Current Activities of IAEA A+M Unit

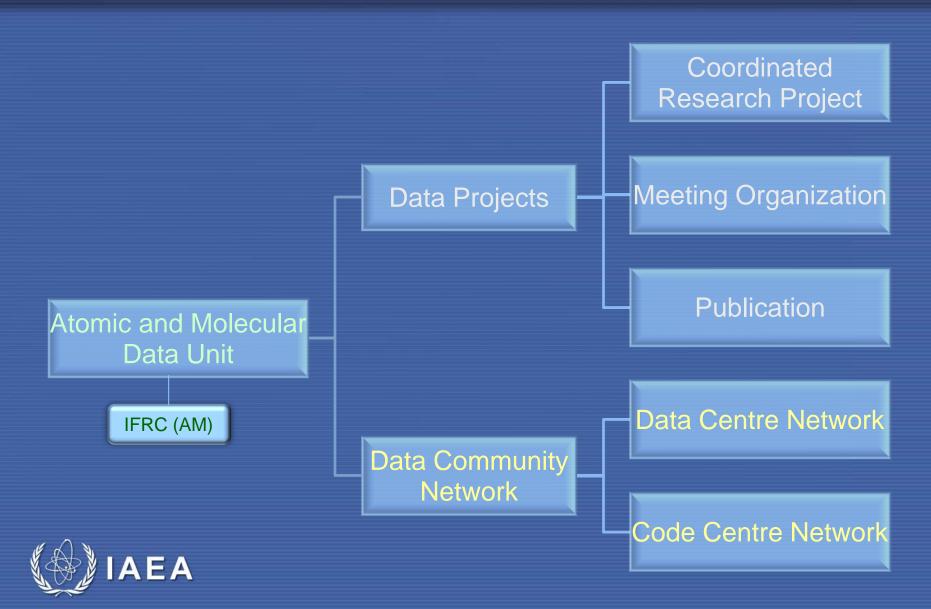
B. J. Braams and H.-K. Chung

Atomic and Molecular Data Unit, Nuclear Data Section Division of Physical and Chemical Sciences

23rd Data Centre Network (DCN) Meeting, November 2-4, 2015



Atomic and Molecular Data Unit Activities



Coordinated Research Projects

Data Generation and Exchange

CRP: Coordinated Research Project

- Main mechanism by which the AMD Unit encourages new research
- Unique Opportunity for Comprehensive and Synergistic Collaboration

Joint research on Atomic, Molecular & Plasma Surface Interaction Data for fusion:

- Representatives from 10 to 15 institutes world-wide
- Duration 3-4 years; 3 Research Coordination Meetings (RCM)

Objectives: To define and to coordinate international research on:

- Generation, compilation and evaluation of data
- Establishment of databases
- Development of new techniques

Outputs:

- Publications, Meeting Presentations and Reports
- <u>Final Reports</u> in "Atomic and Plasma-Material Interaction Data for Fusion" (APID); more recently in a journal (JPCS, Atoms)
- Data and Results in ALADDIN Numerical <u>Database and Knowledge Base</u>



Past, Present and Future CRPs

http://www-amdis.iaea.org/CRP

- 2008-2012: Characterization of Size, Composition and Origins of Dust in Fusion Devices
- 2009-2013: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions
- 2010-2014: Spectroscopic and Collisional Data for W from 1 eV to 20 keV
- 2011-2015: Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma
- 2012-2016: Erosion and Tritium Retention for Beryllium Plasma-Facing Materials
- 2013-2017: Plasma-Wall Interactions with Irradiated Tungsten and Tungsten Alloys in Fusion Devices
- 2015-2019: Plasma-wall Interaction with Reduced-activation Steel Surfaces in Fusion Devices
- 2016-2020: Data for Charge Transfer Processes Related to Neutral Beams in Fusion Plasma



CRP on Spectroscopic and Collisional Properties of Tungsten from 1 eV to 20 keV (2010-2014)

Objectives

- Concerned with W in all plasma regions, edge to core
- Theory and experiment are both represented, with overlap among and between the two
- Aim to produce validated database for tungsten in plasma

Data needs

- Electron-impact, radiative and photoninduced, and heavy particle collision processes
- Cross-sections for kinetic modelling
- Rate coefficients for macroscopic modelling
- Spectroscopic signatures for diagnostics

