International Atomic Energy Agency INDC(NDS)-445

I N D C INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Technical Meeting on
"Atomic and Plasma-Material Interaction Data for Fusion Science Technology"

28-31 October 2002, Jülich, Germany

SUMMARY REPORT

Prepared by: R.E.H. Clark

October 2003

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

INDC(NDS)-445

IAEA Technical Meeting on
"Atomic and Plasma-Material Interaction Data for Fusion Science Technology"

28-31 October 2002, Jülich, Germany

SUMMARY REPORT

Prepared by: R.E.H. Clark

October 2003

Abstract

The proceedings and conclusions of the Technical Meeting on “Atomic and Plasma-Material Interaction Data for Fusion Science Technology” held in Jülich, Germany on October 28-31 are summarized. During the course of the meetings working groups were formed to review the status of specific areas of atomic, molecular and material physics of relevance to fusion and to make recommendations on data needs in fusion from these areas. The reports of those working groups are summarized and the complete reports included as appendices. This meeting brought together over fifty leading scientists in fusion related data. Results of research in a number of topics were presented and very useful discussions were held. The meeting was extremely successful.

Reproduced by the **IAEA** in Vienna, Austria
October 2003

Table of Contents

Appendices

1. INTRODUCTION

The Technical Meeting on "Atomic and Plasma-Material Interaction Data for Fusion Science Technology" was held on October 28-31 October, 2002 at the Institut für Plasmaphysik, Forschungszentrum Jülich, Germany. The objectives of the meeting were:

a) To review the current status of atomic and plasma-interaction data relevant to fusion

b) To make recommendations on data needs and priorities on such data in light of current fusion machine design considerations.

The meeting was attended by over fifty leading scientists in atomic, molecular, plasma and material physics. A complete list of the participants is included as Appendix 1.

2. BRIEF MEETING PROCEEDINGS

The meeting began with opening addresses from G. Eisenbeiss of the host institution, R. Clark of the IAEA, and B. Vierkorn-Rudolph of BMBF. The Meeting Agenda was adopted without change (see Appendix 2). The meeting then continued with six sessions, the first five devoted to reports of current status of data and fusion technology, and the fifth session devoted to working groups which met to review and form specific recommendations for data for fusion technology.

R. Clark acted as chairman of the first session. The focus of this session was the current status of fusion research. The first speaker, D. Campbell of EFDA CSU-Garching, gave a thorough overview of the status and prospects of fusion research, including some considerations that must be addressed in physics issues, as well as engineering problems. H. Bruhns, of the European Commission, then presented a summary of the perspectives of fusion in the European 6^{th} Framework Program, including an emphasis on the importance of energy research in general and some of the specific attractive properties on fusion.

The second session summarized the data needs in fusion reactors and was chaired by D. Reiter and J. Hogan. T. Evans of General Atomics reviewed the data needs and the physics of the DIII-D device. A summary of the energy deposition and the implications of ELMS in fusion devices was given by A. Loarte of Max-Planck-Institut für Plasmaphysik. J. Rice of the Massachusetts Institute of Technology gave a talk on the spectroscopy of heavy elements in the C-Mod device. A discussion of molecular diagnostics of cold edge plasmas was presented by U. Fantz of Lehrstuhl für Experimentelle Plasmaphysik. Following a coffee break, H. Kubo of Naka Fusion Research reported on divertor spectroscopy in the JT-60U machine, with an emphasis on molecules. K. Sato of the National Institute for Fusion Science described VUV emission characteristics in the Large Helical Device. A. Pospeisczczyk of Forschungszentrum Jülich then reviewed the processes taking place in high temperature edge plasamas. This was followed by a presentation by D. Reiter of Forschungszentrum Jülich on computer codes used in modelling fusion reactor edge plasmas. After this talk a poster session was held.

The third session focussed on plasma-surface interaction and material properties data needs in fusion and was chaired by V. Philipps of Forschungszentrum Jülich. U. Samm, of the Institut für Plasmaphysik, Forschungszentrum Jülich, discussed the status and data needs for plasma wall interactions. This was followed by a review of the status of data for sputtering and erosion of plasma facing materials given by J. Roth of Max-Planck-Institut für Plasmaphysik. T. Tanabe, of the Centre for Integrated Research in Science & Engineering, then gave a presentation on hydrogen recycling by spectroscopy in linear plasma machines. Following a coffee break G. Federici of the ITER Garching Joint Work Site discussed tritium inventory in ITER plasma facing components. This was followed by the final talk of this session by V. Barabash of the ITER EDA Garching Work Site on the topic of data status and needs of thermo-mechanical properties of materials in fusion devices.

The fourth session was chaired by R. Janev, J. Roth and A. Haasz and focussed on data generation activities. R.W. McCullough of Queen's University Belfast gave the first presentation on th data generation activities for heavy particle collisions relevant to fusion. This was followed by a talk by L.A. Vainstein of the P.N. Lebedev Physical Institute on computer codes used in calculating electron-ion and electron-atom collision processes. T. Märk of Universität Innsbruck then gave a presentation on electron-molecule collisions. Following a coffee break W. Jacob of Max-Planck-Institut für Plasmaphysik presented a review of sticking coefficients and surface loss probabilities of hydrocarbon radicals on plasma facing surfaces. This was followed by a talk by R. Causey of Sandia National Laboratories on hydrogen retention and recycling in tungsten. A. Haasz of University of Toronto then gave a presentation on hydrogen retention and release with carbon. This was followed by a presentation by R. Doerner of University of California, San Diego on beryllium and liquid metals. Next came a talk by R. Neu of the ASDEX Upgrade team on data generation in fusion devices with erosion yields from spectroscopy as the primary emphasis. This was followed by the final talk of the session by S. Rose of Aldermaston on high energy density plasmas.

The fifth session was chaired by N. Peacock and was on the topic of status of databases. The first talk by R. Clark of the International Atomic Energy Agency described the databases and database establishment programs at the IAEA. H. Summers of University of Strathclyde reviewed the Atomic Data and Analysis Structure, ADAS, project. R.K. Janev of Macedonian Academy of Sciences and Arts and currently at Forschungszentrum Jülich gave a talk on the status of a collision database for atomic and molecular hydrogen in fusion plasmas. This was followed by a presentation by T. Kato of the National Institute for Fusion Science on the NIFS database and the linking of databases within the IAEA Data Centre Network. The final talk of this session was given by W. Wiese of National Institute for Standards and Technology on the NIST atomic structure database.

The sixth session began with the formation of working groups on the topics of:

1. Atomic and Molecular Data.
2. Plasma-Surface Interaction.
3. Material properties.

The participants naturally fell into one of the categories, although there was some overlap between the plasma-surface interaction group and the material properties group. After the formation of the three groups, time was set aside for the groups to meet with the two goals of summarizing the current status of data in the area and recommending data needed for future fusion related research in the next five to ten years. This work continued through the morning of the fourth day. In the afternoon of the fourth day each group gave a report of the work of the group and led discussion on that report. Each group had the additional task of producing a final written version of the report. Those final reports are included as appendices to this Summary Report. At the conclusion of this final session the meeting was adjourned.

3. MEETING CONCLUSIONS AND RECOMMENDATIONS

As mentioned at the end of the previous section the full reports from the working groups are attached as appendices 3-5. In this section we include the main conclusions and recommendations from each group.

3.1. Atomic and Molecular Data

The analysis of the status of atomic and molecular (A+M) spectroscopic and collision databases in view of the needs of current fusion plasma research and design of next-generation fusion devices leads to the following general conclusions:

(1) An impressive body of A+M data information relevant to fusion research has been accumulated during the years and implemented into fusion plasma application codes. The breath of fusion relevant data generation world-wide is strong and, generally, adequately follows the development of fusion research needs.

(2) The IAEA has played and continues to play a critical role in fostering and co-ordinating the A+M data generation efforts and in dissemination of the data to the fusion research community. The IAEA role in establishing and facilitating the interaction between the atomic and fusion communities in A+M data field is also crucial for focusing of data generation efforts on most urgent data needs and for efficient implementation of the results of these efforts in fusion research.

(3) Despite the remarkable achievements in the completion and improvement of A+M databases for fusion, observed in the period since the last IAEA Technical Committee Meeting of this subject in 1992, the spectroscopic and collision A+M databases for fusion still contain significant gaps. The present unsatisfactory status of certain databases is also the result of the shifted priorities for A+M data in the fusion research (related to new divertor operation regimes, materials for plasma facing components, etc).

