although not taking home many things I can *instantly* put to use at home, the school certainly left me with a significant motivation to dive deeper into the detailed physics of my spectra. Thank you all very much for that!!
I would like to thank all the organisers and professors involved in the school for their time and great passion with which they were teaching during this week. I must highlight that I enjoyed Dr. Yuri Ralchenko's lectures immensely and found his lectures captivating and extremely informative and easy to follow. I really enjoyed all the other lectures as well and I am thankful for having the opportunity to meet both the lecturers and the talented students involved in the school. It was a stimulating experience and it motivates me to learn more on the subject of atomic and molecular spectroscopy.
I hope we can access the material in the ictp in the future
Thanks a lot to the organizers for the school.
Is it possible to take videos for such nice courses.
Just a suggestion : maybe a mix between more basic lectures and more advanced conferences should be great for everybody...
No further comments. Just keep it up.
The words on the slides can be larger because some pages were too small to be see clearly.
On the whole, this was a phenomenal experience that has given me a number of explicit research insights directly -- and I am sure many more are to come from continued conversation with lecturers and participants. A side note: many other interesting classes were going on at ICTP simultaneously to our visit; in particular, I received a lot of useful coding advice by communicating with students of a Cooperative Programming course occurring at Guesthouse Adriatico. It would have been interesting for the organizers to explicitly say whose company we were in. Thank you for all your hard work putting on such an excellent program!
It was just a very rich, brainstorming and warmful week despite the weather

Appendix D: Statistics for the Crowdsourcing Challenge on Materials for Fusion

Table 1. Unique locations of data file downloads for the Crowdsourcing Challenge

Belgium	Brussels
Brazil	São Paulo
Canada	Montreal Toronto
France	Paris
Germany	Berlin Frankfurt am Main Hamburg
India	Chennai Mumbai
Italy	Milan Rome
Japan	Tokyo
Netherlands	Amsterdam
Norway	Oslo
Portugal	Lisbon
Serbia	Belgrade
Singapore	Singapore
South Africa	Johannesburg
Spain	Madrid
UAE	Dubai
UK	London Manchester
US	Ashburn Boston Chicago Los Angeles Newark San Francisco San Jose Seattle

Table 2. Subscribers to the Crowdsourcing Challenge. The countries of 115 subscribers could be identified from their affiliation or contact details. The table below. The numbers in parentheses identify the number of subscribers from each country who submitted a solution to the Challenge.

Country	Number of subscribers		Country	Number of subscribers
UK	25(2)		Yemen	1(1)
India	13(1)		Serbia	1
China	11(1)		Tanzania	1
US	9(1)		Timor-Leste	1
Nigeria	6		Czechia	1
Germany	5(3)		Venezuela	1
Italy	4(1)		Mozambique	1
Madagascar	3		Canada	1
Portugal	3		Brazil	1
Nepal	2		Belgium	1
Pakistan	2		Guatemala	1
Egypt	2		UAE	1
Saudi Arabia	2		IAEA	1
France	2		Spain	1
Iran	2(1)		Israel	1
Denmark	2		Japan	1
Austria	2		Morocco	1
Sudan	1		Slovakia	1
Ukraine	1			

Appendix E: Report of the winning submission to the Crowdsourcing Challenge

IAEA Challenge on Materials for Fusion: Analysing Simulated Damage in a Fusion Reactor

U. von Toussaint, J. Dominguez, M. Rampp, M. Compostella

July 14, 2018

Abstract

MD-simulations provide a powerful approach to simulate radiation damage in crystalline materials. The key challenges are to identify, classify and quantify the resulting damage due to the commonly relative small volume fraction of the modified parts of the sample and the potentially unforeseen atomic configurations after irradiation.

1 Personal Details

Name: U. von Toussaint[1], J. Dominguez[1], M. Rampp[2], M. Compostella[2]
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2 Description of solution to the Challenge

MD-simulations provide a powerful approach to simulate radiation damage in crystalline materials. Identification, classification and quantification of the resulting damage is particulary challenging due to

- the commonly relatively small volume fraction of the modified parts of the sample and
- the potentially unforeseen atomic (re-)configurations after irradiation

This motivates a two-staged approach: First apply an algorithm which can robustly identify defects within the sample to focus the attention on the relevant parts of the sample which can subsequently be analysed either by manual inspection and/or by further analysis tools. In the latter case there is often some prior knowledge about the defects to be expected available (e.g. single vacancies under electron irradiation) which should be included in the analysis - but which is almost surely not covering all types of induced defects. Therefore the analysis tools should also be sensitive to new types of defects and should also allow a characterisation/classification.