Research Coordination Meetings

First RCM: 13-15 December 2010

Second RCM: 29-31 August 2012

Third RCM: 06-08 October 2014



Participants

R. SRIVASTAVA IIT Roorkee

A. MÜLLER University of Giessen

N. NAKAMURA University of Electrocommunications

A. RYABTSEV Russian Academy of Sciences

A. . WYART/ Observatoire de Paris

W. TCHANG-BRILLET

P. BEIERSDORFER LLNL

C.-Z. DONG Northwest Normal University

F. KOIKE Kitasato University

V. NIKULIN/ St Petersburg Nuclear Physics Institute

M. TRZHASKOVSKAYA

V. LISITSA, Kurchatov Institute

N. BADNELL, University of Strathclyde

J. COLGAN, Los Alamos National Laboratory

Yu. RALCHENKO, NIST D. KWON KAERI

CRP on A+M Data for State-Resolved Modelling of H, He and their Isotopes in Fusion Plasma (2011-2015)

Objectives

- Species H, H⁺, H₂, H₂⁺, H₃⁺, He, He⁺, He₂⁺, HeH⁺, He₂⁺, H⁻ and isotopic variants; isotope effects are important; He is newly important
- Aim to be comprehensive for volume processes among the mentioned species and e-, hv
- Predominantly theoretical; some experiment

Data needs

- State-resolved cross-sections for kinetic modelling
- Electron-impact, radiative and photon-induced, and heavy particle collision processes

Research Coordination Meetings

First RCM: 10-12 August 2011 **Second RCM**: 3-5 July 2013 **Third RCM**: 14-16 March 2016



Participants

R. CELIBERTO

U. FANTZ

C. JUNGEN

I. SCHNEIDER

V. KOKOOULINE

P. KRSTIC

X. MA

O. MOTAPON

A. OREL

D. REITER

K. SAWADA

X. URBAIN

J.-S. YOON

Polytechnic of Bari, Italy

MPI for Plasma Physics, Garching

Laboratoire Aimé Cotton du CNRS

Université Le Havre

University of Central Florida

Oak Ridge National Laboratory

Chinese Academy of Sciences

University of Douala, Cameroon

University of California at Davis

Forschunszentrum Jülich

Shinshu University

Catholic University of Louvain

National Fusion Research Institute

CRP on Erosion and Tritium Retention in Beryllium Plasma Facing Components (2012-2016)

Objectives

The key processes to be studied are physical and chemical sputtering by H, He and Be, which release beryllium impurities into the plasma, trapping and reflection of hydrogen (H, D, T) on beryllium surfaces, the transport of hydrogen in beryllium and means to extract trapped tritium.

Data needs

- Data for routine interaction of H/He and impurity ions with Be surface, and in transient events (melting, ablation)
- Most important projectiles: H, D, T,
 He, Be, C, N, O, Ne and Ar
- Data of mixed materials, especially, Be-(H,D,T,He), Be-C, Be-N, Be-O and ternary and higher mixtures

Research Coordination Meetings

First RCM, 26-28 Sep 2012 **Second RCM**, 18-20 Aug 2014

Participants

R. DOERNER/

D. NISHIJIMA

D. BORODIN

M. PROBST

S. IRLE/

H. NAKAMURA

K. NORDLUND/

C. BJÖRKAS

Ch. LINSMEIER

W. JACOB

PISCES Lab, UCSD

Forschungszentrum Jülich:

University of Innsbruck: Nagoya University:

University of Helsinki

Forchungszentrum Jülich

IPP, Garching



CRP on Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices

Objectives

To support assessment of the prospects for tungsten-based plasma-facing materials in a fusion reactor environment

Data needs

- •effects of neutron irradiation and charged particle surrogate irradiation on the microstructure of tungsten-based materials.
- •relation between tungsten microstructure after irradiation and plasma-material interaction properties for erosion, tritium retention and tritium migration.
- •Synthesize information, extrapolate to fusion neutron fluence, and provide best expert estimates and uncertainties for tritium retention and tritium transport

