

INDC International Nuclear Data Committee

Summary Report of
IAEA Workshop

Atomic and Molecular Data for Fusion Energy Research

Prepared by
R.E.H. Clark

ICTP, Trieste, Italy
28 August – 8 September 2006

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Abstract

A workshop on Atomic and Molecular (A+M) Data for Fusion Energy Research was held at the International Centre for Theoretical Physics (ICTP) in Trieste, Italy, from 28 August until 8 September 2006. The workshop was attended by fourteen students and three ICTP associates representing eleven Member States. A total of eight lecturers, including six external to the Agency, made presentations to the workshop. All lecturers provided advance copies of the lecture materials, and provided written assignments for the students to provide practical examples of applications of data issues to actual problems related to fusion energy research. All materials were collected on CDs, which were distributed to the students at the conclusion of the workshop. During the course of the workshop, the students were given the opportunity to describe their background and research interests. The workshop did arouse interest in A+M processes related to fusion, and was viewed as successful by both the students and lecturers.

February 2007

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1. Overview

A Workshop on Atomic and Molecular Data for Fusion Energy Research was held on 28 August - 8 September, 2006 at the International Centre for Theoretical Physics (ICTP), Trieste, Italy. The Atomic and Molecular (A+M) Subcommittee of the International Fusion Research Council (IFRC) had recommended holding such a workshop at their review meeting of the IAEA work programme on 24-25 June 2004. This workshop was attended by fourteen students, three ICTP associates, six external lecturers and two IAEA staff. The list of participants at the workshop is given in Appendix 1, and the agenda is provided in Appendix 2.

2. Workshop Proceedings

2.1. Introduction

Six external lecturers, along with two IAEA staff, were scheduled to present lectures to cover a variety of A+M issues related to fusion energy research. All lecturers prepared materials in advance of the workshop and coordinated their presentations to achieve a very good overall view of the important A+M processes relevant to fusion energy research.

At the start of the workshop the participants were welcomed to the International Centre for Theoretical Physics. R. Clark welcomed the participants on behalf of the IAEA and introduced the lecturers and their fields of expertise. The schedule for the two week workshop was also reviewed and adopted (Appendix 2). The general approach was to begin each day with one hour of discussion of the material from the previous day, including solutions to the assigned exercises. This exercise was followed by three lectures, with a break for lunch. The latter part of the afternoon was devoted to work on the exercises, with the lecturers being available for individual help. A substantial computing room was made available for the students at the ICTP with good Internet connection.

2.2. Students

During the discussion time each morning students were invited to give a short description of their background and research interests. Their presentations are summarized briefly in this section.

Elahe Alizadeh from the Atomic Energy Organization of Iran has a background and interest in plasma diagnostic systems with application to controlled fusion. Latefa Boufatah from the Universite de Tiemcen 'Alboubekr Belkaid has an interest in electron-collision theory and calculation of radiative recombination to specific states. Dorian Bridi, from Lebanon, is currently working on aspects of plasma diagnostics at the Institut für Allgemeine Physik, Vienna University of Technology. Jose Miguel Carmona Torres of the Centro de Investigaciones Energeticas Medioambientales Y Tecnologicas, Spain, has an interest in atomic interactions, spectroscopy and charge exchange spectroscopy with fusion applications. Ndeye Arame Boye Faye, an ICTP Associate, of the Universite Des Sciences Departement de Physique, Senegal, has research interests in atomic physics related to plasma research. Min Huang of Fudan University, China, has an interest in calculations of dielectronic capture and has data available from an EBIT machine. Mohktar Kemal Inal of the Universite de Tiemcen, Algeria, had extensive background in atomic processes in hot plasmas, including polarization of X-rays lines of highly charged ions. Ahmed Asaad Ibrahim Khalil of Cairo University, Egypt, has extensive background in industrial plasmas and laser-produced

