



IAEA

60 Years

Atoms for Peace and Development

Review of CRP and Meeting Objectives

Hyun-Kyung Chung,

Atomic and Molecular Data Unit, Nuclear Data Section

CRP F43023 on Data for Atomic Processes of Neutral Beams in Fusion Plasma

IAEA A&M Data Unit support for fusion program worldwide

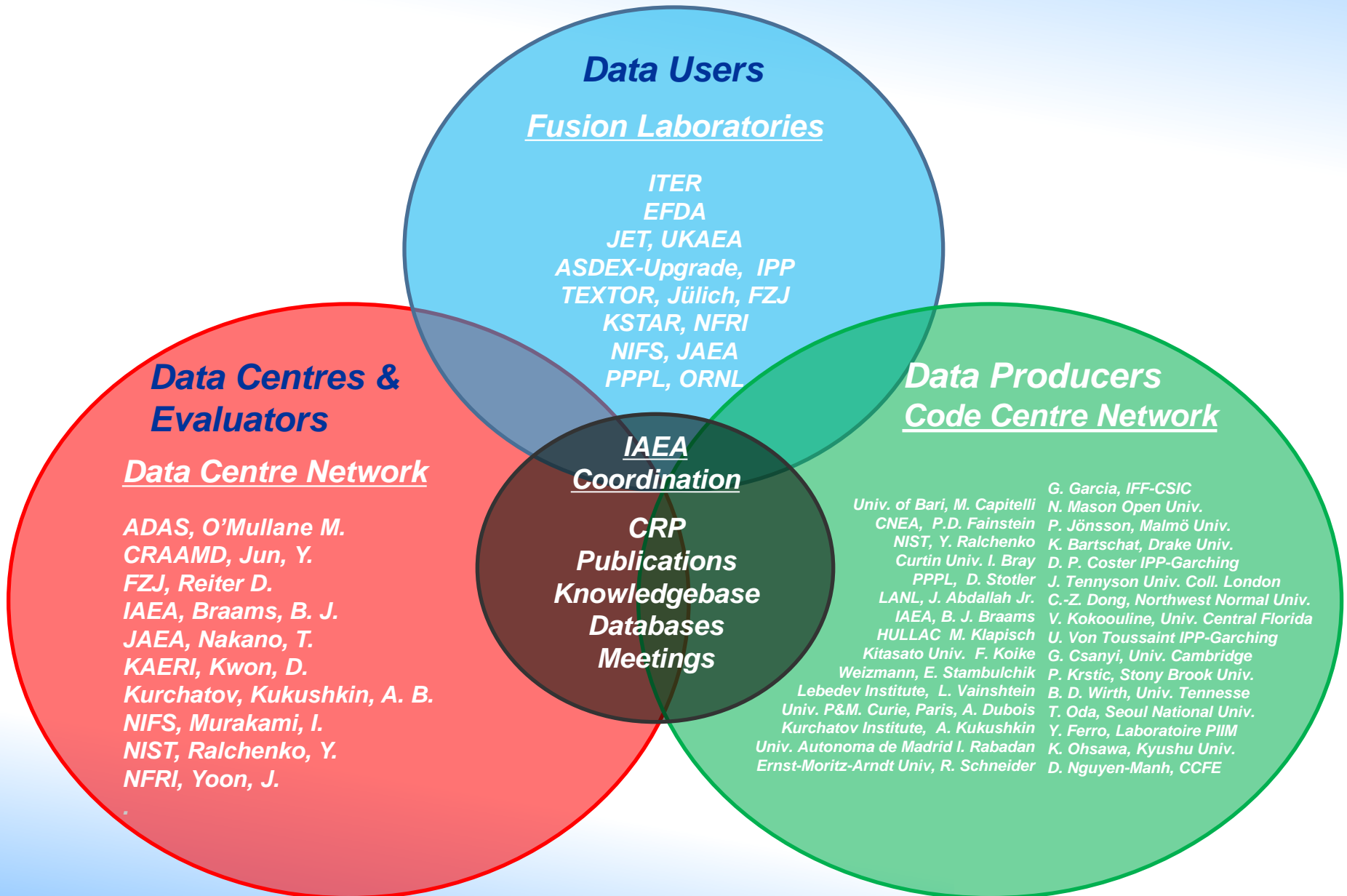
Fusion research requires huge amounts of material data – AM/PSI data

- IAEA A+M Unit formed in 1977
- Review progress and achievements of Atomic, molecular and plasma-surface interaction (A+M/PSI) data for Fusion programme worldwide
- Stimulate international cooperation in measurement, compilation and evaluation of A+M / PSI data for fusion



*Coordinated
Research
Projects (CRP)
Publications
Knowledgebase
Databases
Meetings*

Collaboration Network



A&M Data Services

<https://www-amdis.iaea.org/>

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
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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
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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**).