(4) The most urgent high priority A+M data needs for the current fusion research and design of next-generation, reactor level fusion devices are:

   (a) Improvement (validation) of the collision database for hydrocarbon impurities to understand their transport in edge/divertor plasma, and associated re- (and co-) deposition processes, in order to qualify the suitability of carbon as a plasma facing material;

   (b) Improvement of spectroscopic and collision databases for high-Z materials (particularly W) as they are being considered as plasma facing materials for next generation fusion devices, or as diagnostic impurities (Kr);

(c) Improvement and completion of the coupled H/H_2 collision database for increasing the predictive capabilities of neutral particle transport codes in divertor performance modelling and optimisation, and to increase the reliability of molecular edge plasma diagnostics.

(5) It is strongly recommended that the IAEA considers the initiation of co-ordinated research Projects (CRPs) in the near future on the subjects (a) and (b) above for accelerating the process of establishing the corresponding databases.

3.2. Plasma Surface Interaction Data

In summary, the R&D program needs to address the physics of the erosion mechanisms and the transportation and redeposition of eroded material and to demonstrate T removal on a Tokamak. Many inportant issues for further R&D are given in the detailed discussion above, requiring laboratory work and more wall diagnostics with Tokamak operation time dedicated to wall experiments. Modelling of the results are essential to enable progress on wall physics.

In order to identify topics of highest priority the scenario can be devided into a case involving carbon as first wall material and a case of an all-metal machine.

CFC Target Plates:

- In-situ determination of sources and sinks for carbon erosion. Development of suitable diagnostics on a shot-to-shot basis and investigation of the deposited layer thickness.
- Removal of T from deposited layers. Techniques available from laboratory experiments (oxidation, laser desorbtion) need to be tested and validated in existing fusion devices.

All Metal Machine:

- In-situ determination of the erosion of high-Z target plates by seed impurities. Establish the fact that the reduction in divertor temperature offset the increased erosion by seed impurities.

Investigation of high heat flux performance of high-Z components. This includes test laboratory experiments and the use of high-Z divertor plates in an experiment with relevant ELM scenarios.

3.3. Material Properties

(1) To the PSI-community: use the proposed material candidates for material studies (e.g NB31, W with relevant texture)

(2) It is useful to organize collection of the data in the form of database with as much detailed information as possible.

Appendix 1

IAEA Technical Meeting on
"Atomic and Plasma-Material Interaction Data for Fusion Science Technology"

28-31 October 2002, Jülich, Germany

LIST OF PARTICIPANTS

AUSTRIA
Prof. T. Märk
Universität Innsbruck
Technikerstrasse 25
A-6020 Innsbruck
Tel.: +43-512-507-6240; Fax: +43-512-507-2932
E-mail: tilman.maerk@uibk.ac.at

BELGIUM
Dr. F. Brouillard
Université Catholique de Louvain
Laboratorie de Physique Atomique
Et Moleculaire – FYAM
B-1348 Louvain-la-Neuve
Tel.: +32-10-47-3252; Fax: +32-10-47-2431
E-mail: brouillard@fyam.ucl.ac.be

Prof. Pierre Defrance
Université catholique de Louvain
Département de Physique, Unité FYAM,
Chemin du Cyclotron, 2
B-1348 Louvain-la-Neuve
Tel.: +32-10-47-3348; Fax: +32-10-47-2431
E-mail: defrance@fyam.ucl.ac.be

Dr. Xavier Urbain
Université catholique de Louvain
Département de Physique, Unité FYAM,
Chemin du Cyclotron, 2
B-1348 Louvain-la-Neuve
Tel.: +32-10-47-3348; Fax: +32-10-47-2431
E-mail: urbain@fyam.ucl.ac.be

CANADA
Dr. A.A. Haasz
Professor and Director
University of Toronto
Institute for Aerospace Studies
4925 Dufferin St.
Toronto, Ontario M3H-5T6
Tel.: +1-416-667-7734; Fax: +1-416-667-7925
E-mail: aahaasz@utias.utoronto.ca

CHINA
Dr. Sun Yongsheng
Institute of Applied Physics & Computational
Mathematics
P.O. Box 8009
Beijing 100088
Tel.: +86-1-201-4411-3101; Fax: +86-1-2010-108
E-mail: sunys@mail.iapcm.ac.cn

EUROPEAN COMMISSION
Prof. H. Bru;hns
European Commission, MO 3.58
Rue Montoyer 75
B-1049 Brussels
Tel.: +32-2-295-7923; Fax: +32-2-296-4252
E-mail: Hardo.Bruhns @cec.eu.int

Dr. David Campbell
European Commission – EFDA
CSU-Garching
Boltzmannstrasse – 2
D-85748 Garching
Fax: +49-89-3299-4312

Dr. Gianfranco Federici
ITER Garching Joint Work Site
Max-Planck-Institut für Plasmaphysik
D-85748 Garching
Tel.: +49-89-3299-4228; Fax: +49-89-3299-4110
E-mail: federig@ipp.mpg.de ; federig@itereu.de

FRANCE
Dr. K. Katsonis
Laboratoire de Physique des Gas et des Plasmas
Université de Paris Sud
Batiment 212
F-91405 Orsay Cedex
Tel.: +33-169-156543; Fax: +33-169-417844
E-mail: konstantinos.katsonis@lpgp.u-psud.fr

GERMANY
Dr. V. Barabash
ITER EDA Garching Work Site
Max-Planck-Institut für Plasmaphysik
Boltzmannstrasse 2
D-85748 Garching bei München
Tel.: +49-89-329-94144; Fax: +49-89-329-94110
E-mail: barabav@sat.ipp-garchingmpg.de

Dr. Günter Bertschinger
Forschungszentrum Jülich GmbH
Institut für Plasmaphysik
Postfach 1913
D-52425 Jülich
Tel.: +49-2461-615781; Fax: +49-2461-616664
E-mail: g.bertschinger@fz-juelich.de

Dr. Sebastian Brezinsek
Plasma-Wand-Wechselwirkung
Institut für Plasmaphysik
Forschungszentrum Jülich GmbH
D-52425 Jülich
Tel.: +49-2461-616611; Fax: +49-2461-613331
E-mail: s.brezinsek@fz-juelich.de

Dr. Ursel Fantz
Lehrstuhl für Experimentelle Plasmaphysik
Institut für Physik
Universitätstr. 1
D-86135 Augsburg
Tel.: +49-821-598-3310; Fax: +49-821-598-3302
E-mail: fantz@physik.uni-augsburg.de

Dr. Franz Gerstgrasser
SGL CARBON GmbH
Graphite Specialties
Innovation Management
Drachenburgstrasse 1
D-53170 Bonn
Tel.: +49-228-841-253; Fax: +49-228-841-68-253
E-mail: franz.gerstgrasser@sglcarbon.de

Dr. Wolfgang Jacob
Centre for Interdisciplinary Plasma Science
Max-Planck-Institut für Plasmaphysik
EURATOM Association
P.O. Box 1533
Boltzmannstr. 2
D-85748 Garching
Tel.: +49-89-3299-2618; Fax: +49-89-3299-1149
E-mail: wolfgang.jacob@ipp.mpg.de

Dr. J. Linke
Forschungszentrum Jülich GmbH
Institut für Werkstoffe und Verfahren
Der Energietechnik IWV-2
D-52425 Jülich
Tel.: +49-2461-616880; Fax: +49-2461-613699
E-mail: j.linke@fz-juelich.de

Dr. A. Loarte
Max-Planck-Institut für Plasmaphysik
EFDA CSU Working Site
Boltzmannstr. 2
D-85748 Garching bei München
E-mail: loartea@ipp.mpg.de

Dr. Matej Mayer
Max-Planck-Institut für Plasmaphysik
Boltzmannstr. 2
D-85748 Garching
Tel.: +49-89-3299-1639; Fax: +49-89-3299-2279
E-mail: matej.mayer@ipp.mpg.de

Dr. Philippe Mertens
Institut für Plasmaphysik
Forschungszentrum Jülich
D-52425 Jülich
Tel.: +49-2461-61-5720; Fax: +49-2461-61-5452
E-mail: ph.mertens@fz-juelich.de

Dr. Dirk Naujoks
Max-Planck-Institut für Plasmaphysik
Bereich Plasmadiagnostik
Mohrenstrasse – 41
D-10117 Berlin

Dr. R. Neu
Max-Planck-Institut für Plasmaphysik
Boltzmannstr. 2
D-85748 Garching

Dr. V. Philipps
Forschungszentrum Jülich GmbH
Institut für Plasmaphysik
D-52425 Jülich
Tel.: +49-2461-61-6331; Fax: +49-2461-61-2660
E-mail: v.philipps@fz-juelich.de