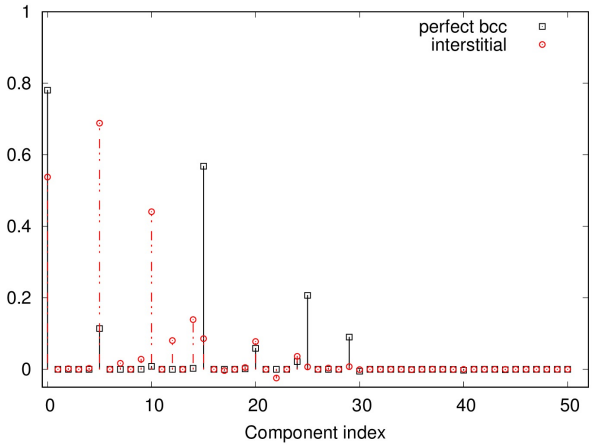

Figure 1: Descriptor vectors for two reference configurations

2.1 Identification of non-lattice structures

The apparently straight-forward identification of a localised atomic configuration as crystalline (i.e. defect free) in MD-sample data is hampered by the fact that the atoms do not reside at the ideal (local reference-frame based) lattice position but commonly show some individual displacement (e.g. due to thermal movement for temperatures T $>$ 0K). In addition, the estimation of a local reference frame may be challenging in its own (i.e. poly-crystalline materials) and can (in our experience) result in a large number of false positives.

In our approach we use the local environment (within some cut-off-radius) of an atom as measure, without relying on an external reference frame. This necessitates a description of the (local) lattice structure which is invariant under rotations (because the orientation is arbitrary). There are several means to achieve this (e.g. just using the distances to the neighbouring atoms) but we focused on the SOAP-based descriptor [2, 3] based on the expansion of the local environment of an atom into a bi-spectral representation. Several successful implementations of MD-potentials based on this descriptor [1] up to chemical accuracy indicate that the descriptor is indeed capturing the relevant features of the local environment. The calculation of the descriptor vector $\vec{d}$ for an atom in some environment can be done efficiently using a command-line interface to the open-source software quippy (http://libatoms.github.io/QUIP/intro.html). For the chosen parameters the descriptor vector was 51-dimensional. In a first step (various refinements have subsequently been considered, i.e. averaging over thermal lattice fluctuations, incorporation of covariances of the descriptor vector components, which also yielded some benefits and reduced the number of adjustable parameters (i.e. thresholds) but are not really crucial for the general approach) the descriptor vector $\vec{d}_{\mathrm{bcc}}$ for a tungsten atom in a perfect tungsten bcc-lattice with the provided parameters has been determined (see Fig. 1). Then, the descriptor vectors for all atoms j in the provided tungsten data-sets have been computed followed by the calculation of the distance s_j to the reference vector $\vec{d}_{\mathrm{bcc}}$. In the beginning we used (for simplicity) the unweighted Euclidean distance between the vectors as measure but evaluated later the (co-

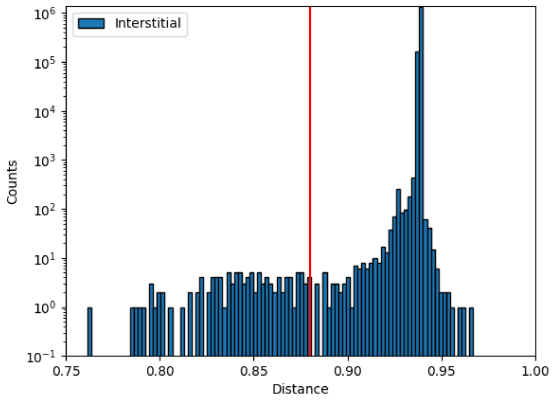

Figure 2: Histogram of the distances of the atom descriptor vectors to the tetrahedral interstitial structure descriptor $\vec{d}_{\mathrm{TI}}$.

)variance of each of the descriptor vector components using the descriptor vectors of a thermalized MD-tungsten sample. This enables the conversion (under some assumptions on the distribution) from a distance to a probability that an atom in a given environment can be considered as a 'lattice' atom. Nevertheless, to avoid cluttering the general approach with too many details: For the present report we just applied a simple threshold at a distance value above which we considered (by visual cross-checking with the atomic structure in real-space) the corresponding atoms as potential defects (or next to a defect).

