CRP and Meeting Objectives

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

Vienna, 26-28 September 2012

Bas Braams and Hyun Chung

Atomic and Molecular Data Unit

IAEA

International Atomic Energy Agency

About the IAEA

The International Atomic Energy Agency

- is a science and technology-based organization in the United Nations family that serves as the global focal point for nuclear cooperation;
- assists its Member States in using nuclear science and technology for various peaceful purposes and facilitates the transfer of such technology and knowledge to developing Member States;
- develops nuclear safety standards and promotes the achievement and maintenance of high levels of safety in applications of nuclear energy, as well as the protection of human health and the environment against ionizing radiation;
- verifies through its inspection system that States comply with their commitments, under the Non-Proliferation Treaty and other non-proliferation agreements, to use nuclear material and facilities only for peaceful purposes.

Fusion energy at IAEA

Physics Section programme on Nuclear Fusion Research.

- Biennial Fusion Energy Conference
- Journal *Nuclear Fusion* (Published by IOP)
- Technical Meetings, Coordinated Research Projects

Nuclear Data Section has Atomic and Molecular Data Unit.

- Databases ALADDIN, AMBDAS
- Database search engine GENIE
- Wiki-style knowledge base
- Technical Meetings, Coordinated Research Projects

NDS also has the

- FENDL: Fusion Evaluated Nuclear Data Library

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A+M Data Unit at IAEA

Main web page: http://www-amdis.iaea.org/

"Atomic and Molecular Data":

- Really A+M+PMI: atomic, molecular and plasma-material interaction data
- Data for magnetic confinement fusion energy

Activities of the Unit

- Maintain numerical and bibliographical databases and knowledge base
- Organize coordinated research projects
- Organize technical and other meetings

A+M Data Unit…

www-amdis.iaea.org

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International Atomic Energy Agency

Atomic Molecular Data Services

Provided by the Nuclear Data Section

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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 Plasma-Surface Data | ALADDIN Numerical Database | AMBDAS Bibliographic Database | GENIE Atomic Data Search Engine | OPEN ADAS Database Search | Rovibronic Energy levels Triplet D_2 | FC Factors & A-values of H_2 & 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 Meetings

Jun 20-22, 2012
Consultant Meeting onData Evaluation and the Establishment of a Standard Library of A+M/PMI Data for Fusion

Aug 29-31, 2012
2nd RCM of CRP on Spectroscopic and Collisional Data for W from 1 eV to 20 keV

Sep 4-7, 2012
Joint IAEA-NFRI Technical Meeting on Data Evaluation for Atomic, Molecular and Plasma-Material Interaction Processes in Fusion NFRI,Daejon,Korea

Sep 26-28, 2012
1st RCM of CRP on Data for Erosion and Tritium Retention in Beryllium Plasma

AMO/PSI Meetings

May 21-25, 2012
20th Plasma-Surface Interaction Conference Aachen, Germany

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Priorities for A+M+PMI data efforts

Atomic data (electron collisions, spectroscopy)

- Important for diagnostics
- Need data evaluation, recommended library

Molecular data (mainly collision data, excited states)

- Important for divertor modelling, optimization
- Focus on data evaluation, recommendation