Dr. A. Pospieszczyk
Institut für Plasmaphysik
Forschungszentrum Jülich
D-52425 Jülich
Tel.: +49-2461-61-5536; Fax: +49-2461-61-3331
E-mail: a.pos@fz-juelich.de

Prof.. D. Reiter
Institut für Plasmaphysik
Forschungszentrum Jülich
D-52425 Jülich
Tel.: +49-2461-615841; Fax: +49-2461-612970
E-mail: d.reiter@fz-juelich.de

Dr. Joachim Roth
Max-Planck-Institut für Plasmaphysik
Boltzmannstr. 2
D-85748 Garching
Tel.: +49-89-3299-1387; Fax: +49-89-3299-2279
E-mail: roth@ipp.mpg.de

Prof. U. Samm
Director, Institut für Plasmaphysik
Forschungszentrum Jülich
D-52425 Jülich
Tel.: +49-2461-61-3085
E-mail: u.samm@fz-juelich.de

Dr. Beatrix Vierkorn-Rudolph
Bundesministerium für Bildung und
Forschung Referat 414
Heinemannstrasse – 2
D-53170 Bonn-Bad Godesberg
Tel.: +49-1888-572174; Fax: +49-1888-5782174
E-mail: beatrix.vierkorn-rudolph@bmbf.bund.de

JAPAN

Dr. Takako Kato
Data and Planning Centre
National Institute for Fusion Science
322-6, Oroshi-cho, Toki-shi
Gifu-ken, 509-5292
Tel.: +81-57-258-2265; Fax: +81-57-258-2628
E-mail: takako@nifs.ac.jp

Dr. Mineo Kimura
Professor of Physics
Graduate School of Science and Engineering
Yamaguchi University
UBE, Yamaguchi 755-8611
Tel.: +81-836-85-9805; Fax: +81-836-85-9801
E-mail: mineo@po.cc.yamaguchi-u.ac.jp

Dr. H. Kubo
Naka Fusion Research
Japan Atomic Energy Research Institute (JAERI)
801-1 Mukoyama, Naka-machi, Naka-gun
Ibaraki-Ken 311-0193
Tel.: +81-29-270-7349; Fax: +81-29-270-7419
E-mail: kubo@naka.jaeri.go.jp

Dr. Kuninori Sato
Associate Professor
National Institute for Fusion Science
322-6, Oroshi-cho, Toki-shi
Gifu-ken, 509-5292

Dr. Tetsuo Tanabe
Centre for Integrated Research in Science
& Engineering
Nagoya University
Furo-cho, Chikusa-ku
Nagoya 464-8603
Tel.: +81-52-789-5157
Fax: +81-52-789-5177 (or) 5158
E-mail: tanabe@cirse.nagoya-u.ac.jp

MACEDONIA

Dr. R.K. Janev
Macedonian Academy of Sciences and Arts
Bulevar K. Misirkov, 2
P.O. Box 428
91000 Skopje
Tel.: +389-91-114200; Fax: +389-91-114685
E-mail: rjanev@manu.edu.mk

Currently at:
Institut für Plasmaphysik
Forschungszentrum Jülich
D-52425 Jülich
Tel.: +49-2461-615878; Fax: +49-2461-612660
E-mail: r.janev@fz-juelich.de

NETHERLANDS

Dr. R. Hoekstra
Kernfysisch Versneller Institut
University of Groningen
Zernikelaan 25
NL-9747 AA Groningen
Tel.: +31-50-633-600; Fax: +31-50-634-003
E-mail: hoekstra@kvi.nl

RUSSIAN FEDERATION

Dr. V.Kh. Alimov
Institute of Physical Chemistry
Russian Academy of Sciences
Leninsky Prospect 31
119991 Moscow
Tel.: +7-095-330-2192; Fax: +7-095-334-8531
E-mail: alimov@ipc.rssi.ru

Dr. M. Panov
Atomic Collision Laboratory
Ioffe Physical -Technical Institute of
Russian Academy of Sciences (RAS)
Politechnicheskaya 26
St. Petersburg 194021
Tel.: +7-812-2479146; Fax: +7-812-2471710
E-mail: m.panov@mail.ioffe.ru

Dr. L. Vainshtein
Fizicheskij Institut P.N. Lebedeva
Akademii Nauk Russia
Leninskij Prospekt 53
119991 Moscow
Tel.: +7-095-135-2429; Fax: +7-095-135-2429
E-mail: vanish@sci.lebedev.ru

SPAIN

Dr. Luis Méndez
Laboratorio Asociado al CIEMAT de Fisica
Atomica y Molecular en Plasmas de Fusion
Universidad Autonoma de Madrid
Canto Blanco, 28049 Madrid
Tel.: +34-91-397-5259; Fax: +34-91-397-4187
E-mail: l.Mendez@uam.es

UNITED KINGDOM

Dr. P.T. Greenland
14 Bailie Close
Abingdon
Oxon Ox14 5RF
Tel.: 44-1235-521760; Fax: +44-1235-521760
E-mail: ptg@globalnet.co.uk

Dr. R.W. McCullough
Atomic and Molecular Physics Research Division
Department of Pure and Applied Physics
The Queen's University of Belfast
Belfast, BT7 1NN
Northern Ireland
Tel.: +44-28-90-273541; Fax: +44-28-90-310785
E-mail: rw.mcculough@qub.ac.uk

Dr. N.J. Peacock
Culham Fusion Laboratory
Culham, Abingdon
Oxfordshire, OX14 3DB
Tel.: +44-1-235-463561; Fax: +44-1-235-463682
E-mail: nicol.peacock@ukaea.org.uk

Dr. Steve Rose
Building N56
AWE
Aldermaston
Reading RG7 4PR
Tel.: +44-118-982-6193; Fax: +44-118-982-4844
E-mail: steven.rose@awe.co.uk

Dr. H.P. Summers
Department of Physics and Applied Physics
University of Strathclyde
107 Rottenrow
Glasgow, Scotland G4ONG
Tel.: +44-141-548-4196; Fax: +44-141-552-2891
E-mail: summers@phys.strath.ac.uk

UNITED STATES OF AMERICA

Dr. M. Crisp
Office of Fusion Energy Sciences
Office of Science, SC-55
U.S. Department of Energy
19901 Germantown Road
Germantown, MD 20874-1290
Tel.: +1-301-353-4883
Fax: +1-301-903-1225
E-mail: michael.crisp@science.doe.gov

Dr. Predrag Krstić
Oak Ridge National Laboratory
Physics Division
P.O. Box 2008
Oak Ridge, TN 37831-6373
Tel.: +1-865-574-4701; Fax: +1-865-574-4745
E-mail: krsticp@ornl.gov

Dr. John E. Rice
Plasma Science and Fusion
Massachuetts Institute of Technology (MIT)
Massachuetts Avenue, NW17-174
Cambridge, MA 02139-4307
Tel.: +1-617-253-6052
E-mail: rice@psfc.mit.edu

Dr. W.L. Wiese
Bldg. 221, Room: A267
Atomic and Plasma Radiation Division
US Department of Commerce
National Institute for Standards and Technology
Gaithersburg, MD 20899
Tel.: +1-301-975-3201; Fax: +1-301-990-1350
E-mail: wolfgang.wiese@nist.gov

IAEA

Dr. R.E.H. Clark
IAEA Atomic and Molecular Data Unit
Wagramerstrasse – 5
P.O. Box 100
A-1400 Vienna, Austria
Tel.: +43-1-2600-21731; Fax: +43-1-26007
E-mail: r.e.h.clark@iaea.org

Appendix 2

IAEA Technical Meeting on
"Atomic and Plasma-Material Interaction Data for Fusion Science Technology"

28-31 October 2002, Jülich, Germany

MEETING AGENDA

Monday 28 October

09:30-10:00	Host Institution: G. Eisenbeiss IAEA Representative: R. Clark BMBF Representative: B. Vierkorn-Rudolph	

Session 1: Current Status of Fusion Research

Chairman: R. Clark

10:00-10:30	D. Campbell	Status and prospects of fusion research
10:30-11:00	*Coffee Break*	
11:00-11:30	H. Bruhns	Perspectives of fusion in the European 6th Framework Programme
11:30-13:00	*Lunch*	

Session 2: A+M Data needs in Fusion Reactors

Chairman: D. Rieter

13:00-13:30	T. Evans	Advanced physics, A+M needs for DIII-D diagnostics
13:30-14:00	A. Loarte	Energy deposition from ELMs in fusion devices
14:00-14:30	J. Rice	Spectroscopy of high Z elements in C-Mod
14:30-15:00	U. Fantz	Molecular diagnostics of cold edge plasmas
15:00-15:30	*Coffee Break*	

