Databases and Coordinated Research Projects in the IAEA Atomic and Molecular Data Unit

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

2011 ADAS Workshop

Auburn University, 6-8 October 2011

IAEA

International Atomic Energy Agency

Overview of A+M Data Unit Activities

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

IAEA

Data Centres Network (DCN)

- The DCN includes 12 national data centres or related activities:

  Terms of Reference:

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

  Established Program: Collection, Dissemination, Critical assessment (evaluation) and generation of A+M, PSI (PMI) data.
- The DCN activities are coordinated by the IAEA A+M Data Unit and periodically reviewed (every two years) by IFRC A+M Subcommittee.
- Key issues for DCN presently: maintenance of bibliographical database, coordination of data validation (data evaluation) work, development of "data needs" document, extension of knowledge base (wiki) effort.

IAEA

Code Centres Network (CCN)

- New effort (since 2008) to provide access to A+M codes relevant for fusion plasma modelling
- An IAEA web page provides summaries of the code capabilities and links to Centre web pages
- Some on-line code capabilities; other CCN partners provide contact information
- Flexible group of participants; we intend to use CCN as an umbrella for other code activities

IAEA

CCN Participants

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

IAEA

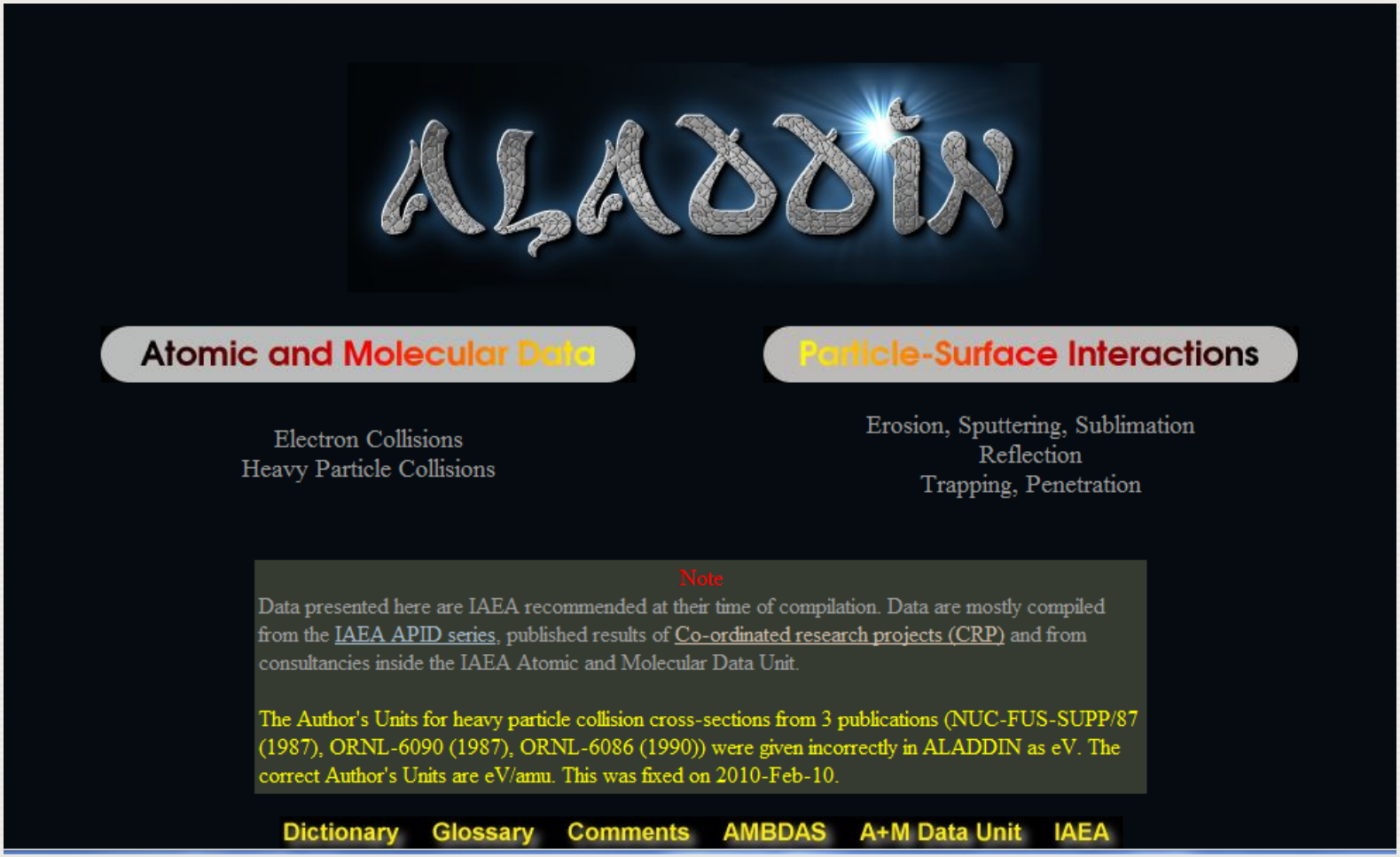
XML Schema for Atoms, Molecules and Solids (XSAMS)