2.2 Identification of defect sites

Having localised potential defect sites the next task is to identify these defects (e.g. is it an interstitial atom etc.). As a proof of concept we computed the descriptor vectors for a common type of defect: an interstitial atom at a tetrahedral site $\vec{d}_{\mathrm{TI}}$. The corresponding descriptor vector is given in Figure 1. Then we computed the distance of the atom descriptor vectors to $\vec{d}_{\mathrm{TI}}$. An example of the histogram of the distances for the tetrahedral interstitial case is given in Figure 2 (please note the log-scale). Using again a simple threshold in the tail left of the bulk of the atoms yielded the interstitial atoms (20 atoms). For other known types of defects the same cycle can be repeated and for each type a distance (or probability) can be computed. The approach presented so far provides only information at atom locations. To alleviate this shortcoming and to identify under-dense regions in addition also the field quantity $f\,(x,y,z)$ = distance_from_(x, y, z)_to_nearest_atom was computed (using the open source code KDTREE2). Values exceeding a lattice dependent threshold provide a clear indication of void regions (with a higher sensitivity than e.g. atom centric Voronoi-volumes, where empty volumes are shared between neighbouring atoms).

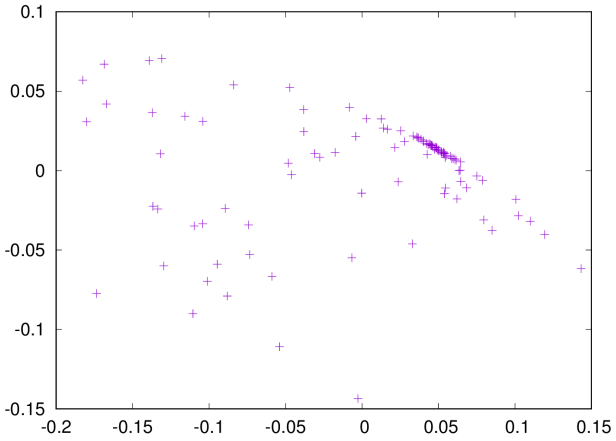

Figure 3: Display of the two most relevant principal components of the unclassified 51-dimensional atom descriptor vectors. Please note the cluster at (0.05,0.02).

2.3 Classification of unknown defect types

The proposed approach identifies deviations from a locally regular lattice structure and provides means to identify known defect types by comparison with suitable descriptor vectors. However, there may be unexpected or unknown defect structures. To tackle this problem we used the following approach: For all atoms (76 atoms) which had been identified as non-lattice atoms and did not belong to one of the known defect types a principal component analysis (PCA) has been performed. A projection into the 2-dimensional PCA-space of the 51-dimensional descriptor vectors yielded Figure 3, which clearly exhibits a cluster around (0.05,0.02) - the corresponding descriptor vector was labelled 'defect-type a'. Subsequently, the underlying atomic configurations have been analysed in real space and revealed an almost triangular arrangement of three voids. In this way also unexpected defect configurations can be identified, e.g. also in a semiautomatic manner by applying a cluster algorithm to the PCA-projections of varying dimension.

2.4 Visualization

For interactive exploration of the data in the three-dimensional space of the MD sample we employ the free visualization software package VisIt [4]. Standard functionalities of VisIt allow us to conveniently filter a subset of relevant atoms, based on the criterion $d_j > D_{\min}$, with cutoff $D_{\min} \approx 0.1$. All atoms that satisfy this criterion are rendered as spheres, with a radius proportional to the cube root of the atom-centric Voronoi-volume and colouring according to a (non-linear) mapping of distance measures for three different descriptor vectors ('defect-type a','void','tetrahedral interstitial') to RGB colour space. A volume rendering of the scalar function $f(x, y, x)$ is used to visualize under-dense regions as semi-transparent clouds. An example using the tungsten sample with the 50 keV-collision cascade employing the descriptor vector based selection and