Chairman: J. Hogan

15:30-16:00	H. Kubo	Divertor spectroscopy with attention to molecules in JT-60U

16:00-16:30	K. Sato	VUV emission characteristics in LHD plasmas
16:30-17:00	A. Pospieszczyk	High temperature plasma edge diagnostics
17:00-17:30	D. Reiter	Fusion reactor plasma edge modelling codes
17:30-19:00	*Poster-Session*	

<u>Tuesday 29 October</u>

<u>*Session 3: Plasma-Surface Interaction and Material Properties Data Needs in Fusion Reactors*</u>

<u>Chairman</u>: V. Philipps

9:00-9:30	U. Samm	Plasma wall interaction modelling: status and data
09:30-10:00	J. Roth	Review and status of sputtering, erosion of plasma facing materials
10:00-10:30	T. Tanabe	Hydrogen recycling studies by spectroscopy in linear plasma machines
10:30-11:00	*Coffee Break*	
11:00-11:30	G. Federici	Tritium inventory in the materials of the ITER plasma-facing components
11:30-12:00	V. Barabash	Data status and needs on thermo-mechanical properties of structural materials in fusion devices
12:00-13:30	*Lunch*	

<u>*Session 4. Data Generation Activities*</u>

<u>Chariman</u>: R. Janev

13:30-14:00	R.W. McCullough	Data generation activities for heavy particle collisions relevant to fusion
14:00-14:30	L.A. Vainstein	Electron-ion/atom collision processes: review of data generating codes
14:30-15:00	T. Märk	Electron-molecule collisions
15:00-15:30	*Coffee Break*	

Chairman: J. Roth

15:30-16:00	W. Jacob	Sticking coefficients and surface loss probabilities of hydrocarbon radicals on plasma facing surfaces
16:00-16:30	R. Causey	Hydrogen retention and recycling in tungsten
16:30-17:00	A. Haasz	Hydrogen retention and release in/from carbon
17:00-17:30	R. Doerner	Beryllium and liquid metals

Wednesday 30 October

Session 4 (continure)

Chairman:A. Haasz

09:00-09:30	R. Neu	Data generation in fusion devices: Erosion yields from spectroscopy
09:30-10:00	S. Rose	High energy density plasmas
10:00-10:30	*Coffee Break*	

Session 5. Status of Databases

10:00-10:30	R.E.H. Clark	A+M databases and database establishment programs
10:30-11:00	H. Summers	The Atomic Data and Analysis Structure, ADAS
11:00-11:30	R.K. Janev	Status of collision database for atomic and molecular hydrogen in fusion plasmas
12:00-13:30	*Lunch*	
13:30-14:00	T. Kato	NIFS database and cooperation with IAEA DCN
14:00-14:30	W. Wiese	NIST Atomic structure database (energy levels, transition probilities, wavelengths)
14:30-15:00	*Coffee Break*	

Session 6 Formation of working groups
Groups of 1. A+M data 2. PSI 3. Material properties

Visit to TEXTOR

Thursday, 31 October

Morning:

Working groups meet separately

12:00-13:30 *Lunch*

Afternoon

Joint session:

1. Reports of working groups conclusions and recommendations with respect to status and needs
2. Discussion of Reports and possible amendments
3. Adoption of meeting conclusions and recommendations

Adjournment of the Meeting

Appendix 3

Working Group Report on:
Atomic and Molecular Data: Status and Needs for Research on Present and Design of next Generation Magnetic Fusion Devices

1. Introduction

Atomic and molecular (A+M) structural, radiative and collisional data continue to play a vital role in fusion energy research and development. This role is particularly pronounced in the areas of impurity control, power and particle exhaust and plasma diagnostics. Power and particle control continues to be a critical issue in the design of next generation, reactor level fusion devices, and present approaches to its solution extensively rely on the use of radiative and collision properties of atomic and molecular species (present, or deliberately introduced) in the plasma. Reduction of plasma power and particle fluxes on critical plasma facing components (divertor plates) requires appropriate levels of radiative (and other types of) plasma cooling and plasma momentum dissipation in the edge and divertor regions, which can be achieved only through atomic collision processes. On the other hand, diagnostics of both core and periphery (edge, SOL, divertor) plasmas of magnetic fusion devices, based on radiation and other features of atomic (ionic) and molecular (in cold edge regions) species, remain a basic tool for obtaining information on basic plasma parameters, as well as on plasma dynamics.

A significant development during the last ten (or so) years, i.e. since the last IAEA Technical Committee Meeting in Cadarache (France) 1992, has been the achievement of detached plasma regimes in divertors of operating large fusion devices, accompanied with significant reductions of the plasma fluxes on divertor plates. The achievement of detached plasma regimes requires low divertor plasma temperatures (below ~ 3-5 eV in the near-wall regions) and high neutral particle densities. Under such conditions, collision processes of molecular hydrogen and other molecular impurities play a prominent role in divertor plasma kinetics (including the volume plasma recombination), thus opening a new large area of (molecular) data needs for the fusion research. These needs were further emphasised by the development of molecular (radiation band) based edge plasma diagnostic techniques, that require information on vibrationally resolved molecular collision processes.

The present report addresses the status of A+M spectroscopic and collisional data (availability and needs) in the context of key fusion research and design areas of impurity control, power and particle exhaust and plasma diagnostics. The A+M data aspects of neutral beam plasma heating are also covered by the scope of the report. It is convenient to consider the data status and needs for the core and edge/SOL/divertor plasma related studies/design issues separately.

2. Atomic Data for Core Plasma Studies

The core plasma related studies and design issues for which atomic data are essential include: plasma diagnostics, impurity transport and radiation, and neutral beam plasma heating.

2.1. Plasma Diagnostics

The atomic data status and needs will be assessed for the following major core plasma diagnostic methods/techniques:

a. X-ray and VUV spectroscopy;
b. Charge exchange recombination spectroscopy (CXRS);
c. Beam emission spectroscopy;
d. Active-beam alpha-particle diagnostics;
e. Neutral particle emission analysis.

2.1.a. X-ray and VUV spectroscopy

These diagnostic techniques are based on the analysis of emitted radiation of highly stripped impurities in the core plasma. Both intrinsic and deliberately medium- and high- Z impurities (depending on core plasma temperatures) are used for diagnostic purposes. The types of intrinsic impurities depend on used first wall materials and in presently operating fusion devices they include (besides the low-Z, Be, B, C, and O): Ti, Cr, Fe, Co, Ni, Cu and Mo. Use of tungsten (W) is envisaged for ITER. Injected impurities include: Ne, Si, Ar and Kr (for ITER). Collision processes involved in the ion level population/depopulation kinetics include: electron-impact excitation, ionisation and dielectronic recombination of impurity ions, radiative transitions, and electron capture from the residual atomic hydrogen (if the concentration of the latter is higher than a few times 10^{-5} n_e, as in beam heated plasmas).

Data Status and Needs

Spectroscopic data (energy levels, transition probabilities) are available for low-Z ($Z \leq$ 10) impurities in all charge states, but are incomplete for some of the medium-Z impurities (10.Z.30), especially for the higher charge states, and rather scarce for the high-Z (Z/30) impurities. The spectroscopic database for the iron group (Cr, Fe, Ni) is in fairly good shape from the view point of completeness, but uncertainties in transition probabilities are still quite large (often more than 50%). The energy level data for high-Z impurities (Kr, Mo, W, Ta, Xe) are limited only to lower charge states, and the information on transition probabilities is rather fragmentary and not always reliable.

Data generation capabilities to fill at least some of the data gaps do, however exist (EBIT sources, computer packages such as HULAC, etc.), but appropriate motivation should be provided to engage them in a data generation effort.

The collision database for highly stripped (H-,He-Li-like) medium-Z core plasma impurities is in fairly good shape, particularly for the iron group of elements. Because of the relatively small number of target electrons and strong electron-ion (Coulomb) interaction, existing and wide-spread computer codes (based on Coulomb-Born distorted wave, or other approximations) can easily provide the necessary electron-impact collision data of adequate accuracy. However, still discrepancies in the data (and code results), exist for the He-like, w, x, y and z satellite lines, the ratios of which (z/(x +x y), (x + y + z)/w) are normally used in the diagnostic procedure. The e-impact data for Be-, B- C-like isoelectronic sequences are less available, or have much larger uncertainties, and are needed in VUV diagnostics of less hot (~3-5 keV) core plasmas.