- Project initiated in October 2003 during the DCN meeting
  - Working group composed of NIST, ORNL, IAEA, Obs Paris-Meudon
  - 2008: collaboration from Russia: Russian Federal Nuclear Centre (VNIITF)
  - 2009: VAMDC (Virtual Atomic and Molecular Data Centre, July 2009)
- Regular Consultants' Meetings organized by A+M Data Unit
- Presentations at ICAMDATA in October 2008, China
- Release of XSAMS version 0.1, 22 September 2009
- XSAMS has been adopted by VAMDC for their databases (24 teams)
- Present development of XSAMS is led by VAMDC
- Recent additions: Line shapes, Molecular spectroscopy, PAH
- Adoption of XSAMS version 1.0, 4 October 2011

IAEA

Numerical database ALADDIN

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



IAEA

Atomic data from FLYCHK

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

FLYCHK: Generalized Model of Atomic Processes In Plasmas

On-line Capability of NLTE kinetics Code

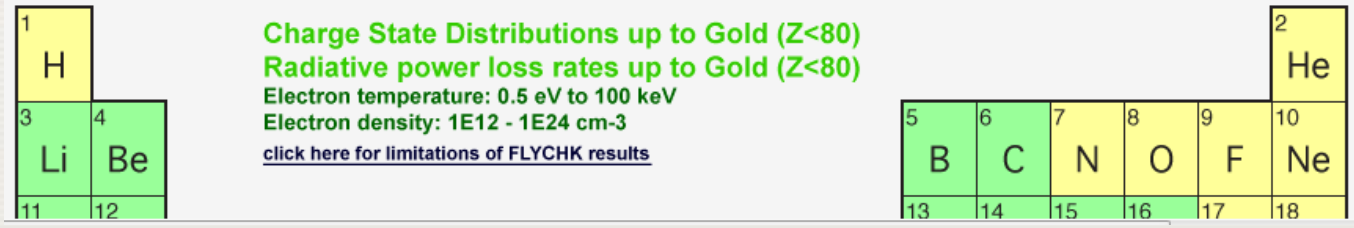
The FLYCHK code provides a simple and general modeling capability to generate atomic level populations and charge state distributions for low-Z to mid-Z elements under NLTE(Non-Local Thermodynamic Equilibrium) conditions. The code is currently available at the **password-protected NIST website.** For more information on details, validity and limitations of the code, please click **the FLYCHK information page** .

Steady-State Charge State Distributions

Average charge states <Z> of atoms from Z=1 (Hydrogen) to Z=79 (Gold) are calculated by FLYCHK code and plotted over a wide range of plasma conditions. The calculation is done for the steady-state plasmas with electron temperatures from 0.5 eV to 100 keV and electron densities from 10^{12} cm^{-3} to 10^{24} cm^{-3}. Click the element in the periodic table and a page will apear with the information on <Z>, Charge State Distribution and Total Radiative Power Loss Rates of the element.