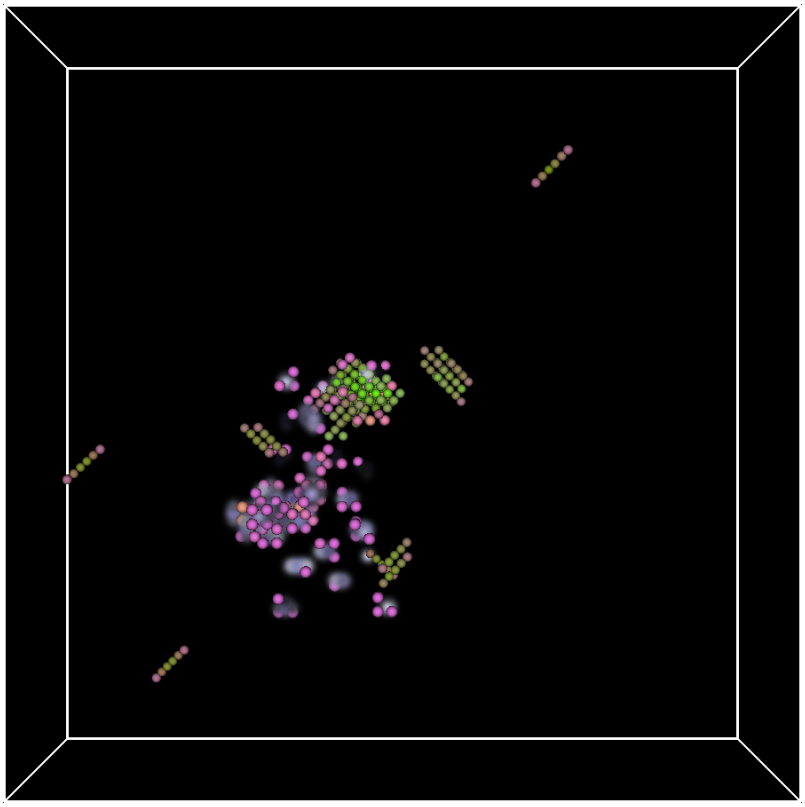

Figure 4: Visualization of the defect structure of the 50 keV-tungsten sample, indicating the different defect types using an RGB-color scheme as well as voids and the atomic Voronoi volume.

coloring is given in Figure 4. The linear displacment chains (caused by an interstitial) are clearly visible, which is simultaneously indicated by an reduced atomic Voronoi volume (slightly smaller sphere radius). Next to individual voids the pink colored atoms highlight this type of defect, whereas the orange color indicate lattice atoms in a 'type-a' environment, i.e. multiple atoms are missing in the neighbourhood. The green color channel (essentially proportional to the sum of the void and interstitial descriptor vectors distances) is sensitive to stronger lattice distortions (because the atomic environment has components of more than one base descriptor vector). For producing the final images and movies we make extensive use of the VisIt python interface.

Other used tools for the various visualizations (all are open source):

- xmgrace (http://plasma-gate.weizmann.ac.il/Grace/) : 2-d plots, histogram-calculation
- gnuplot (http://www.gnuplot.info/): for fast 3-d visualization

- Ovito (https://ovito.org/): a versatile open visualization tool for atomistic data

3 Please provide a detailed summary of the files in the uploaded archive

The following files are included:

- README : short overview over the data analysis chain and the used codes
- compute_vectors.py : Python code for computing the descriptor vectors
- distance_difference.py : Python code for computing the vector distance
- bcc_w.xyz : file with atomic coordinates as test data set
- W_descriptor_vectors.txt : two reference descriptor vectors (for bcc-lattice and for tetrahedral interstitial)
- reference_vector.dat : a reference descriptor vector (ready to be processed with distance_difference.py
- w_50keV.mp4 : Movie file for the detected and colour-coded defects for the 50 keV tungsten sample
- fe_10keV.mp4 : Movie file for the detected and colour-coded defects for the 10 keV iron sample
- w_200keV.mp4 : Movie file for the detected and colour-coded defects for the 200 keV tungsten sample
- *_VRGB.png : individual frames of the detected and colour-coded defects of the test-cases under different angles (15 in total, 5 for each considered case)
- w_50keV_submission.xyz.gz : the xyz-file of the 50 keV-tungsten test case augmented with the distances to the respective reference descriptors (this file contains the main result). It has 50 MB - if it cannot be attached to the submission due to size restrictions in the upload it can also be downloaded from http://www.rzg.mpg.de/~udt/w_50keV_submission.xyz.gz . The files for the other two cases can also be found there: http://www.rzg.mpg.de/~udt/w_200keV_submission.xyz.gz and http://www.rzg.mpg.de/~udt/fe_10keV_submission.xyz.gz .