The e-impact collision database for high-Z core plasma impurities is in much worse shape and, to a large extent, mimics the situation in the corresponding spectroscopic database. Especially the data for W^{q+}-ions, which will have a large number of bound electrons even in ITER-like plasma, are of critical importance. There are electron-impact ionisation data for W^{q+} ions up to q = 13-15, but almost no data for other electronic processes.

The charge exchange data of hydrogen atoms on impurity ions will be discussed in the next sub-section in connection with CXRS.

2.1.b *CXRS diagnostics*

Critical for the H- and He-beam (beam energies 80-200 keV/amu) based core plasma diagnostics are the processes contributing to the beam intensity attenuation and the state-selective (n, l - resolved) electron capture on (intrinsic or injected) impurities. The collision database for processes involved in beam attenuation kinetics (mainly beam atom excitation, ionisation and charge exchange by plasma protons and impurity ions) is complete for both H- and He-beam atoms. For the beam energies of interest, the total charge exchange cross sections of H on core plasma impurities are known with good accuracy. For the light impurities (completely stripped in the core plasma), the n, l - resolved electron capture cross sections are also known. These cross sections are known within a good approximation also for the highly stripped medium- and high-Z impurities (q≥15) for which the A^{q+} ion can be considered as "fully stripped".

For He-beam based CXRS, however, n, l - resolved electron capture cross sections are available only for some of light (fully stripped) impurities, and almost absent for the medium- and high-Z (fully or incompletely stripped) impurities. There exist, however, adequate theoretical (e.g. the CTMC, AOCC and CDW methods) and experimental (e.g. the TES method at QUB, Belfast, photon emission spectroscopy method at KVI, Groningen) tools to successfully address this problem. One of the effective ways of introducing diagnostic impurities in the core plasma is the pellet injection technique (TESPEL), used e.g. on the LHD device. The type (atomic number) of injected diagnostic impurity is dictated by the requirement of significant CXRS signal in the observed spectral range (X-ray, VUV or even the visible, like in LHD), which is related to the value of beam energy (through the energy dependence of CX cross section). For H-beam energies of about ~ 150 keV and plasma temperatures ~ 1-5 keV, optimal CXRS TESPEL signals in the visible range are expected for injected impurities with Z = 12-22. The n- and l-distributions of captured electrons change significantly with the variation of Z, and these dependences are still poorly characterised (and understood).

2.1.c *Beam emission spectroscopy*

This method involves emission measurement from the beam atoms (H or He) and the corresponding collision database is required only for the processes determining atomic level populations. As discussed in 2.1.b, for both H and He beams, the collision databases are available, but improvements are necessary in the case of He-beams for the transitions between excited states induced by proton and impurity ion impact. (In the present database, various cross section scaling relationships are being used for these processes.)

2.1.d *Active-beam alpha particle diagnostics*

For the measurement of the slow-down velocity distribution of fusion alpha particles in an ignited plasma, the detection of the 304 Å line emission from excited He (n = 2) atoms has been proposed. The excited atoms are produced by double charge exchange of fusion alpha particles on energetic He-beam atoms. The cross section for this process is required in the energy range from 3,5 MeV down to a few keV. Experimental cross section data for this process are still missing, although they are feasible. Accurate cross section measurements and calculations do, however, exist for the resonant two-electron capture (producing He (n = 1), which can be useful for the interpretation of charge-exchange He-neutrals in neutral particle analysers (see next sub-section). Theoretical calculations of the cross section for He(n = 2) production by double charge in the above mentioned energy range are possible by combination of several methods (CDW, AOCC and MOCC).

2.1.e *Neutral particle emission analysis*

Neutral particle analysers have recently been used on JET and other large fusion devices for the energy analysis of emitted energetic neutrals from core plasmas. The interpretation of neutral particle signals (e.g. energetic H-atoms) requires information on all collision processes involved in the charged particle neutralisation (e.g. charge exchange) and "escape" kinetics (e.g. re-ionisation). Production of energetic H neutrals in the plasma core is due to either CX on "residual" H atoms, or CX on incompletely stripped impurity ions. Cross section data for the latter process (for different A_Z^{q+}, $q \leq (Z-1)$) are extremely fragmentary. In an ignited plasma, fusion alpha particles will also undergo CX on incompletely stripped ions, as will do their He^+ product ions. This chain of CX processes may affect the life-time of fusion alphas in a reactor. The CX cross sections of He^{2+} and He^+ on incompletely stripped core plasma impurities are also extremely scarce.

2.2. Impurity Transport and Radiation Losses

Impurity transport and radiation losses are dominated by electron-ion collision processes. (Charge exchange on "residual" hydrogen is important only at high H-concentration, $n_H > 10^{-5} n_e$.) There exist several codes for impurity transport and radiation loss calculations (MIST, STRAHL, etc) in which the corresponding atomic databases are different. Consequently, the predictions of these codes also differ. The quality of underlying collision databases in these codes is also often unknown (as in STRAHL), or when it is known, it does not reflect the present state of accuracy of the data (like in MIST).

While unification of atomic databases in impurity transport and radiation losses codes, and their upgrades to reflect the current state of availability and accuracy of the data is recommendable, the Working Group is aware that there could be practical difficulties in achieving such a goal.

The Working Group recommends, however, that IAEA Atomic and Molecular Data Unit make an effort in identifying the data sources and data quality of atomic databases in existing impurity transport and radiation codes. The Working Group also recommends that the access to atomic databases of these codes be made more easily feasible.

2.3. Neutral Hydrogen Beam Heating

As discussed in sub-section 2.1.b, the collision database for neutral hydrogen beam attenuation kinetics is in good shape (for beam energies above ~ 150 keV). However, the processes in the related ion sources and beam neutralisers still need further characterisation. The Working Group felt, however, that these topics were outside the scope of its task.

3. Atomic and Molecular Data for Edge/SOL/Divertor Plasma

The key areas where atomic and molecular processes play a critical role in the edge/SOL/divertor plasma studies are: radiative cooling of the plasma edge, edge/divertor plasma diagnostics, and neutral particle transport (and the related particle exhaust). Under the high neutral density conditions in divertors, plasma opacity for certain lines may also become important and involve some photonic processes.

3.1. Radiative Cooling and Plasma Energy Loss

Radiative cooling of edge and divertor plasmas due to intrinsic impurities (Be, B, C, O, Si, Cr, Fe, Ni, Cu, Mo, W) is insufficient to achieve adequate levels of power exhaust and additional plasma cooling is required by injecting (seeding) recyclable impurities in these regions such as N, Ne, Ar, Kr, Xe. Due to lower plasma temperatures (~ 500 - 100 eV in the edge /SOL region and ≤ 100 eV in divertor region), the impurity ions are incompletely stripped. Their radiative power maximises roughly at charge states $q \sim Z/2$, where Z is the impurity atomic number. Impurity radiative losses are generally determined by electron-impact processes, with CX playing a relatively minor role.

The collision database for all low-Z impurities ($Z \leq 10$) is in fairly good shape (except for the lowest and neutral charge states of B and Ne). For the medium-Z impurities ($10 < Z \leq 30$), the collision database becomes less adequate with decreasing ion charge state q, with exception of the iron group of elements for which the situation is somewhat better. Significant database improvements are especially needed for the low charge states of Si, Ar, Cr and Cu. For the high-Z impurities (Mo, Kr, Xe, W) the data are only fragmentary, and a significant effort is required to generate the required data. Here, again, the charge states with $q \leq Z/2$ are the most important from edge plasma radiative cooling viewpoint and they must be given a priority in data generation.

The spectroscopic database for edge radiative cooling impurities to a larger degree resembles that for collision processes, but it is still somewhat more complete for the medium Z elements. Charge exchange processes of edge neutrals (H, H_2, He) on edge impurity ions may lead to the population of excited ionic states (increasing for higher ion charge states), the energy of which is then radiated. The database for state-selective electron capture of H, H_2 and He on incompletely stripped edge impurities is still inadequate, although a significant body of data is already available. The experimental and theoretical potential for generation of required data is available (experimental groups at KVI, Groningen; QUB, Belfast; ORLN, Oak Ridge; and theoretical groups in Madrid, Bordeaux, Yamaguchi University, P.N.Lebedev Institute, Moscow; and elsewhere), and is largely involved in the current data generating CRP activities of IAEA.