Rate Coefficients at Coronal Equilibirum for Plasma Modeling Applications

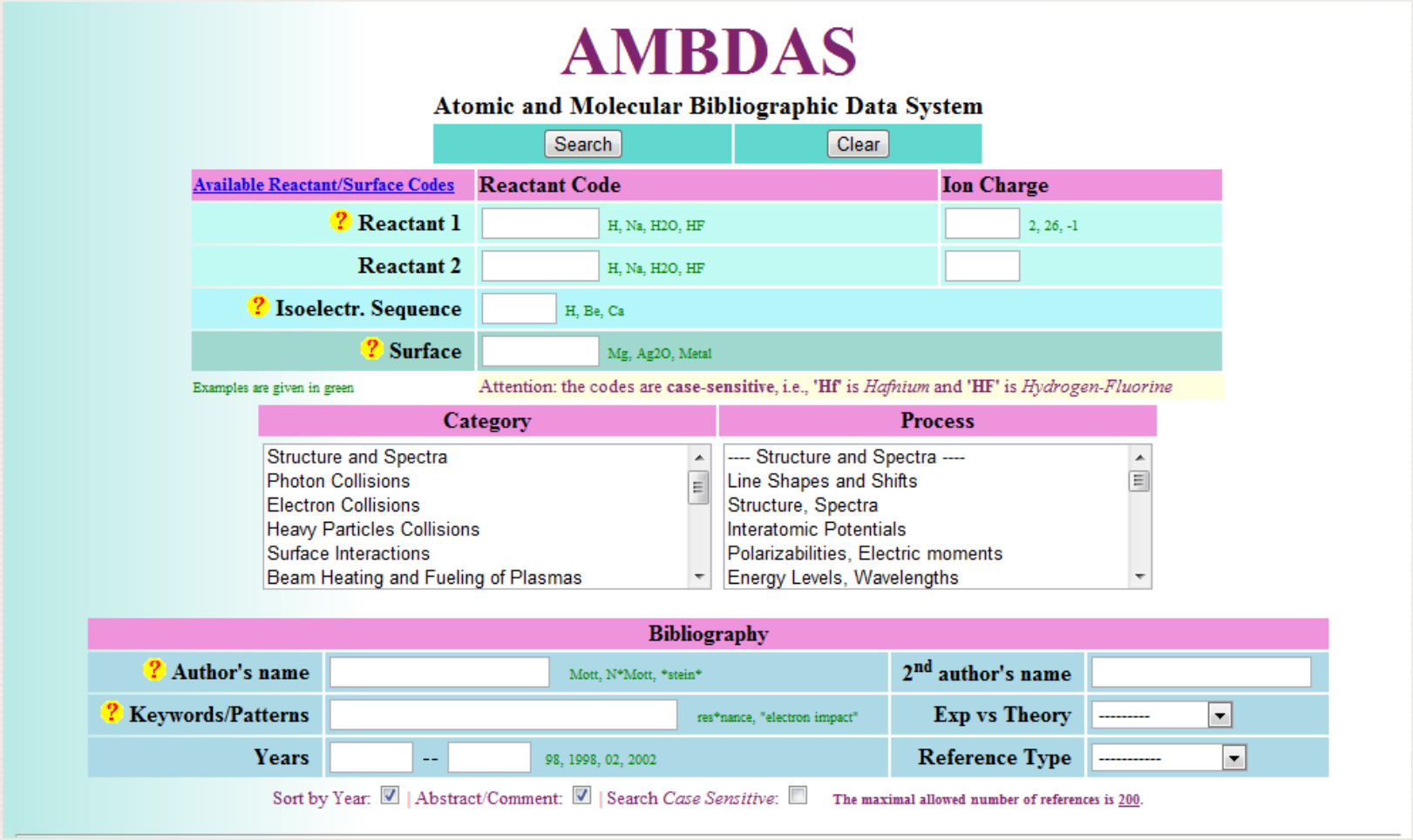
To help plasma modeling applications, Rate coefficients of Direct Ionization, Excitation-Autoionization, Radiative Recombination and Dielectronic Recombination at coronal conditions are generated for a wide range of plasma temperatures from 0.5 eV to 100 keV. Also avaialble are the Radiative Loss rates per Charge State, both Line radiation and Recombination radiation. They are available at the same page as Charge state distributions. The details of the methods are found at **the FLYCHK Rates information page** .