Research Coordination Meetings

First RCM, 26-28 November 2013 Second RCM, 8-11 September 2015



<u>Participants</u>

- G. H. Lu et al., Beihang University, Beijing.
- C. Liu, X. Wu et al., ISSP-CAS, Hefei.
- G. Luo, C. Zhang et al., IPP-CAS, Hefei.
- M. Barthe, C. Becquart et al., CNRS.
- C. Grisolia, B. Rousseau et al., CEA.
- M. Mayer, T. Schwarz-Selinger et al., IPP Garching.
- B.Unterberg, J. Linke, Forschungszentrum Jülich.
- S.Deshpande, P. M. Raole et al., IPR, Gandhinagar.
- A.Hasegawa et al., Tohoku University.
- Y. Hatano, Y. Oya et al., Toyama University.
- M. Sakamoto, H. Watanabe et al., U. of Tsukuba.
- T.Oda, H. Shim et al., Seoul National University.
- Y. Gasparyan, A. Pisarev et al., MEPhl, Moscow.
- B. Khripunov, A. Ryazanov et al., Kurchatov Ins
- S. Markelj et al., Josef Stefan Institute, Ljubljana.
- S. Dudarev et al., CCFE, Abingdon.
- B. D. Wirth et al., U. of Tennessee, Knoxville.
- J.Allain, D. Ruzic et al., University of Illinois.
- M.Shimada, B.Merrill et al., Idaho National Lab.

CRP on Plasma-wall Interaction with Reducedactivation Steel Surfaces in Fusion Devices

Background

- Main wall in DEMO or in a reactor will not be beryllium (too high erosion); tungsten is also unattractive (radiation issues). Some kind of low-activation steel looks attractive for the main wall, but more data are needed to assess just where it could be used.
- Special issue with steel: the alloy could be "self-passivating" with respect to erosion.

CRP Topics and Objectives

- Develop information about the microstructure of steel surfaces exposed to fusion neutrons and energetic plasma particles.
- Develop information about the relation between steel microstructure after irradiation and properties for erosion, tritium migration and ways to extract trapped tritium.
- To synthesize new information and provide best expert estimates and uncertainties for plasmamaterial interaction properties for steel surfaces in a fusion reactor environment.

Participants

- Peng Wang, Lanzhou Institute of Chemical Physics
- W. Jacob and T. Schwarz-Selinger, IPP Garching
- Y. Hirooka and N. Ashikawa, NIFS
- A. Golubeva and A. Spitsyn, Kurchatov Institute
- R. Doerner and D. Nishijima, UCSD PISCES Lab
- V. Maklai and I. Garkusha, IPP Kharkov
- D. Terentyev and L. Malerba, SCK-CEN

Meeting Plan

- First RCM: 9-11 December 2015
- Second RCM: Appr. Q2, 2017



CRP on Data for Charge Transfer Processes Related to Neutral Beams in Fusion Plasma

Planned CRP; tentative title

Proposal is due in Q2 2016; CRP could start in Q4 2016 or Q1 2017

Core topics and objectives

Develop data for collision processes of neutral beams in fusion plasma

Scope to be better defined

- Heating and diagnostic neutral beams
- H/D/T beams for sure; He, Li beams most likely; maybe other (Ne, Ar, ...)
- Charge transfer processes and related (CXRS) spectroscopy
- Beam excitation and related (BES) spectroscopy
- Motional Stark Effect (MSE) diagnostics
- Processes in the beam generation, negative ion production and neutralization? (Probably not)

Meeting schedule

- Consultancy meeting to help define the scope in March 2016
- First RCM could be near the end of 2016 or early 2017



CRP beyond 2016 (very tentative)

Procedure

- Preliminary proposal or proposals are submitted in the course of 2016
- Definitive proposal about 9 months before the intended start of the CRP
- Instead of a CRP we can choose to organize one or more technical meetings

Possible topic: Data for plasma interaction with liquid metal surfaces

- Most interest: Li, Ga, Sn
- Interest in plasma contamination and tritium retention
- Possible interest in related spectroscopy

Possible topic: Codes and data for vapour shielding in fusion plasma

- Relevant for disruptions, other pulsed heat load on walls
- Also relevant for pellet injection (D/T; impurity seeding)
- Classic problem of radiation transport
- Likely involvement from the WDM/HDM/ICF community