3.2. Edge/Divertor Plasma Diagnostics

The currently most often used methods for edge/divertor plasma diagnostics, that require atomic/molecular spectroscopic and collisional information are:

a) H_α - diagnostics
b) Atomic-line emission spectroscopy
c) Beam-emission spectroscopy
d) Molecular diagnostics

3.2.a H_α - diagnostics

This is one of the standard edge/divertor plasma diagnostics based on the Balmer-α (3 → 2) emission of atomic hydrogen. This diagnostic not only provides information on edge/divertor plasma parameters, but through the features of radiated emission (Doppler shifts, etc.) can also provide an insight in the dominant n = 3 population processes. One of the pre-requisites in the application of this diagnostic is obviously an accurate collisional-radiative (CR) model for H. The database for electron-impact (and radiative) processes in this model is available (although in practice the simplified semi-empirical cross section formulae are frequently used). In a divertor plasma with high hydrogen molecule content, significant contributions to the H(n = 3) level population may come also through various collision processes involving the molecules species (e.g. charge exchange of protons on excited neutral molecules dissociative excitation of hydrogen molecules and their ions by electron impact, mutual recombination of H^+ and H^-, etc.). In the current edge plasma application of H_α - diagnostic methods, molecular processes are included in a non-systematic (frequently an ad hoc) manner.

A successful application of this method for a variety of edge plasma conditions requires establishment of a complete H/H_2 coupled CR model, that includes also the collision processes of vibrationally excited H_2 and H_2^+ species, as well as the collision processes of electronically excited H and H_2 with plasma electrons and protons. Processes involving the formation and destruction of H^- and H_3^+ species, particularly in the cold divertor plasma regions ($T_e \leq 5$ eV), must also be included in the coupled H/H_2 CR model. Such H/H_2 CR model serves also as a basis for the Fulcher-band molecular diagnostics, and the corresponding collision database will be discussed in more detail in Sect. 3.2.d). Here we only note that despite of the significant recent efforts on establishing a coupled H/H_2 CR model, the corresponding collision database is still by far incomplete. This assessment remains true even for a reduced H/H_2 CR model, in which vibrational kinetics is omitted (or accounted for an effective way), which is sufficient for the H_α - diagnostic purposes.

3.2.b Atomic line emission spectroscopy

Atomic (or ion) line emission spectroscopy is one of the standard method for diagnosing the edge/divertor plasmas. Lines of either intrinsic or seeded atomic impurities can be used depending on the chosen spectral range and plasma conditions. The selection of a diagnostic impurity also depends on the availability of spectroscopic and collisional data. The use of this technique requires a full CR model for selected impurity in a given charge state, as well as a fairly good collision database for at least the nearby charge states of that impurity.

As indicated earlier, the e-impact collision databases for low-Z impurities are in fairly good shape (with the exception of lowest and neutral charge stages of B and Ne). Medium- and high-Z impurities can be present in edge/divertor regions only in low charge states, the collision data for which are still either inadequate or extremely scarce. Even the most advanced computer codes become ineffective and unreliable for the low-charge high-Z impurities (such as W or Xe). Experimental methods (e.g. for determination of excitation cross sections) may be hampered by the lack of spectroscopic (energy level) information of these systems. It is felt that a concerted internationally co-ordinated effort is required for establishing the database for some selected high-Z impurities of significant relevance for fusion (such as W).

3.2.c *Molecular diagnostics*

The abundance of H_2 and molecular impurities (C_x, H_y, CO, CO_2, etc) in cold edge/divertor plasma regions gives a basis for use of spectroscopic diagnostic techniques based on molecular band radiation. Two such techniques have been developed and used in several fusion devices: the Fulcher-band H_2 emission spectroscopy, using the

$d^3A_u \rightarrow {}^3\Sigma$ (n = 3 → n = 2)

transition, and the 420.0 - 440.0 nm emission band in CH, using the $A^2\Delta \rightarrow X^2A$ transition. Besides providing information about edge/divertor plasma parameters, the Fulcher-band spectroscopy also provides information about the vibrational temperature of H_2 divertor gas, while the CH emission spectroscopy provides information on the hydrocarbon fluxes entering the plasma from the carbon-based wall materials. Band emissions from C_2 and other hydrocarbon molecules are currently under consideration for use in plasma diagnostic purposes at several tokamaks.

Fulcher-band Diagnostics. The H/H_2 Database

As mentioned in Sect. 3.2.a, reliable interpretation of the Fulcher-band diagnostic measurements requires a very accurate and elaborated coupled H/H_2 CR model with inclusion of vibrational kinetics. This model includes all collision processes among: e, H^+, H(n ≥ 1), H_2(v), H_2^*(n;v), H_2^+(v), H_3^+(v) and H^-, as well as the radiative and non-radiative (such as auto-ionisation, pre-dissociation) decay processes. Explicit inclusion (i.e. without using scaling relationships) of excited H_2 molecular states with n ≤ 3 (and n = 4, for the higher term series), together with the v-v' resolved transitions among them, is mandatory for the Fulcher-band diagnostics and for the reliability of H/H_2 CR model. v-v' resolved excitation cross sections are presently available only for the transitions from the ground $X^1\Sigma_g$ to first few single states. Similar v-resolved cross sections are also available for the dissociative electron attachment on H_2(v), for dissociative recombination and excitation in e + H_2^+(v) collisions, dissociative excitation of H_2(v) and for the charge exchange and dissociation in H^+ + H_2(v) collisions.

The major gaps in the coupled H/H_2 database are for the processes:

(1) v-v' resolved e-impact excitation and ionisation of H_2^*(n ≤ 3), including the transitions between excited states;

(2) v-v' and channel resolved processes involving the formation and destruction of $H_3^+(v)$ ion (in particular its formation in $H_2^+(v)$ + $H_2(v)$ collision and dissociative recombination with electrons producing $H_2(v)$;

(3) processes involving e, H^+ and H° with excited $H^*(n \geq 2)$ and $H_2^*(n \geq 2)$;

(4) non-radiative decay processes of excited H_2^* states (pre-dissociation, auto-ionisation).

For a (D,T) divertor plasma the extension of the H/H_2 database would require appropriate modifications to account for vibrational level dependence of v-v' resolved processes, and isotope (mass) dependence of certain processes (such as dissociative attachment, pre-dissociation, isotope exchange, etc).

There is a significant effort currently taking place world wide to generate the missing data in the H/H_2 coupled database. Part of this effort takes place within two ongoing IAEA CRPs. Significant contributions to this effort can be expected from the theoretical groups at University of Bari, University College London, ORNL (Oak Ridge), University of Nebraska (Lincoln), and from the experimental groups at University of Louvain-la-Neuve, University of Stockholm (CRYRING), the Weizman Institute of Science (Rehevot), etc.

CH* Emission Spectroscopy and the Hydrocarbon Database

The CH* (420.0 - 440.0 nm) emission spectroscopy, or any similar diagnostics based on C_2 or other hydrocarbon molecule band emissions, provides a way to determine the hydrocarbon fluxes entering the plasma. The (inverse) photon efficiency coefficient, D/XB, relating the photon and hydrocarbon fluxes, is highly sensitive to the cross sections of collision processes of hydrocarbon species with plasma electrons and protons. Chemical carbon erosion and its re-(co-)deposition is one of the critical issues in the use of carbon (in form of graphite, or C-C or CFC composites) as a plasma facing material in next generation fusion devices.

The spectrum of hydrocarbon molecules C_xH_y that may be present in divertor plasmas can range from CH to C_3H_8. The most important processes of these molecules and their ions with plasma electrons are: direct and dissociate ionisation and excitation, and dissociative recombination. Proton charge exchange on these molecules is also important, and has a resonant character for the molecules with large number of H atoms. Experimental cross section database for these processes is rather limited, particularly for dissociative processes and higher ($C_{2,3}H_y$) hydrocarbons.

Most of the existing information is for total ionisation and dissociative recombination cross sections, and only in a limited number of case partial cross sections or reaction branching rations are available. The theoretical cross section information on these processes is also scarce and limited only to total ionisation.

An effort has recently been made at NIFS (Toki) and FZ-Jülich to establish a cross section database for all electron and proton impact processes of C_xH_y molecules by using the available experimental information and certain semi-empirical scaling relation-ships. Obviously, there is a need for experimental validation of this database. Uncertainties exist in the present database particularly in the channel branching ratios of dissociative processes, and energy distribution of reaction products. Characterisation of vibrational excitation of reaction products is also missing in the present database.

It is felt that an internationally co-ordinated effort on the establishment of an experimentally validated collision database for hydrocarbon molecules would be highly desirable, and it is recommended that the IAEA takes an initiative in this direction. Experimental groups that can significantly contribute to this effort are at the University of Innsbruck, University of Heidelberg, INP Greifswald, University of Stockholm (CRYRING), and the Weizmann Institute of Science (Rehevot).