IAEA

Bibliographical database AMBDAS

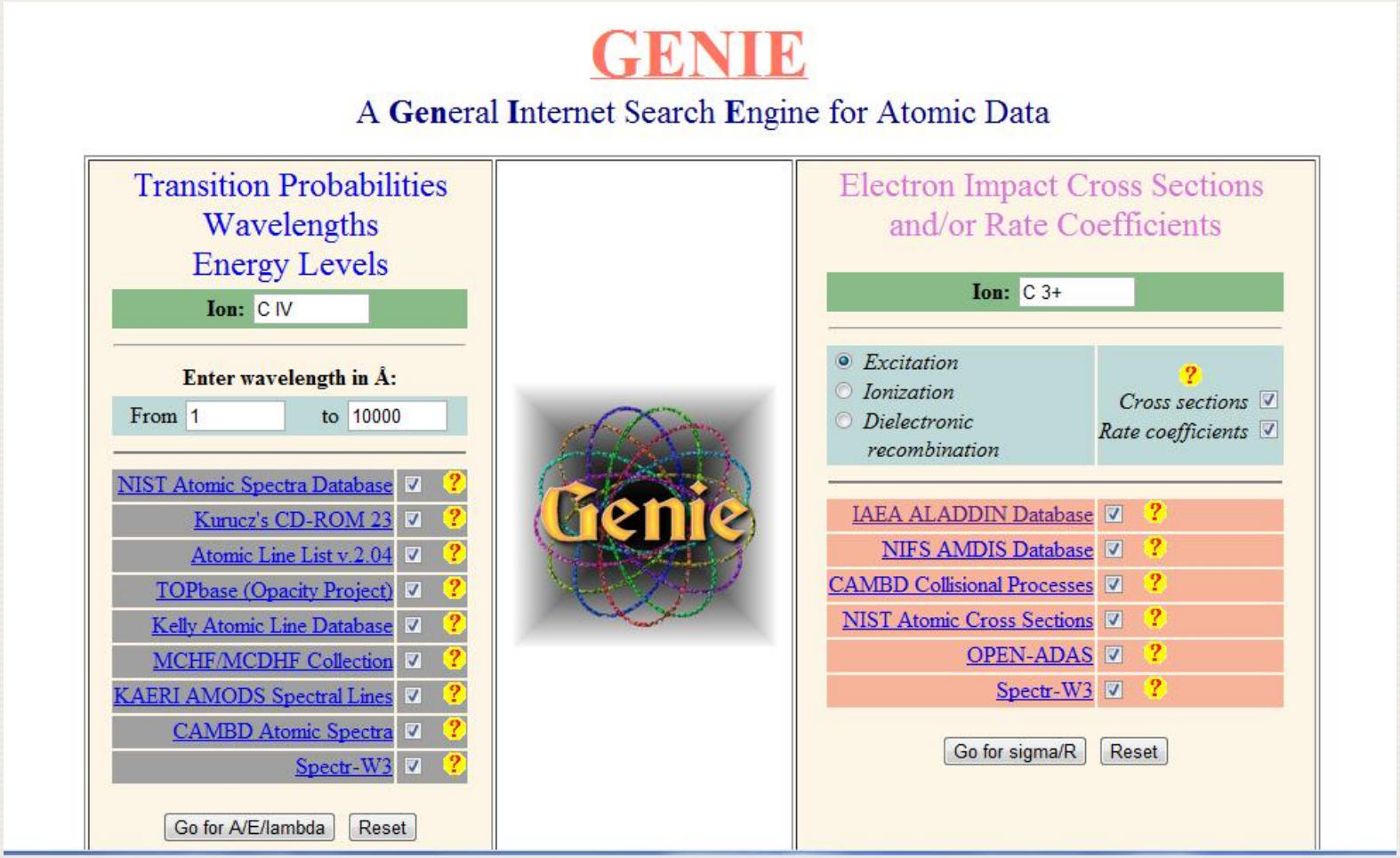
http://www-amdis.iaea.org/AMBDAS



IAEA

Database search engine GENIE

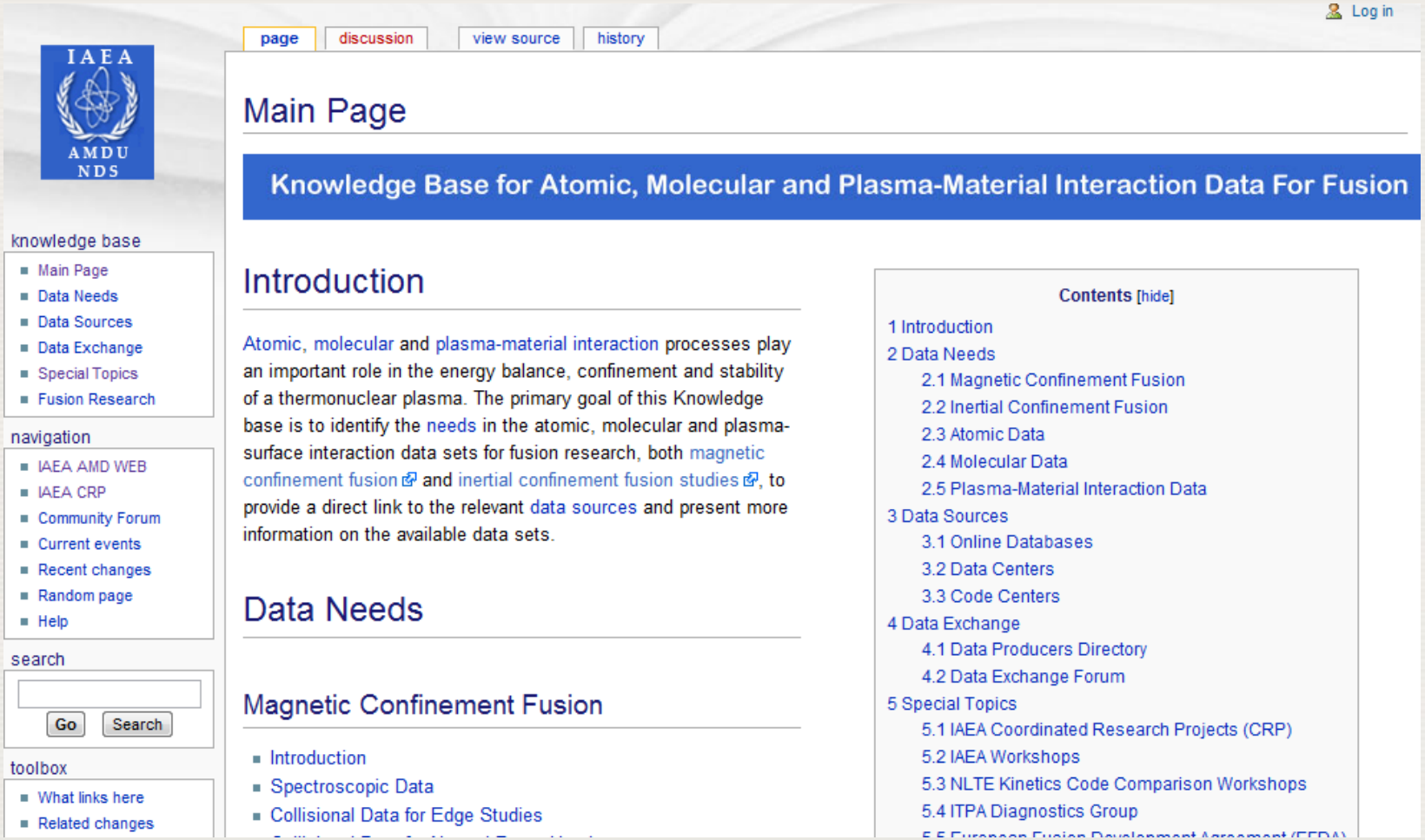
http://www-amdis.iaea.org/GENIE



IAEA

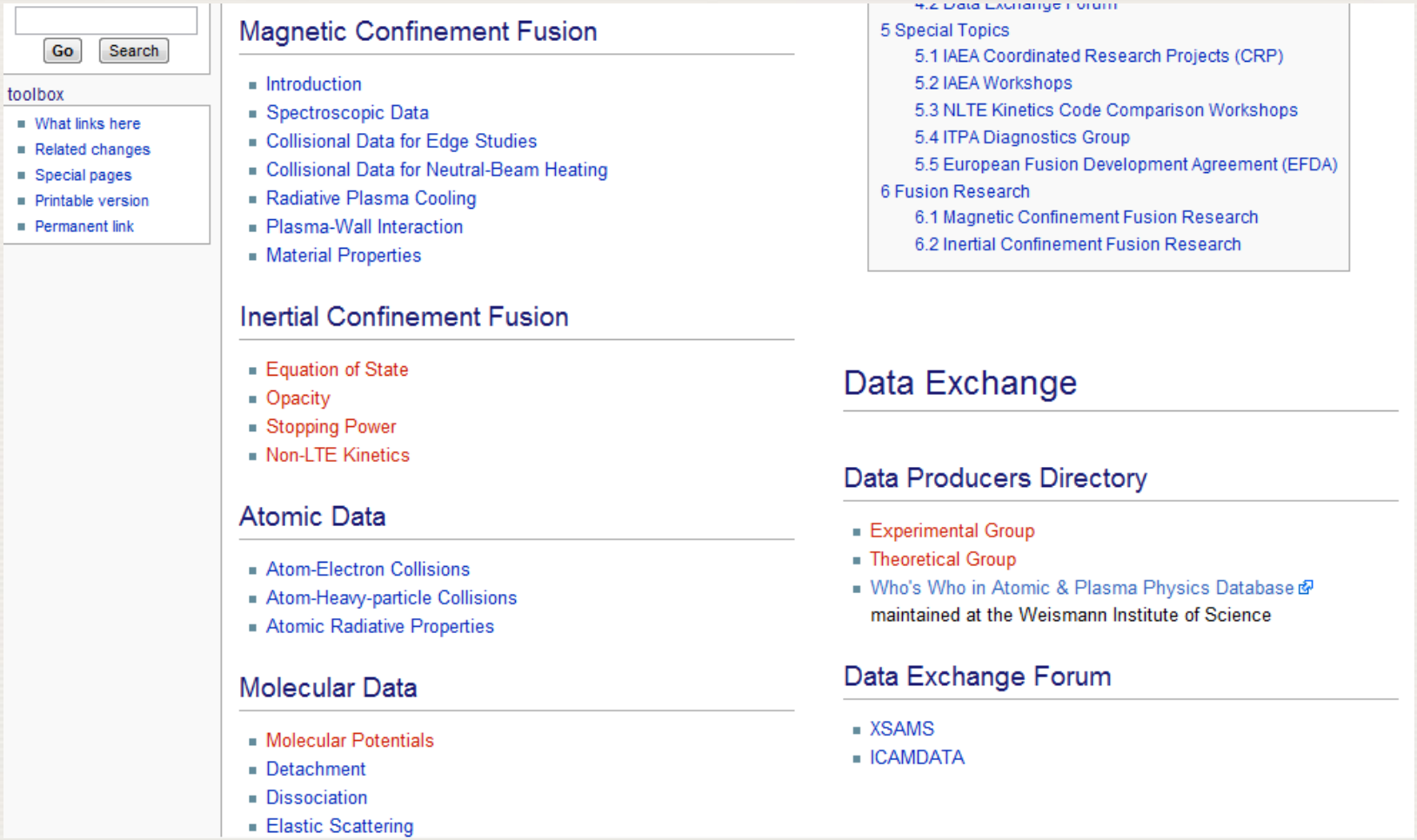
Knowledge Base (Wiki)

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



IAEA

Wiki, cont'd… http://www-amdis.iaea.org/w



Go Search

toolbox

- What links here
- Related changes
- Special pages
- Printable version
- Permanent link

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

Inertial Confinement Fusion

- Equation of State
- Opacity
- Stopping Power
- Non-LTE Kinetics

Atomic Data

- Atom-Electron Collisions
- Atom-Heavy-particle Collisions
- Atomic Radiative Properties

Molecular Data

- Molecular Potentials
- Detachment
- Dissociation
- Elastic Scattering

4.2 Data Exchange Forum

5 Special Topics
- 5.1 IAEA Coordinated Research Projects (CRP)
- 5.2 IAEA Workshops
- 5.3 NLTE Kinetics Code Comparison Workshops
- 5.4 ITPA Diagnostics Group
- 5.5 European Fusion Development Agreement (EFDA)

6 Fusion Research
- 6.1 Magnetic Confinement Fusion Research
- 6.2 Inertial Confinement Fusion Research

Data Exchange

Data Producers Directory

- Experimental Group
- Theoretical Group
- Who's Who in Atomic & Plasma Physics Database maintained at the Weismann Institute of Science