Meetings in 2013

- Final RCM on "Light Element (H, He, Li, Be) Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions"
 - 20-22 Mar 2013, IAEA Headquarters, Vienna, Austria
- TM on "International Code Centres Network"
 - 6-8 May 2013, IAEA Headquarters, Vienna, Austria
- 2nd RCM on "A & M Data for State-Resolved Modeling of Hydrogen and Helium and Their Isotopes in Fusion Plasma"
 - 3-5 July 2013, IAEA Headquarters, Vienna, Austria
- The 2nd SLSP Code Comparison Workshop
 - 5-9 August 2013, K+K Maria Theresia Hotel, Vienna, Austria
- TM on "Technical Aspects of A & M Data Processing and Exchange 22nd Meeting of the A & M Data Centres Network"
 - 4-6 Sep 2013, IAEA Headquarters, Vienna, Austria
- 1st RCM on "Plasma-Wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices"
 - 25-29 Nov 2013, IAEA Headquarters, Vienna, Austria
- CM on "Data Evaluation of N₂ Molecules"
 - 5-6 Dec 2013, IAEA Headquarters, Vienna, Austria



Meetings in 2014

- TM of the International Fusion Research Council Subcommittee on A & M Data for Fusion
 - 28-29 April 2014, IAEA Headquarters, Vienna, Austria
- Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical A & M Scattering Data
 - 7-9 July 2014, Cambridge, MA, USA
- 2nd RCM on ""Data for Erosion and Tritium Retention in Beryllium Plasma Facing Materials"
 - 18-19 Aug 2014, IAEA Headquarters, Vienna, Austria
- CM on "Plasma Interaction with Steel Surfaces"
 - 20 Aug 2014, IAEA Headquarters, Vienna, Austria
- 16th International Conference on Radiative Properties of Hot Dense Matter (RPHDM)
 - Sep 29- Oct 3, 2014, Vienna, Austria
- 3rd RCM on "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV"
 - 6-8 October 2014, IAEA Headquarters, Vienna, Austria
- Joint ICTP-IAEA Conference on Models and Data for PMI in Fusion Devices
 - 3-7 Nov 2014, Trieste, Italy
- IAEA Technical Meeting on A & M and PMI Data for Fusion Science and Technology
 - 15-19 December 2014, Daejeon, Korea



Meetings in 2015

- The 3rd Spectral Line Shapes in Plasma Workshop
 - 2-6 March 2015, Marseille, France
- Joint ICTP-IAEA Advanced School and Workshop on Modern Methods in Plasma Spectroscopy
 - 16-27 March 2015, Trieste, Italy
- CM on "Guidelines for Uncertainty Quantification of theoretical atomic and molecular data"
 - June 22-23 2015, IAEA Headquarters, Vienna, Austria
- CM on "Evaluation and Uncertainty Assessment for Be, C, Ne Atomic Data"
 - July 13-15 2015, IAEA Headquarters, Vienna, Austria
- TM on "International Code Centres Network on Simulation of PMI Data"
 - July 29-31 2015, IAEA Headquarters, Vienna, Austria
- 2nd RCM on "PWI for Irradiated Tungsten and Tungsten Alloys in Fusion Devices"
 - September 8-11 2015, Seoul National University, Seoul, Korea
- Joint IAEA-KAERI CM on "Recommended Data for Processes of Tungsten Ions"
 - September 14-16 2015, Korea Atomic Energy Research Institute, Daejeon, Korea
- TM on "Technical Aspects of A & M Data Processing and Exchange, 23rd Meeting of the A & M Data Centres Network"
 - November 2-4 2015, IAEA Headquarters, Vienna, Austria
- 1st RCM on "Plasma Interaction with Reduced-Activation Steel Surfaces in Fusion Devices"
 - December 9-11 2015, IAEA Headquarters, Vienna, Austria



Meetings in 2016 (highlights)