4 Please provide a description of the tools required to compile, install and use the submitted code and the used OS

All software used by us is open source and all the data operations have been performed under different Linux operating systems (OpenSUSE, Ubuntu, Debian). Standard command-line tools like awk have been used for low-level file

conversions.
The main codes for the computation have been:

- Quippy and QUIP are used to compute the *descriptor vector* of the environment of an atom. QUIP is FORTRAN based and Quippy provides a Python interface to the QUIP routines. An installation guide is given here: https://libatoms.github.io/QUIP/install.html. Essentially standard Linux system tools are needed (Fortran compiler) and a very recent Python environment (e.g. Anaconda).
- KDTREE2: Fortran 95 and C++ software by Matthew B. Kennel to efficiently search for neighbours in a multi-dimensional Euclidean space (source: https://github.com/jmhodges/kdtree2). KDTREE2 has been used to compute the nearest-neighbour distance to the closest atom (Academic free licence).
- voro++: an open source software library for the computation of the Voronoi tessellation (http://math.lbl.gov/voro++/about.html) which has been used to compute the volume of the Wigner-Seitz cell of the atoms.
- LAMMPS: The molecular dynamics code LAMMPS has been used to compute the variance of the descriptor vectors under thermal atomic movement. The code is available at https://lammps.sandia.gov/.

5 Under which software licence is the code submitted to IAEA

All mentioned and used code packages are open-source under various software licences (BSD-type, GPL-type and Academic free licence) - please see the respective web-sites for the details. The data processing based on the other tools is then very simple and can be put under any GPL-licence (e.g. GPL3).

6 Further comments

The presented approach works very well and efficient in practice and we deliberately refrained from labour-intensive fine-tuning of thresholds. As already pointed out, the manual setting of thresholds can eventually be minimised by converting the distances into probabilities, e.g. by using the covariance matrices of the descriptor vectors and the associated χ-distribution. Then statistical approaches like (Bayesian) model selection are straightforward to apply. Several further refinements are conceivable:

- We did not change (i.e. optimize) the settings of the SOAP-descriptor vector. Here is definitely room for improvement. We also did not examine other descriptors.
- Other available quantities (like energy of the atoms) can easily be incorporated into the proposed detection scheme.

- The suggested approach is not limited to a static situation - it can also be applied to trace the time dependence of defect evolution: i.e. which meta-stable defect types (on MD-time scales) are in a collision cascade and do these defects anneal or as which type of stable defect do they end up?

- In addition it is worth mentioning that these additional descriptors are also perfectly suited for a machine learning approach because they enhance the space the algorithms can work on with high-level features. In a supervised case a domain expert identifies the atomic configurations of interest (either from scratch based on prior experience or guided by simulations) and thus enriches the reference descriptor vector set. But also unsupervised schemes are straightforward: cluster detection methods can be applied continously in a time-dependent simulation in the descriptor space. If a cluster is detected this can be followed up by backprojection into the real-space to identify the corresponding configuration (e.g. crack initiation) and the cluster can eventually be added to the set of descriptor vectors.

References

[1] Albert P. Bartók, Sandip De, Carl Poelking, Noam Bernstein, James R. Kermode, Gábor Csányi, and Michele Ceriotti. Machine learning unifies the modeling of materials and molecules. *Science Advances*, 3(12), 2017.

[2] Albert P. Bartók, Risi Kondor, and Gábor Csányi. On representing chemical environments. *Phys. Rev. B*, 87:184115, May 2013.

[3] Albert P. Bartók, Risi Kondor, and Gábor Csányi. Erratum: On representing chemical environments [phys. rev. b 87, 184115 (2013)]. *Phys. Rev. B*, 96:019902, Jul 2017.

[4] Hank Childs, Eric Brugger, Brad Whitlock, Jeremy Meredith, Sean Ahern, David Pugmire, Kathleen Biagas, Mark Miller, Cyrus Harrison, Gunther H. Weber, Hari Krishnan, Thomas Fogal, Allen Sanderson, Christoph Garth, E. Wes Bethel, David Camp, Oliver Rübel, Marc Durant, Jean M. Favre, and Paul Navrátil. VisIt: An End-User Tool For Visualizing and Analyzing Very Large Data. In *High Performance Visualization–Enabling Extreme-Scale Scientific Insight*, pages 357–372. Oct 2012.

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