Data Exchange Forum

- XSAMS
- ICAMDATA

IAEA

Wiki, cont'd… http://www-amdis.iaea.org/w

- Atomic Radiative Properties

Molecular Data

- Molecular Potentials
- Detachment
- Dissociation
- Elastic Scattering
- Molecule-Electron Collisions
- Molecule-Heavy-Particle Collisions
- Molecular Radiative Transitions

Plasma-Material Interaction Data

- Introduction
- Erosion
- Sputtering
- Sublimation
- Reflection
- Trapping
- Desorption
- Particle Induced Electron Emission
- Wall Material Properties
- Penetration
- Dust
- Arcing

Data Sources

Data Exchange Forum

- XSAMS
- ICAMDATA

Special Topics

IAEA Coordinated Research Projects (CRP)

The Coordinated Research Projects (CRPs) are normally three to five-year joint projects of a group of (10-15) laboratories, research teams or institutions, performing coordinated research to achieve certain well defined goal. The CRPs generally produce a significant amount of new data on the collision processes or structural properties of elements or materials relevant to fusion energy research, or perform detailed critical assessments of the existing data and selection of sets of "recommended" data (or best available at the time of assessment). The CRP results of adequate accuracy and completeness are stored in the IAEA numerical database ALADDIN and published in the IAEA publication "Atomic and Plasma-Material Interaction Data for Fusion":APID Series.

- CRP(2002-2006): Tritium Inventory in Fusion Reactors
- CRP(2004-2008): Atomic and Molecular Data for Plasma Modelling

IAEA

Wiki, cont'd… http://www-amdis.iaea.org/w

Data Sources

Online Databases

Bibliographic Database

- AMBDAS IAEA AMD Unit
- Atomic Spectra Bibliographic Databases at NIST has three databases: Bibliographic Database on Atomic Transition Probabilities, Bibliographic Database on Atomic Spectral Line Broadening and Shifts and Bibliographic Database on Atomic Energy Levels and Spectra
- CFADC Bibliography The Controlled Fusion Atomic Data Center, Oak Ridge National Laboratory

Numerical Databases

- ALADDIN Atomic, Molecular and Plasma-Surface Interaction data
- GENIE Search Engine for numerical databases
- NIST NIST Atomic Spectra Database
- NIST NIST Molecular Spectroscopy database
- MOLAT Paris-Meudon Observatory
- SPECTR-W^3 Russian Federal Nuclear Center (RFNC-VNIITF)

Online Code Capabilities

- FLYCHK Generalized modeling capability of atomic processes

- CRP(2004-2008): Atomic and Molecular Data for Plasma Modelling
- CRP(2005-2009): Atomic Data for Heavy Element Impurities in Fusion Reactors
- CRP(2007-2011): Data for Surface Composition Dynamics Relevant to Erosion Processes
- CRP(2008-2012): Characterization of Size, Composition and Origins of Dust in Fusion Devices
- CRP(2009-2013): Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions
- CRP(2010-2014): Spectroscopic and Collisional Data for W from 1 eV to 20 keV
- CRP(2011-2015): Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma

IAEA Workshops

- Workshop on A+M Data for fusion Energy Research ICTP Trieste, 2009
- Workshop on A+M Data for fusion Energy Research ICTP Trieste, 2006
- Workshop on A+M Data for fusion Energy Research ICTP Trieste, 2003

NLTE Kinetics Code Comparison Workshops

- Background
- Workshop Results

IAEA

Wiki, cont'd… http://www-amdis.iaea.org/w

- MOLAT Paris-Meudon Observatory
- SPECTR-W^3 Russian Federal Nuclear Center (RFNC-VNIITF)

Online Code Capabilities

- FLYCHK Generalized modeling capability of atomic processes in plasmas

Data Centers

- Atomic Data and Analysis Structure ADAS, UK
- Oak Ridge National Laboratory CFADC, ORNL, USA
- China Research Association of Atomic and Molecular Data CRAAMD China
- ENEA ENEA, Italy
- GAPHYOR LPGP LPGP, France
- IAEA, Atomic and Molecular Data Unit Austria
- Japan Atomic Energy Agency JAEA, Japan
- Korea Atomic Energy Research Institute KAERI, Korea
- Kurchatov Institute Russia
- Max-Planck-Institut fur Plasmaphysik Germany
- National Institute for Fusion Science NIFS, Japan
- National Institute of Standards and Technology NIST, USA
- Virtual Atomic and Molecular Data Centre VAMDC, Europe
- Russian Federal Nuclear Centre All-Russian Institute of Technical Physics RFNC-VNIITF, Russia

Code Centers

NLTE Kinetics Code Comparison Workshops

- Background
- Workshop Results

ITPA Diagnostics Group

- Official Site to ITPA Diagnostics Group
- Introduction to ITPA Diagnostics Special Working Group on First Wall Diagnostics
- Direct Link to Special Working Group on First Wall Diagnostics

European Fusion Development Agreement (EFDA)

- Official Site:http://www.efda.org/
- European Fusion Development Agreement
- EU Plasma Wall Interaction Task Force and Meetings
- Task Agreements on In-Vessel Dust and Tritium Management

Fusion Research

IAEA

Database issues

- ALADDIN: Provide only recommended data, or leave that evaluation outside ALADDIN? Recent DCN meeting showed new interest in data evaluation, esp. at NFRI.
- AMBDAS: Future maintenance of bibliography on collisional processes.
- GENIE: Good tool for a survey search, unified query language.
- XSAMS: Being implemented on many A+M databases for astrophysics and atmospheric science. Fusion?
- Knowledge Base (Wiki): Most accessed by far, flexible mechanism; content to grow.