- 3rd RCM on Atomic and Molecular Data for Hydrogen and Helium in Fusion Plasma
 - 14-16 March 2016, IAEA Headquarters, Vienna, Austria
- CM on data evaluation for heavy particle collision processes; CM on processes of neutral beams in fusion plasma
 - 17-18 March 2016, IAEA Headquarters, Vienna, Austria
- 3rd RCM on Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials
 AprilMay/June 2016, IAEA Headquarters, Vienna, Austria
- Joint ICTP-CAS-IAEA School and Workshop on Plasma-Material Interaction in Fusion Devices
 - 18-22 July 2016, Hefei, China
- <u>?? TM on Uncertainty Assessment for calculated atomic, molecular and plasma-material</u> interaction data
 - Oct-Nov 2016, IAEA Headquarters, Vienna, Austria
- ?? TM on benchmarking experimental and theoretical A+M collision data
 - Oct-Nov 2016, IAEA Headquarters, Vienna, Austria
- CM on recommended data for hydrogen and helium in fusion plasma
 - Q4 2016, IAEA Headquarters, Vienna, Austria
- CM on Data Exchange (XSAMS, etc.)
 - Q4 2016, IAEA Headquarters, Vienna, Austria
- 1st RCM on Data for Collision Processes related to Neutral Beams in Fusion Plasma
 Q4 2016, maybe Q1 2017, IAEA Headquarters, Vienna, Austria

Publications

http://www-amdis.iaea.org/publications/

- IAEA-INDC(NDS) Reports (http://www-nds.iaea.org/publications/)
 - Reports are published for every meeting
- International Bulletin on Atomic and Molecular Data for Fusion
 - Bibliographic Information on Atomic, Molecular and Plasma-Surface Interaction Data
 - No publication since 2013
- Atomic and Plasma-Material Interaction data for Fusion (APID Series)
 - Data and papers related to results produced by CRPs and Consultants groups
 - All volumes are available on-line (http://www-amdis.iaea.org/publications/APID/)
 - Edition in preparation

Volume 17: CRP on "Atomic Data For Heavy Element Impurities in Fusion Reactors Volume 18: CRP on "Light Element A & M and Radical Behaviour in the Divertor and Edge Plasma Regions" Volume 19: CRP on "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV"

- Special issues at Atoms Journals
 - Critical Assessment of Theoretical Calculations of Atomic Structure and Transition Probabilities (2014)
 - Spectral Line Shapes in Plasmas Print Edition available (March 2014)
 - Atomic Data for Tungsten (July 2015)



Network Collaboration for AM/PSI Data for Fusion

Data Users

Fusion Laboratories

ITER
EFDA
JET, UKAEA
ASDEX-Upgrade, IPP
TEXTOR, Jülich, FZJ
KSTAR, NFRI
NIFS, JAEA
PPPL, ORNL

<u>IAEA</u> Coordination

CRP
Publications
Knowledgebase
Databases
Meetings

Data Producers

Code Centre Network

Curtin Univ. I. Bray
Kitasato Univ. F. Koike
Univ. Autonoma de Madrid I. Rabadan
Univ. P&M. Curie, Paris, A. Dubois
Univ. of Bari, M. Capitelli
Kurchatov Institute, A. Kukushkin
Lebedev Institute, L. Vainshtein
Ernst-Moritz-Arndt Univ, R. Schneider
NIST, Y. Ralchenko
PPPL, D. Stotler
LANL, J. Abdallah Jr.
IAEA, B. J. Braams
HULLAC M. Klapisch
CNEA, P.D. Fainstein
Weizmann, E. Stambulchik

Data Centres & Evaluators Data Centre Network

ADAS, Summers H.
CRAAMD, Jun, Y.
FZJ, Reiter D.
IAEA, Braams, B. J.
JAEA, Nakano, T.
KAERI, Kwon, D.
Kurchatov, Kukushkin, A. B.
NIFS, Murakami, I.
NIST, Ralchenko, Y.
NFRI, Yoon, J.



Atomic Molecular Data Information Services

http://www-amdis.iaea.org



International Atomic Energy Agency

Atomic Molecular Data Services

Provided by the Nuclear Data Section

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☆ IAEA Meetings

Molecule and Radical

Mar. 20-22, 2013 3rd RCM of CRP on "Light Element Atom,

Behaviour in the

Plasma Regions' May 6-8, 2013

Centre Network

Jul 3-5, 2013

Atomic and

Modelling of

Hydrogen and

Helium and Their Isotopes in Fusion

Plasma

22nd Meeting of the

Sep 4-6, 2013

Molecular Data

Centres Network

AMO/PSI Meetings

and Oscillator Strengths

2013: Atomic Spectra

for Astrophysical and

Laboratory Plasmas

Belgium Sep 30- Oct 4,

(ASOS-11), Mons,

2013:66th Annual

Workshop

Gaseous Electronics

Conference

Nov 4- 8, 2013: The 8th NLTE Code Comparison

Atomic and

Nov, 2013 1st RCM of CRP on

Plasma-Wall

August 5-9,

Divertor and Edge

Meeting of the Code

2nd RCM of CRP on

Molecular Data for

State-Resolved

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Activities

IFRC Subcommittee CRP Publications Meetings Workshops Data Centre Network Code Centre Network XSAMS

★ Contacts

Links Contacts

Atomic and Molecular Data Unit Activities

The Atomic and Molecular Data Unit operates within the Nuclear Data Section of the International Atomic Energy Agency, Vienna, Austria. The primary objective of the Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other plasma science and technology applications.