plasmas. Zaal Machavariani of Tbilisi State University, Georgia, has worked on atomic and molecular processes including electron-atomic inelastic collisions. Darian Mahmoodi of Azad University, Iran, is pursuing research in controlled fusion, particularly self-organization and multi-scale physics. Ousmanou Motapon of the Universite de Douala, Cameroon, has been applying multi-channel quantum defect theory to molecular processes relevant to plasmas. Abha Rai, from India, is studying at the Max Planck Institute for Plasma Physics, Germany, and is working on fusion-orientated computational material science, focusing on the modelling of hydrogen transport. Muhammad Aslam Rana of Quaid-I-Azam University, Pakistan, is working on atomic and molecular physics related to plasma research. Mohammad Ikram Safi of Hazara University, Pakistan, is carrying out research on emission spectroscopy of cold plasmas. Tamo Francois Olivier Waffeu of the Universite de Douala, Cameroon, is undertaking graduate studies that focus on the dissociative recombination of molecular ions. Abdelhaly Muhammad Sallah of Al-Azhar University, Egypt, is an ICTP associate who participated in most of the workshop activities.

The students all gave well-articulated summaries of their backgrounds. The short presentations served to generate more detailed discussions among the students at coffee breaks and during exercise sessions. The presentations were collected and made available through the A+M Unit web server.

2.3. Lecturers

There were a total of eight lecturers, of which six originated from outside the IAEA. They represent expertise in electron collisions with atoms and molecules, ion collisions, and particle surface interactions. The presentations were well planned and fit the level of the students very well. The exercises were extremely valuable and gave the students a feel for the application of A+M data to real problems on existing fusion devices.

R. Clark of the IAEA gave six lectures that focused on structure and electron impact processes in atoms and ions, as well as using such data in the modelling of plasmas in fusion machines. Detailed processes included electron impact excitation and ionization, photon ionization, autoionization as well as energy level and radiative decay data. The database at the A+M Data Unit was described and students were given exercises to look at specific online databases for some of the processes and to use several online codes to arrive at some parameters for fusion-related plasma conditions.

D. Humbert of the IAEA presented three lectures that focused on electronic database issues. The first lecture was on the general goals of the A+M Unit and the Data Centre Network (DCN). In successive lectures he detailed the electronic tools for finding and retrieving numerical and bibliographic data from a number of online databases, including those of the DCN. He pointed out the strengths and weaknesses of a number of online tools, and presented exercises for the students to appreciate the differences in a variety of data sources.

J. Davis of the Institute for Aerospace Studies, University of Toronto, Canada, presented three lectures on co-deposition and plasma interaction with co-deposited materials. He provided a very good overview of the co-deposition process in tokamak devices and implications for ITER and other machines. He explained the various transport mechanisms in fusion devices and characterized films arising from these processes. He then reviewed the plasma interactions with co-depositions and mixed materials, including erosion processes and possible removal processes for such films.

T. Schwarz-Selinger of the Max-Planck Institut für Plasmaphysik, Germany, gave presentations on plasma interactions with materials. He closely co-ordinated his presentations with Davis, so that there was a good set of lectures on plasmas interacting with pure materials as well as mixed materials. Schwarz-Selinger outlined the major processes that occur when plasma constituents interact with a pure material, and described methods for analysing such interactions. He introduced the students to a number of available means of predicting the overall effects of plasma-surface interaction. Of particular note was the availability of the well known SRIM computer package. Several realistic exercises were assigned to the students with parameters drawn from working or planned fusion devices.

R. McCarroll of the Université Pierre et Marie Curie, France, gave six lectures on photon and heavy particle collision processes for molecules. He summarized the basic processes of photons and ions colliding with atoms, molecules or ions. He went through the details of how cross sections for such processes are calculated and the reason for the behaviour of such cross sections. He showed how the potentials for such processes could be approximated, and described the various approximations that can be made in such calculations. He presented exercises to the students that allowed them to carry out some estimates of parameters in such processes that were informative and provided some realistic estimates.

J. Abdallah of the Los Alamos National Laboratory, USA, reviewed the basics of modelling plasmas. He first summarized the different plasma regimes of local thermodynamic equilibrium (LTE), coronal equilibrium and collisional-radiative (CR) plasmas, which require solution of large sets of rate equations. He pointed out that most fusion plasmas require the full CR treatment. He then detailed the various types of data needed to solve the CR problem and the generation of rate coefficients from cross sections. Abdallah also presented some simplified two-level atom problems to illustrate how the rate equations are solved. Finally, he presented a number of applications of full CR models to actual laboratory plasmas with comparisons of calculated and observed spectra.