IAEA

CRP: Coordinated Research Project

Joint research on A+M/PMI topic for fusion:

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

Objectives:

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

Data and results:

- Journal publications
- Final reports in “Atomic and Plasma-Material Interaction Data for Fusion” (APID)
- Numerical data in ALADDIN
- Looking forward to results in Knowledge Base

IAEA

Present and Planned CRPs

2007-2011: Data for Surface Composition Dynamics Relevant to Erosion Processes

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

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

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

2011-2015: Atomic and Molecular Data for State-Resolved Modelling of H and He and their Isotopes in Fusion Plasma

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

2013-2017 (tentative): Plasma Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices

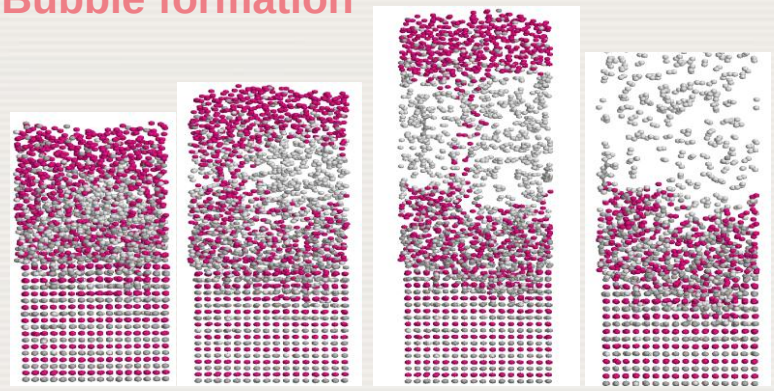
IAEA

CRP on Data for Surface Composition Dynamics Relevant to Erosion Processes (2007-2011)

Overall objective

- To better understand erosion processes and to find new methods to control erosion
- To collect and generate new data relevant to erosion dynamics in fusion reactors
- Investigated materials mainly the ones foreseen for ITER: C, W, Be

Bubble formation



100 eV 90% D +10% W on
W-terminated tungsten-carbide
Kai Nordlund, University of Helsinki

First outputs and outcomes

- Some new data included in ALADDIN
- New ALADDIN web interface for PSI

First RCM, 17-19 October 2007

Second RCM, 11-13 March 2009

Final RCM, 13-15 September 2010

IAEA

CRP on Size, Composition and Origin of Dust in Tokomaks (2008-2012)

Objectives

- To determine the size, composition and origin of dust in tokamaks
- Understand dust transport
- Improve dust estimates
- Understand tritium retention in dust
- Investigate dust removal techniques
- Focus on dust from C, W and Be

First RCM: 10-12 December 2008
Second RCM: 21-23 June 2010
Third RCM: 30 Nov – 02 Dec 2011

Plans for a real dust database! (Effort centred at IPP Garching; based on automated analysis of 10s of thousands of individual dust images.)

Flaking of co-deposited layer on lower part of limiter, TFTR, Nov 1998

IAEA

CRP on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions (2009-2013)

Objectives

To generate new data for radiative and collisional processes in ions of atoms and molecules of hydrogen, helium, lithium, beryllium, boron, carbon, nitrogen and oxygen at temperatures and densities typical of the edge and divertor region of fusion reactors

Data needs

- In diagnostics for plasma parameters such as temperature and density
- In plasma modelling
- Special focus on processes including ro-vibrational states of molecules
- Fine structure energy levels of molecules

First RCM: 18-20 November 2009

Second RCM: 23-25 May 2011

Third RCM: Q1 2013

IAEA

CRP on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions (2009-2013)

Participants

Pierre DEFRANCE	UCL, Louvain-la-Neuve, Belgium
Dmitry FURSA/Igor BRAY	Curtin University of Technology, Perth, Australia
Ratko JANEV	Macedonian Academy of Sciences and Arts
Luis MENDEZ/Ismanuel RABADAN	UAM, Madrid, Spain
James MITCHELL	Université de Rennes I, France
Michael PINDZOLA/Teck LEE	Auburn University, AL, USA
David SCHULTZ	ORNL, USA
Hidekazu TAKAGI	Kitasato University, Sagamihara, Japan
Jianguo WANG	IAPCM, Beijing, China
Baoren WEI	Fudan University, Shangai, China
Ioan SCHNEIDER	Université de Le Havre, France
Viorica STANCALIE	INFLPR, Romania