Databases on Atomic and Molecular Data for Fusion.

Atom, Molecule lasma-Surface Data

ALADDIN Numerical Database

Bibliographic

Atomic Data Search Engine Database

OPEN ADAS Rovibronic Energy levels

H₂ & Isotopes

Online Computing Capabilities

Code Centres **Portal**

LANL Atomic **Physics**

FLYCHK Non-LTE **Kinetics**

Heavy **Particles** Collisions

Averaged e- Impact Cross-section

Effective e- Ionization Rates

ATOM-AKM e - Collision Data

· Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data for Fusion

Our Unit achieves its objectives by coordinating the activities of the International Atomic and Molecular Data Center Network (DCN) and Code Center Network (CCN), initiation and conducting international Coordinated Research Projects (CRP), organization of various types of Expert's Meetings, publication of technical reports on meetings and research activities and using other forms (research contracts, research agreements, consultancies) for stimulation of the generation, collection and critical assessment of the required atomic, molecular (A+M) and plasma-material interaction (PMI) data information.

The activity of Our Unit is supervised and biennially reviewed by the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC A+M Subcommittee), an advisory body to the Agency's Director General.

IAEA Nuclear Data Section



and more































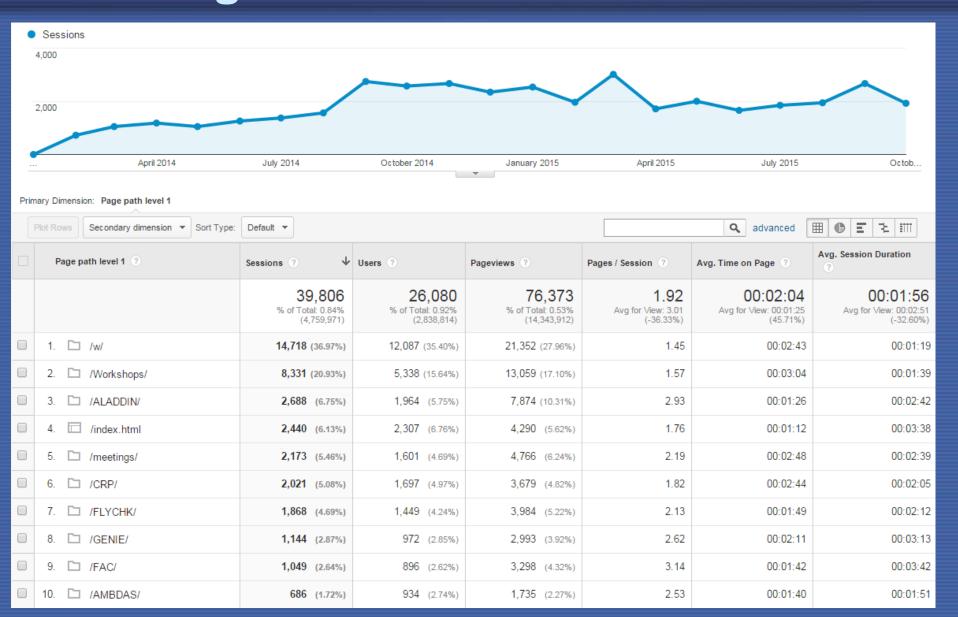




Codes

© Copyright 2007-2013, International Atomic Energy Agency - Nuclear Data Section, Vienna International Centre, P.O. Box 100, A-1400 Vienna, Austria Telephone (+431) 2600-0. Facsimile (+431) 2600-7. E-mail: online@iaeand.iaea.org, Read our Disclaimer

More than 2000 sessions per month after migration to cloud servers



Data Centre Network (DCN) Activities

http://www-amdis.iaea.org/DCN

Domain: atomic and molecular (A+M), particle surface interaction (PSI) and bulk material properties (plasma-material interaction - PMI) data for fusion and other applications.