IAEA Nuclear Data Section

 IAEA-NDS Mission, Staff and more	 Nuclear Data Services	 Meetings Workshops	 Newsletters	 Coordinated Research Projects	 Nuclear Reaction Data Center Network	 Nuclear Structure & Decay Data Network	 Technical Documents INDC Reports Publications	 Computer Codes
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- IAEA Meetings
 - December 19-21, 2016
TM on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications
 - Feb 27 - March 3, 2017
Joint ICTP-IAEA School on Atomic Processes in Plasmas, Trieste, Italy
 - Mar 20-24, 2017
The 4th Spectral Line Shapes in Plasma Workshop, Vienna, Austria
 - 1Q, 2017
CM on Recommended data for hydrogen and helium in fusion plasmas
 - 2Q, 2017
3rd RCM of CRP on Plasma-Wall
- AMO/PSI Meetings
 - Sep 11-16, 2016
18th International Conferences on the Physics of Highly Charged Ions, Kielce, Poland
 - Sep 25-29, 2016
10th International Conference on Atomic and Molecular data and Their Applications, Gunsan, Korea
 - Sep 29-30, 2016
ADAS workshop 2016, Gunsan, Korea
 - Oct 10-14, 2016
69th Annual Gaseous

IAEA Coordinated Research Projects *60 Years* *Atoms for Peace and Development*

- **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
 - Data in Knowledge Base

ALADDIN: Numerical data (XYZ)

Go to data selection Reset request

Process

Reflection
Chemical Sputtering
Physical Sputtering
Radiation Enhanced Sublimation
Penetration

Projectile

H
D
T
[3]He

Surface

Be
Graphite
a-Carbon
CFC

Chemical Component

Be
C
W
H

Data Description

Mean Penetration Depth vs. angle and energy
Sputtered energy and energy reflection coeff. vs. angle and energy
Sputtering yields and particle reflection coeff. vs. angle and energy
Sputtering yields vs. incident flux density

Data Type

Derived
Experimental
Theoretical

First Author

Behrisch R.
Doerner R.P.
Eckstein W.
Haasz A.A.

Publication

IAEA-APID-7A (1998)
IAEA-APID-7B (2001)
INDC(NDS)-249 (1991)
INDC(NDS)-287 (1993)

Date

2012
2011
2009
2007

DUST database after a CRP

ID

Password

[User Registration](#)
[ID/Password](#)



IAEA Database
on micro-size Dusts and Nanoparticles

Accessing Database



NFRRI 국가핵융합연구소
National Fusion Research Institute

Accessing Database

Managing Database

Device Info

Campaign Info

Sample Info

Analysis Info

Device Name :	<input type="text"/>
Campaign :	<input type="text"/>
sample Name :	<input type="text"/>
Size (from, to) :	<input type="text"/> - <input type="text"/> μm
First Wall Material :	Carbon <input type="button" value="v"/>
<input type="button" value="Search"/> <input type="button" value="Reset"/>	

DFT/MD database

- DFT database (Oda)

Click on the links inside the tabbed menu:

W	Be	C
---	----	---

Tungsten
Z=74

W	W-H	W-H-He	W-N
---	-----	--------	-----

Click on the links inside the tabbed menu:

W	Be	C
---	----	---

W-H
contents

Potential Model	First-principles calculation
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- MD database (Dudarev, Sand)

DFT database (Oda)

Click on the links inside the tabbed menu:

W Be C

Tungsten

Z=74

W W-H W-H-He W-N

Click on the links inside the tabbed menu:

W Be C

W-H

contents

Potential Model First-principles calculation

MD database (Dudarev, Sand)

November 16-17, 2017 TM of the code centre network on molecular dynamics data of collisional cascades after irradiation

- ★ Atomic coordinates in ASCII readable text file
 - Possible additional information: velocities, potential energy,...
- ★ Simple format: XYZ file

```
601526
Frame number 11687 40002. fs boxsize 212.068400 212.068400 212.068400
W -103.659726 79.923029 -103.661777 -8.900047
W -103.660175 79.923225 -100.496878 -8.900130
W -103.659834 79.922949 -97.330699 -8.900268
W -103.660790 79.923151 -94.167560 -8.898738
W -103.660363 79.922767 -91.003001 -8.900769
W -103.659343 79.923741 -87.837000 -8.899446
W -103.659576 79.923071 -84.671184 -8.900672
W -103.659617 79.923131 -81.507449 -8.900600
W -103.660214 79.922650 -78.343085 -8.900321
W -103.659035 79.923771 -75.177067 -8.900647
W -103.660728 79.923978 -72.012728 -8.899717
W -103.658488 79.923953 -68.845823 -8.900009
W -103.660177 79.924804 -65.681139 -8.902425
W -103.660350 79.924767 -62.515246 -8.900812
W -103.659059 79.923857 -59.350034 -8.900000
W -103.660107 79.923701 -56.185375 -8.900031
```

Atomic and Molecular Data Unit CRPs



2009-2014: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions.