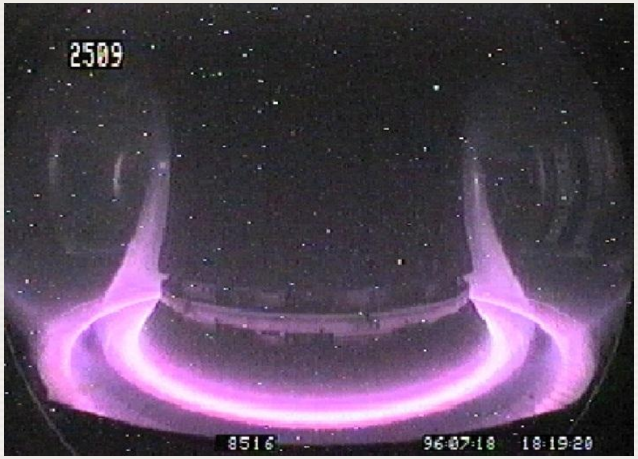
Plasma-material interaction data

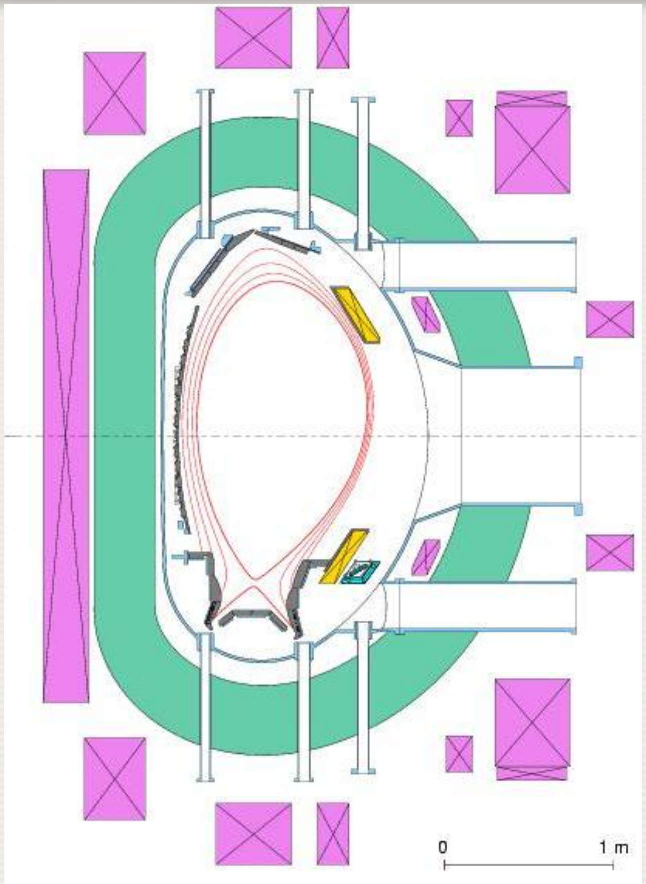
- Important for design, viability of fusion
- Focus on data production
- Difficult to obtain and parameterize data

Edge plasma physics

- Need to exhaust plasma power
  - Avoid melting, blistering, other damage
  - Limit erosion
- Need to exhaust impurities and He
  - Impurities include eroded wall material and deliberate cooling gas (N, Ne, Ar)
- Need to conserve tritium
  - Tritium must not be absorbed in the walls

Edge plasma physics…





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Possible wall materials

Carbon-based (CFC, Graphite)

- Good: High resistance to erosion, low nuclear activation, low radiation in plasma
- Bad: Absorbs tritium; probably rejected for ITER and a reactor

Tungsten

- Good: Very high resistance to erosion, does not absorb tritium
- Bad: High activation, radiates very strongly as a plasma impurity
- Question: How does tritium retention change after neutron irradiation?

Beryllium

- Good: Low tritium absorption (but some uncertainty about this), low nuclear activation, low radiation in plasma
- Bad: Low resistance to erosion; probably not suitable for a reactor

Low activation stainless steels

- Plausible choice for main wall in a reactor

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Three CRPs on PMI

“Erosion and tritium retention in beryllium plasma-facing materials” (2012-2016/2017)

- Experiments with Be are difficult (toxic); note the PISCES linear device at UCSD and now also JET.
- Sputtering and erosion is influenced by surface conditions (oxide layer, impurities)
- Sputtering and redeposition of BeH, BeH_2 may enhance trapping of tritium
- Want to understand tritium retention properties from first principles quantum mechanics and molecular dynamics

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Three CRPs on PMI…

"Plasma-surface interaction with irradiated tungsten and tungsten alloys in fusion devices" (2014-…)

- Main concern is with tritium in irradiated tungsten
- Need to characterize neutron damage at high dpa
- Need to characterize damage for relevant surrogate irradiation (neutron fluence in a reactor is very high)
- Need to study tritium migration in damaged tungsten
- Consider also transmutation of W to Re and Os
- Very difficult problem for first principles calculations
- Very difficult for experiment; really needs IFMIF

Three CRPs on PMI…

"Plasma-surface interaction with reduced activation steel surfaces" (2015-…)

- Steel may replace beryllium as main wall material in a reactor
- Need to characterize erosion, tritium retention properties
- Must take into account radiation damage
- Must take into account transmutation
- Timeline is relevant for IFMIF and for DEMO planning

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Objectives for this meeting

Review our work

Review data and database needs

- Including organizational aspects. How to organize data for real beryllium surfaces to make it useful for modelling

Review opportunities

- Including possibilities for large scale computing

Develop work plan

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Database Aims

27 September 2012

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International Atomic Energy Agency

Various classes of data and users

Erosion and tritium retention on JET

Suppose: JET has a record of operation of the device over a campaign. Plasma configuration (dynamic), measured profiles including impurities, ELM behaviour; all data extrapolated to the main wall.

So: n_e, T_e, n_Z, T_i and whatever other plasma data are needed; spatially resolved along the main wall and time resolved over a campaign.

Now want to predict and then test erosion and tritium retention anywhere on the beryllium wall.

What kind of PMI data are needed to make this feasible?

Is it realistic?

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Various classes of data and users…

Erosion and tritium retention on JET…

Most basic data: sputtering, reflection, penetration; but we have a variable (space and time) composition of the wall material.

Dimensionality of the database?

Alternatively, just run dynamic BCA? SDTRIMSP with chemistry? Local redeposition via ERO, WALLDYN?

In that case, do we need to (can we) extract data from MD and DFTB-MD to optimize the BCA treatment?

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Hydrogen transport calculations

Diffusion model? What parameters are needed? What functional dependencies? What is the role of a database?

Kinetic Monte Carlo? Same questions: what parameters, what functional dependencies, what kind of database?