3.2.d *Beam emission spectroscopy*

Diagnostic neutral beams of H, He and Li of energies usually below ~ 80 keV/amu are being used for this type of edge plasma diagnostics. The beam atom level population kinetics is determined by the collision processes of neutral atoms with plasma electrons, protons and impurity ions.

The collision database for H-beam emission diagnostics is well established except for some uncertainties in the cross sections for impurity ion induced transitions between excited H-states (currently described by scalings). Similar is the situation also with the He- and Li-beam emission diagnostics. For these two diagnostic techniques, total charge exchange cross sections for He and Li on some low charged impurity ions are also missing.

3.3. Neutral Particle Transport Modelling

Understanding and accurate description of neutral particle transport in edge/divertor plasmas is a critical issue since it is related to particle removal problem and in particular to helium exhaust. Elaborate kinetic Monte Carlo transport codes (such as DEGAS, EIRENE, UEDGE, etc) are currently being used for neutral particle transport modelling in edge/divertor plasmas, sometimes coupled with the plasma transport codes (e.g. the B2-EIRENE code package). These codes presently play an essential role in divertor performance optimisation and design. The code capabilities include tracking and the final results of all collision induced transformations of particle charge states, their kinetic and internal energy, their momentum, and their generation or destruction in reactions. The collision database for modelling the neutral particle transport by these codes, besides the cross section information on all relevant inelastic collision processes, must include information on the energy and angular distributions of reaction products, as well as on elastic scattering characteristics.

An accurate modelling of hydrogen (H and H_2) transport by these codes requires a complete H/H_2 coupled collision database, including the elastic (momentum transfer) cross sections in ion-neutral and neutral-neutral collisions. The status of H/H_2 database was discussed in Sect. 3.2.c), together with the data needs. The cross section database for ion-neutral and neutral-neutral elastic collisions in the H/H_2 system is available (including the hydrogen isotopomers) and of good accuracy.

The collision database for He transport in divertors is in a fairly good shape, but significant gaps still exist. These are related particularly to processes involving collisions of helium ions and atoms with excited hydrogen (atomic and molecular), as well as to particle exchange reactions of helium species with molecular hydrogen.

Transport modelling of atomic and molecular edge plasma impurities requires and adequate collision database including the information on elastic scattering characteristics. The status of collision databases for atomic and C_xH_y molecular impurities has already been discussed in previous sections.

3.4. Plasma-Opacity

Under the high neutral density conditions in divertors, plasma opacity for certain lines may also become important and involve some photonic processes. At FZJ the photon transport modelling for Lyman-α radiation including Zeeman and Stark splitting has been carried out. The processes involved are very similar to those applied in photon transport models for the sun. The existing models there should be checked for their use in high neutral density divertors and the results also compared with experimental findings in Alcator C-Mod.

3.5. Line Shapes

Intensive work has been done in the recent past on modelling the influence of the magnetic field on the line shapes of fusion relevant particles. The data base from the University of Durban, Natal, ZA includes 60 lines from 115nm – 910nm for H I, B II, Be I-III, C I-V, He I, O I, Kr I, Mg II, Na I, Ca I-II, Ne I-II and Si I-IV with possible variations possible for T_i , B, (field direction) and observation angle. However, for the interpretation clear data for temperatures, densities and particle release velocities should be available in order to derive energy distributions, drift and rotational motions from the deconvoluted data. The profile of the current density in a tokamak and hence the poloidal magnetic field plays an extremely important role in the transport properties of the plasma. Examples are the observations of transport barriers, filaments, magnetic islands and improved confiment regimes, all in a way related to the specific topology of the magnetic field. A diagnostic to measure this (poloidal) magnetic field in the core of the plasma is essential for understanding and controlling the confinement of the plasma. A real-time and local measurement of this magnetic field is in principle possible by employing the motional Stark effect (MSE) experienced by energetic hydrogen atoms injected into the tokamak. A known Zeeman pattern would strongly facilitate the interpretation.

4. Conclusions and Recommendations

The analysis of status of atomic and molecular (A+M) spectroscopic and collision databases in view of the needs of current fusion plasma research and design of next-generation fusion devices leads to the following general conclusions:

(6) An impressive body of A+M data information relevant to fusion research has been accumulated during the years and implemented into fusion plasma application codes. The breath of fusion relevant data generation world-wide is strong and, generally, adequately follows the development of fusion research needs.

(7) The IAEA has played and continues to play a critical role in fostering and co-ordinating the A+M data generation efforts and in dissemination of the data to the fusion research community. The IAEA role in the establishing and facilitating the interaction between the atomic and fusion communities in A+M data field is also

crucial for focusing of data generation efforts on most urgent data needs and for efficient implementation of the results of these efforts in fusion research.

(8) Despite the remarkable achievements in the completion and improvement of A+M databases for fusion, observed in the period since the last IAEA Technical Committee Meeting of this subject in 1992, the spectroscopic and collision A+M databases for fusion still contain significant gaps. The present unsatisfactory status of certain databases is also the result of the shifted priorities for A+M data in the fusion research (related to new divertor operation regimes, materials for plasma facing components, etc).

(9) The most urgent high priority A+M data needs for the current fusion research and design of next-generation, reactor level fusion devices are:

(a) Improvement (validation) of the collision database for hydrocarbon impurities to understand their transport in edge/divertor plasma, and associated re- (and co-) deposition processes, in order to qualify the suitability of carbon as a plasma facing material;
(b) Improvement of spectroscopic and collision databases for high-Z materials (particularly W) as they are being considered as plasma facing materials for next generation fusion devices, or as diagnostic impurities (Kr);
(c) Improvement and completion of the coupled H/H_2 collision database for increasing the predictive capabilities of neutral particle transport codes in divertor performance modelling and optimisation, and to increase the reliability of molecular edge plasma diagnostics.

(10) It is strongly recommended that the IAEA considers the initiation of co-ordinated research Projects (CRPs) in the near future on the subjects (a) and (b) above for accelerating the process of establishing the corresponding databases.

Conclusions and Recommendations: Topic PMI

Safe management and accounting of tritium in ITER and future fusion power reactors will be crucial for the acceptance of fusion as an environmentally benign power source. Tritium retention in plasma-facing components (PFCs) with CFC has emerged as a primary concern for next-step fusion devices fuelled with mixtures of D and T, with strong implications for in-vessel component design, material selection, operational schedule and safety. A key decision for ITER is the choice of plasma-facing materials. Despite the prevalence and strong historic trend of operating tokamaks to rely on carbon-based PFCs (mainly to optimise plasma performance - in combination with oxygen gettering techniques such as boronisation or siliconisation - and to enable access to large plasma operational space), its application to a D-T next-step must be restricted due to its strong chemical affinity to hydrogen-isotopes, which affects erosion lifetime and tritium inventory.

During the last few years there have been remarkable advances in experiments and theory (for a comprehensive review see ref. [i]). However, there are still several issues, identified by this working group that require further work and whose resolution requires a co-ordinated R&D effort, involving extensive participation by all parts of the fusion community.

They are summarized below.

A) Erosion Mechanisms

– *Physical sputtering*
Physical sputtering of pure elements at relatively low temperatures is well understood and can be simulated in computer codes, but recently metals such as Li and Ga shows an increase of the erosion rates, and a dependence of the yield from the incidence flux, for a broad range of temperatures near the melting point.

Investigate physical sputtering of metals like W, Be (Fe, Ni or Al for cross-calibration) at high temperatures (e.g., near the melting points) and compare with current theories and models.
A main argument for the use of high-Z plasma facing materials, such as W, is the high threshold energy for erosion by hydrogen ions. However, low edge and divertor temperatures can only be obtained if significant power fractions are distributed by impurity radiation. If carbon is absent as a strong radiator in the plasma edge, radiation from seeded impurities (such as Ne, Ar) may be necessary, which can cause higher physical sputtering down to very low plasma temperatures. Investigate in fusion experiments the W-erosion by seeded impurities like Ar, Ne, which are candidate for external plasma impurity seeding in ITER. Establish whether the decrease in divertor temperature will offset the increased sputtering yield of seed impurities.

– *Chemical sputtering.*
Reassess the spectroscopy data from fusion devices by improving the knowledge of the spectroscopic conversion coefficient (D/XB) for the relevant fusion conditions (n_e, T_e). New data from fusion devices should include the in-situ determination of D/XB using puffing of hydrocarbon molecules.