2010-2015: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV.

2011-2016: Data for Hydrogen and Helium and Their Isotopes in Fusion Plasma.

2012-2017: Erosion and Tritium Retention in Beryllium Plasma-facing Materials.

2013-2018: Plasma-wall Interaction with Irradiated Tungsten and Tungsten Alloys.

2015-2020: Plasma-wall Interaction with Reduced-activation Steel Surfaces.

2016-2021: Data for Atomic Processes of Neutral Beams in Fusion Plasma.

For consideration: Atomic Models and Data for Vapour Shielding in Fusion.

For consideration: Data for Plasma Interaction With Liquid Metal Surfaces.

2013-2017: Plasma-Wall Interaction With Irradiated Tungsten and Tungsten Alloys in Fusion Devices



<https://www-amdis.iaea.org/CRP/IrradiatedTungsten/>

Objective: To provide best expert estimates and uncertainties for tritium retention in tungsten-based materials in a fusion reactor

Main topics:

- Characterization of microstructure of irradiated tungsten;
- Hydrogen trapping and migration in damaged tungsten.

Meetings:

- First Research Coordination Meetings (RCM) 26-28 Nov 2013.
- Second RCM at SNU, Korea, 8-11 Sep 2015
- Third RCM in about Q2 2017.
- Final report developed in 2017, published in 2018.

Participants: 19 projects;

... Irradiated Tungsten CRP: Participants



60 Years

Atoms for Peace and Development

- Guang-Hong Lu et al., Beihang University, Beijing. **Hong-Bo Zhou**
- Changsong Liu, Xuebang Wu et al., ISSP-CAS, Hefei.
- Guangnan Luo, Chonghong Zhang et al., IPP-CAS, Hefei. **Haishan Zhou**
- Marie-France Barthe, Charlotte Becquart et al., CNRS.
- Christian Grisolia, Bernard Rousseau et al., CEA. **Elodie Bernard**
- Matej Mayer, Thomas Schwarz-Selinger et al., IPP Garching.
- Bernard Unterberg, Jochen Linke et al., Forschungszentrum Jülich. **Marius Wirtz**
- Shishir Deshpande, P. M. Raole et al., IPR, Gandhinagar.
- Akira Hasegawa et al., Tohoku University.
- Yuji Hatano, Yasuhisa Oya et al., Toyama University.
- Mizuki Sakamoto, Hideo Watanabe et al., University of Tsukuba.
- Takuji Oda, Hyung-Jin Shim et al., Seoul National University.
- Yury Gasparyan, Alexander Pisarev et al., MEPhI, Moscow.
- Boris Khripunov, Alexander Ryazanov et al., Kurchatov Institute, Moscow.
- Sabina Markelj et al., Josef Stefan Institute, Ljubljana.
- Segei Dudarev et al., CCFE, Abingdon.
- Brian D. Wirth et al., University of Tennessee, Knoxville. **Rick Kurtz**
- Jean-Paul Allain, David Ruzic et al., University of Illinois.
- Masashi Shimada, Brad Merrill et al., Idaho National Laboratory.

Discussions at the 2RCM

- DPA definition and estimates
- Benchmark and common protocol for TPD/TDS experiments
- TDS/TPD simulations comparison exercise
- Fundamental Modeling:
 - electronics structure calculations and development of interaction potentials and rate coefficients based on electronic structure
 - verification and validation of models
- Damage production and characterization

Objectives for the Final RCM

- Review of recent work by participants
 - Report from each group
- Discussions and reviews
 - TDS simulation comparison exercise (Shimada)
 - TDS Round Robin experiment review (Lee and Schwarz-Selinger)
 - Overall CRP objectives (Thursday)
 - Fundamental modelling and its connection to experiments. (Dudarev, Oda)
 - Production and characterization of damage (Hasegawa, Kurtz)
 - Hydrogen (tritium) retention in damaged tungsten (Mayer, Shimada)
- Final report
 - A comprehensive review report from CRP participants or
 - An individual report from each CRP group
- Database Issues (Thursday afternoon)
- Future activities



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Thank you!