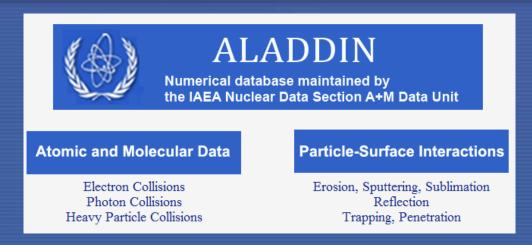
Established Program: Collection, Dissemination, Critical assessment (evaluation) and generation of A+M, PSI (PMI) data

- ALADDIN: Numerical database
- AMBDAS: Bibliographic database
- Dust Particle database
- GENIE: Search Engine
- XSAMS: XML Schema for A+M/PSI Data



ALADDIN: Numerical Database

Data Dissemination http://www-amdis.iaea.org/ALADDIN



- Originally designed to host "evaluated and recommended" data only
- Currently a mix of evaluated data with CRP participants' data
- Will host evaluated and recommended data
 - CM on "Evaluation and Uncertainty Assessment for Be, C, Ne Atomic Data"
 - Joint IAEA-KAERI CM on "Recommended Data for Processes of Tungsten Ions
- New Interface using GOOGLE free search forms is under development



AMBDAS: Bibliographic database

Data Dissemination http://www-amdis.iaea.org/AMBDAS

- Data Sources
 - AM/PSI Data entries relevant to fusion
 - Spectroscopic data from NIST (A. Kramida & J. Fuhr)
 - NFRI, KAERI and IAEA collaboration for electron collisional data
 - Consultancies for plasma-material interaction data
- Data in the "International Bulletin on A & M Data for Fusion" available through AMBDAS
- New environment for bibliographical data collection
 - Web of Science
 - The SAO/NASA Astrophysics Data System



Planned Databases: Dust particles

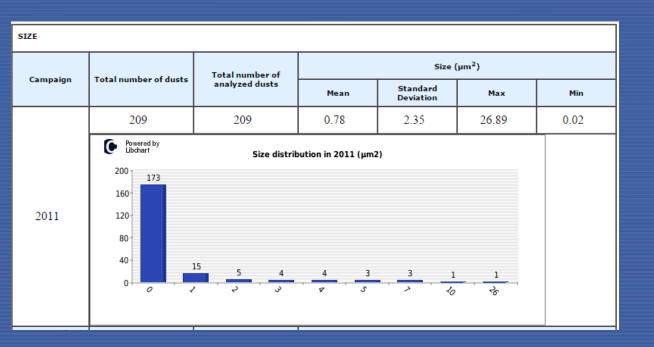
in collaboration with IPP-Garching and NFRI (Hong)

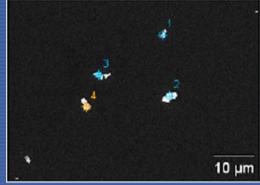
Why dust database is important?

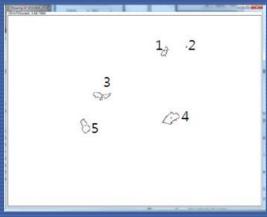
- Radioactivity (ITER: 50 mSv =350 Kg W dusts)
- Chemical activity (hot surface)
- Fuel retention (ITER: 700g T in-vessel)
- Uncontrolled "pellet" injection.
- Damage of in-vessel components

Standardization

- Collection method
- Characterization method and settings
- Analysis tools and methods
- File upload and maintenance strategy







GENIE: Web search engine for atomic data

Data Exchange & Dissemination http://www-amdis.iaea.org/GENIE

Radiative properties – search on 9 databases

Collisional databases – search on 6 databases

Will work on the GENIE statistics outputs for collaborators

GENIE

A General Internet Search Engine for Atomic Data

Transition Probabilities Wavelengths Energy Levels Ion: CIV		Electron Impact Cross Sections and/or Rate Coefficients Ion: C 3+
Enter wavelength in Å: From 1 to 10000	Genie	 Excitation Ionization Dielectronic recombination Cross sections ▼ Rate coefficients ▼
NIST Atomic Spectra Database Kurucz's CD-ROM 23 Atomic Line List v.2.04 TOPbase (Opacity Project) Kelly Atomic Line Database ?		IAEA ALADDIN Database
MCHF/MCDHF Collection KAERI AMODS Spectral Lines CAMBD Atomic Spectra Spectr-W3 ?		OPEN-ADAS ✓ ? Spectr-W3 ✓ ? Go for sigma/R Reset
Go for A/E/lambda Reset		