Characterise the eroded species. Heavier hydrocarbons may contribute strongly to the erosion efficiency and may have a different redeposition behaviour as CD_4.

– Deposition/erosion of C layers.
Detailed information on the sticking coefficient of various hydrocarbon radicals under plasma parameters typical for the divertor and boundary plasma, for given surface temperature.
Type of deposited film (D/C, density, re-erosion).

– Erosion of mixed-materials.
Erosion due to non-recycling impurities, such as C and Be, together with incident fuel ions may lead to protective layer formation or to enhanced erosion.

Investigate experimentally effects such as diffusion, segregation and phase formation not included in present code simulations.

Experiments in plasma simulators using simultaneous impurities and hydrogen ion incidence are needed to clarify the influence of mixed fluxes on physical sputtering and chemical erosion.

B) Material Transport and Redeposition

In many fusion devices, the dominant source locations for impurities, such as main vessel walls or divertor target plates, are still undefined. Dedicated spectroscopic and surface experiments are needed to establish a database for different fusion devices, unambiguously identify carbon sources and sinks and extrapolate to ITER. See also diagnostics and modelling (below).

C) Tritium Retention and Removal

– Retention in W.
Hydrogen release from pure tungsten is not recombination limited and the inventory is expected to be small for ITER conditions.
Surface contamination reducing the recombination coefficient may increase inventory and permeation.

For fusion reactors, the contribution to trapping at damage sites created by neutrons will also need to be considered. Due to the residual radiation in tungsten after exposure to neutrons, it is not expected that experiments will be available on the tritium retention in neutron irradiated tungsten. Simulation of n-irradiation with ion beams will be an important issue.

– H-retention in mixed-material layers.
Continue investigate H/D retention in Be/C and W/C mixed materials.

– In-situ tritium removal techniques
No relevant method to remove tritium has been established on a working tokamak (in contrast to almost every other technical aspect e.g. remote handling). Clearly, there is a need for engineering-scale demonstration experiments of deuterium removal in existing machines. Without established fast and efficient tritium removal method a satisfactory schedule of burning plasma operations in a machine with carbon PFCs appears impractical.

Determine the effectiveness of He/O_2 glow discharges. In the absence of magnetic fields, laboratory experiments using He/O glow discharges have produced rapid, controlled co-deposit removal - only line-of-sight surfaces - with minimal O-contamination. Erosion rates of about 1 µm/h have been observed for co-deposit specimens obtained from TFTR. By comparison, He/O GDC performed in machines resulted in much lower T removal rates, possibly due to the re-deposition of the reaction products before being pumped out of the Tokamak. Laboratory studies have determined this erosion to be a 2-step process: oxidation, followed by particle-induced desorption, with the maximum erosion rate limited by the latter. The feasibility of He/O_2 glow discharges has to be established in fusion devices.

Inject oxygen in JET at the end of C12 (end of 2003, just before long machine opening) and study its effectiveness in removing C/D2. Temperatures in excess of 500 K are required for rapid thermal desorption of CO from carbon surfaces.

Develop and test new ideas.

D) Modelling of Erosion/redeposition and Tritium Co-deposition Effects

Predictive numerical codes are now available to simulate various aspects of PMIs and are recognised to be a vital tool in designing next-step tokamaks. Some of these codes have been successfully benchmarked against results from dedicated PMI experiments in current tokamaks. However, the comparison between data and models is sometimes difficult because some of the physical effects are still poorly understood and not included in the models. Atomic and molecular processes are being constantly upgraded and need to be implemented in the codes.

In addition, erosion/re-deposition processes depend strongly on local plasma conditions that in most cases are not known very well.

Lack of manpower has hampered progress in the field. More researchers needs to be involved in this field.

E) Improved Edge and Wall Diagnostics

Diagnostic advances are urgently needed to better characterise the plasma edge and wall, to validate existing codes against experiments, and to improve our predictive capability for a next-step. So-called "*archaeological studies*", primarily based on analysis of long term samples, removed during maintenance procedures or upgrades, have long provided the mainstay of plasma-wall interaction studies. Unfortunately, although they allow levels of erosion and surface modification to be accurately determined, relating the data obtained to specific conditions in the plasma-wall interaction region is difficult as the samples typically represent an integration over many shots and many different experimental campaigns.

There is a strong case for the development of new, more advanced wall diagnostic techniques and time resolved measurements (e.g., sensitive Langmuir probes, charge-exchange neutral measurements, IR camera, erosion/deposition collector probes, microbalances, laser desorption to measure D/C ratio of hydrocarbon films, sticking probes, molecular spectroscopy,) and substantially increased operational time allocated to plasma-wall interaction studies in existing devices to quantify the erosion and deposition effects and to better understand the underlying causes.

Instrumentation and careful time resolved measurements will be also needed in ITER to control the inventory during operation.

SUMMARY

In summary, the R&D program needs to address the physics of the erosion mechanisms and the transportation and redeposition of eroded material and to demonstrate T removal on a Tokamak. Many inportant issues for further R&D are given in the detailed discussion above, requiring laboratory work and more wall diagnostics with Tokamak operation time dedicated to wall experiments. Modelling of the results are essential to enable progress on wall physics.
In order to identify topics of highest priority the scenario can be devided into a case involving carbon as first wall material and a case of an all-metal machine.
CFC Target Plates:

In-situ determination of sources and sinks for carbon erosion. Development of suitable diagnostics on a shot-to-shot basis and investigation of the deposited layer thickness.

Removal of T from deposited layers. Techniques available from laboratory experiments (oxidation, laser desorbtion) need to be tested and validated in existing fusion devices.

All Metal Machine
In-situ determination of the erosion of high-Z target plates by seed impurities. Establish the fact that the reduction in divertor temperature offset the increased erosion by seed impurities.
Investigation of high heat flux performance of high-Z components. This includes test laboratory experiments and the use of high-Z divertor plates in a experiment with relevant ELM scenarios.

Appendix 5

Working Group Report on Material Properties

Status of Material and Components

- target values for steady high heat fluxes in ITER have been realized (up to 20 MWm^{-2} for CFC and W armored components),
- for this condition armor materials and their design (brush type for W, monoblock for CFC and W) have been selected,
- one of the remaining key issue for armor materials is their behavior at transient events (ELMs, disruptions, VDEs, etc.),
- effects due to neutron irradiation (up to approx. 1 dpa) have been considered; the resulting material degradation remains within acceptable limits,
- the available data for ITER recommended materials have been summarized,
- material data obtained so far are mainly limited to the operation regime of ITER; limited data are so far available for devices beyond ITER with n-fluences >> 1dpa (DEMO, PROTO)

High temperature properties (~ $\leq T_m$, T_s) of armor materials (C, CFC, W, W-alloys, others)

- thermal conductivity
- specific heat
- sublimation
- evaporation curve
- recrystallization (W)
- secondary electron emission
- reflection

> Comment
> reference materials must be studied
> CFC: NB-31, sintered W (Plansee),Be: S65

Physical properties of mixed materials (combination of W, C, Be, B?, Si?,….)

- diffusion coefficient (to the bulk)
- specific heat
- thermal conductivity
- density
- others

Physical properties of doped materials (C+B, C+ Ti,....,W + ...)

- others
- thermal conductivity up to high T

Thermal performance of armor materials / plasma facing components

- high heat fluxes (thermal fatigue)
- ELMs, disruptions, VDEs (thermal shock):
- evaporation: experiment and modeling
- particle erosion (CFC: brittle destruction, W: melt droplet ejection)
- interaction of thermal shock and thermal fatigue

Coatings (W, Be, B_4C?)

- PVD
- plasma spray (improve thermal conductivity)

Neutron effects

- thermal performance of high-Z armor for DEMO / PROTO (i.e. >>1 dpa)
- thermal and mechanical parameters up to high T
- transmutation effects (e.g. W à Re)

Recommendations

1. To PSI-community: use the proposed material candidates for material studies (e.g. NB31, W with relevant texture)
2. It is useful to organize collection of the data in the form of database with as much as possible detailed information
3. Role of IAEA????

---

[i] G. Federici, C.H. Skinner, et al., Nucl. Fusion **41** (2001) 1967.

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1) 26007
telephone: (43-1) 2600-21710

Online: TELNET or FTP: iaeand.iaea.org
username: IAEANDS for interactive Nuclear Data Information System
usernames: ANONYMOUS for FTP file transfer;
FENDL2 for FTP file transfer of FENDL-2.0;
RIPL for FTP file transfer of RIPL.
NDSONL for FTP access to files sent to NDIS "open" area.
Web: http://www-nds.iaea.org