IAEA

CRP on Spectroscopic and Collisional Properties of Tungsten from 1 eV to 20 keV

Concerned with W in all plasma regions, edge to core

- Electron-impact, radiative and photon-induced, and heavy particle collision processes
- Cross-sections for kinetic modelling
- Rate coefficients for macroscopic modelling
- Spectroscopic signatures for diagnostics
- Theory and experiment are both represented, with plenty of overlap among and between the two
- Aim to produce validated database for tungsten in plasma

First RCM: 13-15 December 2010
Second RCM: Q2 2012
Third RCM: Q4 2013; wrap-up in 2014

IAEA

CRP on Spectroscopic and Collisional Properties of Tungsten from 1 eV to 20 keV

Participants

R. Srivastava, IIT Roorkee, India
A. Müller, University of Giessen, Germany
N. Nakamura, University of Electrocommunications, Japan
A. Ryabtsev/R. Kildiyarova, Russian Academy of Sciences, RF
W. Tchang-Brillet/A. Wyart, Observatoire de Paris, France
P. Beiersdorfer, Lawrence Livermore National Laboratory, USA
C.-Z. Dong, Northwest Normal University, China
F. Koike, Kitasato University, Japan
M. Trzhaskovskaya/V. Nikulin, St Petersburg Nuclear Physics Institute, RF
V. Lisitsa, Kurchatov Institute, RF
N. Badnell, University of Strathclyde, UK
J. Colgan, Los Alamos National Laboratory, USA
Yu. Ralchenko, National Institute of Standards and Technology, USA

IAEA

CRP on Atomic and Molecular Data for State-Resolved Modelling of H and He and their Isotopes in Fusion Plasma

- Species H, H^+, H_2, H_2^+, H_3^+, He, He^+, He^{2+}, HeH^+, He_2^+, H^- and isotopic variants; isotope effects are important; He is newly important
- Kinetic modelling: we want state-resolved cross-sections
- Aim to be comprehensive for volume processes among the mentioned species and e^-, hv
- Predominantly theoretical; some experiment

First RCM: 10-12 August 2011

Second RCM: Q1 2013

Third RCM: Q3 2014; wrap-up in 2015.

IAEA

CRP on Atomic and Molecular Data for State-Resolved Modelling of H and He and their Isotopes in Fusion Plasma

Participants

Roberto CELIBERTO and Mario CAPITELLI, Polytechnic of Bari, Italy
Ursel FANTZ and Dirk WÜNDERLICH, MPI for Plasma Physics, Garching
Christian JUNGEN, CNRS and U Paris-Sud, and Ioan SCHNEIDER, U Le Havre
Viatcheslav KOKOOULINE and Talat RAHMAN, University of Central Florida
Predrag KRSTIC, Oak Ridge National Laboratory
Xinwen MA, Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou
Ousmanou MOTAPON, University of Douala, Cameroon
Ann E. OREL, University of California at Davis
Detlev REITER, Forschunszentrum Jülich
Keiji SAWADA, Shinshu University, Japan
Xavier URBAIN and Pierre DEFRANCE, Catholic University of Louvain, Belgium
Jung-Sik YOON and Mi-Young SONG, National Fusion Research Institute, Korea

IAEA

CRP on Erosion and Tritium Retention in Beryllium Plasma-Facing Materials

- Timely for input from JET ITER-Like Wall (ILW) and for planning for ITER.
- Focus on sputtering, reflection and trapping due to regular interaction of H/He and impurity ions with Be surface [*].
- Interested in mixed materials, esp. Be-C and Be-O.
- Mix of experiment and modelling.
- Schedule: RCMs in Q1 2012, Q4 2013, Q2 2015.
- [*] The Physics Section has a CRP on “Investigation of Materials under High Repetition and Intense Fusion Pulses” (2011-2016).

IAEA

Planned CRP on plasma interaction with irradiated tungsten and tungsten alloys

- Strongly recommended by the IFRC subcommittee on A+M data as our second CRP for the 2012-2013 programme
- Tungsten alloys are foreseen for next step beyond ITER
- In any case, W transmutes to W-Re-Os
- Neutron irradiation causes voids and dislocations; changes PMI properties in ways that have not been much studied
- CRP on irradiated tungsten and tungsten alloys in 2013-2017 will support planning for DEMO

IAEA

Summary of database work

Numerical database ALADDIN: Record of IAEA-sponsored work; we wish to broaden it. Data validation and recommendation issues.

Bibliographical database AMBDAS: Have been totally dependent on NIST and ORNL. Input to the collisions part is being revisited.

Database search engine GENIE: Valuable single query interface to multiple database

New knowledge base (wiki): The most visited part of our web site. Essentially single-person effort so far; we hope to broaden the effort.

IAEA

Summary of CRP work

- CRPs are the main mechanism by which the A+M Data Unit encourages new research
- Recent budgets allow us to start about one new CRP per year
- Focus is on A+M and PMI data for Fusion
- Advice on topics from IFRC subcommittee is important
- Considerations for choice of topics:
  - ITER relevance is good, exclusively ITER not so good
  - Need to be able to assemble broad team
  - Must be active topic; we don’t fund the research
  - We like focussed topic for best synergy

IAEA