XSAMS: XML Schema for A+M/PSI Data

Data Exchange http://www-amdis.iaea.org/xsams

Sep 2009: <u>First release version 0.1 of the schema</u>

Mar 2010: XSAMS Meeting in NIFS, Japan

Nov 2010: XSAMS Meeting at IAEA

Jan 2011: <u>Version 0.1.1 (bug fixes)</u>

Source forge project http://sourceforge.net/projects/xsams/

Oct 2011: XSAMS Meeting at NIST

Feb 2012: XSAMS Meeting with VAMDC, University of Vienna

VAMDC continues to develop XSAMS.

Technical Discussions on XSAMS for DCN databases



Code Centre Network (CCN)

http://www-amdis.iaea.org/CCN

Joint effort to gather and provide access to any information relevant for modellers in fusion plasma science

Purpose

To provide solutions to anyone willing AM/PSI data which can not be easily accessed on the web or which simply do not exist.

Tools

Online computing

Downloadable codes

Direct contacts with the CCN for any expertise

IAEA Activities

Organization of meetings and workshops for code developers

Dissemination of community available codes and code results

Online computing capabilities



Code Centre Network (CCN) Meetings

http://www-amdis.iaea.org/CCN

- The 3rd CCN Meeting in May 2013:
 - Uncertainty estimates of theoretical atomic and molecular data
 - General approach to establish guidelines of uncertainty estimates
- The 4th CCN Meeting in July 2015:
 - Uncertainty estimates of plasma-material interaction data
 - Review the status of PMI codes :DFT, MD, KMC, Multi-scale modeling codes
- Code comparison workshops
 - Spectral Line Shapes in Plasmas Code Comparison Workshops (2012, 2013,2015)
 - Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data (July 2014)
 - Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices (November 2014)
 - Workshop on Uncertainty Quantification in Physics and Chemistry (May, 2015)



IAEA Online Codes and Code Results

- Average Approximation http://www-amdis.iaea.org/AAEXCITE/
 - Electron impact excitation cross sections for any ion and configuration
- Heavy particle collisions http://www-amdis.iaea.org/HEAVY/
 - Excitation, ionization and charge exchange for bare nucleus on hydrogenic target
- Effective Ionization/Recombination Rates http://www-amdis.iaea.org/RATES/
 - Level population distributions and radiative power rates from CR modeling
- LANL atomic data from CRP http://www-amdis.iaea.org/LANL/
 - Si, Cl, Ar ions (~ 2 GB)
- FAC atomic physics codes and atomic data http://www-amdis.iaea.org/FAC/
 - He Si atoms (~ 30 GB)
- GRASP2K code distribution https://int-amdis.iaea.org/GRASP2K
- FLYCHK Collisional-Radiative code results http://www-amdis.iaea.org/FLYCHK
 - Charge state distributions and radiative loss rates for Z=1-79 for Te=0.5 eV- 100 keV



Knowledge Base: Inputs only from IAEA



knowledge base

- Main Page
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- Data Exchange
- Special Topics
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navigation

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Main Page

Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data For Fusion

Introduction

Atomic, molecular and plasma-material interaction processes play an important role in the energy balance, confinement and stability of a thermonuclear plasma. The primary goal of this Knowledge base is to identify the needs in the atomic, molecular and plasma-surface interaction data sets for fusion research, both magnetic and inertial confinement fusion studies, to provide a direct link to the relevant data sources and present more information on the available data sets.

Data Needs

Magnetic Confinement Fusion

- Introduction
- Spectroscopic Data
- Collisional Data for Edge Studies
- Collisional Data for Neutral-Beam Heating
- Radiative Plasma Cooling
- Plasma-Wall Interaction
- Material Properties

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Issues for Technical Discussions

- Data Evaluation Activities
- Maintenance of Bibliographical Data on Collisional Processes
- Implementation of XSAMS and VAMDC node software
- Priority List of A+M/PSI data for Fusion
- Database development