D. Reiter from the Institut für Plasmaphysik, Germany, presented an overview of the modelling molecular processes in fusion plasmas. He described the B2-EIRENE codes, giving examples of applications of those codes to fusion problems. He discussed the data used in the codes and their origin. He showed a number of examples of how improved data sets can give rise to a better understanding of plasma behaviour in the divertor region. He showed a number of examples of molecular effects producing significant differences in plasmas at the edge regions, and ways in which particular molecular properties can be used to control plasma conditions.

T. Märk of the Universität Innsbruck gave a thorough review of processes involving molecules in fusion plasmas. He provided an extensive overview of the many processes known or likely to be important in plasma edge regions. He detailed the current status of data for each of the processes, and explained the theoretical methods for calculations and the difficulties of such calculations. A good overview was given of the experimental techniques for measuring a number of processes involving molecules. The leading locations of research in these areas were outlined. Of particular note was a comparison of available data for molecular processes in existence at the time of the previous workshop (2003) and the present time. A great deal of additional data have been added, but it was clear that much work remains to be done for molecules of high interest in fusion research.

The lecturers all gave very professional presentations with well thought out exercises drawn from actual or planned fusion devices. The students benefited from these exercises in

observing databases applied to real problems and seeing the dependence on solutions to the availability of reliable A+M data. All the materials from the lecturers were collected on CDs and distributed to the students before the close of the workshop.

3. Recommendations and Conclusions

This was the second ICTP workshop organized by the A+M Unit on atomic and molecular data for fusion energy research. The workshop was judged to be as successful from the students' perception as well as the lecturers. The students were satisfied with the two-week duration of the workshop. All students had favourable comments regarding the lectures, were pleased to receive the entire set of materials on CD to take with them to their home institutions.

Continuing workshops on A+M processes have been recommended by the A+M Subcommittee of the IFRC. Following the success of the first workshop, this second workshop was proposed, approved and proved to be very successful, both for the students and the lecturers. The two A+M workshops have been very valuable for introducing new researchers to the A+M data needed to understand fusion plasma modelling efforts. Such workshops should continue on a regular 3-year basis.

**IAEA Workshop on
Atomic and Molecular Data for Fusion Energy Research**

28 August – 8 September 2006, ICTP, Trieste, Italy

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**IAEA Workshop on
Atomic and Molecular Data for Fusion Energy Research**

Organizers: R.E.H. Clark (IAEA); C. Tuniz (ICTP)

28 August – 8 September 2006, ICTP, Trieste, Italy

Agenda

Meeting Room: Adriatico Guest House Lundqvist Lecture Hall

Monday, 28 August

- | | |
|---------------|--|
| 08:30 – 09:30 | REGISTRATION |
| 09:00 – 10:00 | <u>Robert E.H. Clark</u>
Introduction |
| 10:00 – 11:00 | <u>Thomas Schwarz-Selinger</u>
Plasma Wall Interaction in Magnetic Fusion |
| 11:00 – 11:30 | <i>Morning Coffee</i> |
| 11:30 – 12:30 | <u>Denis Humbert</u>
Atomic and Molecular Data on the Web |
| 12:30 – 13:30 | <i>Lunch</i> |
| 13:30 – 14:30 | <u>Robert E.H. Clark</u>
Electron Impact Processes in Atomic Ions |
| 14:30 – 15:00 | <i>Afternoon Coffee</i> |
| 15:00 – 17:30 | <u>Workshop Participants</u>
<u>Exercises</u>
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1)) |

Tuesday, 29 August

- | | |
|---------------|--|
| 09:00 – 10:00 | <u>All</u>
Discussion |
| 10:00 – 11:00 | <u>Denis Humbert</u>
Atomic and Molecular Data on the Web |
| 11:00 – 11:30 | <i>Morning Coffee</i> |
| 11:30 – 12:30 | <u>Thomas Schwarz-Selinger</u>
Plasma Wall Interaction in Magnetic Fusion |

- 12:30 – 13:30 *Lunch*
- 13:30 – 14:30 J.W. Davis
Codeposition and Plasma Interaction with Codeposited/Mixed
Materials
- 14:30 – 15:00 *Afternoon Coffee*
- 15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

Wednesday, 30 August

- 09:00 – 10:00 All
Discussion
- 10:00 – 11:00 Ronald McCarroll
Photo-fragmentation of Atoms and Molecules
- 11:00 – 11:30 *Morning Coffee*
- 11:30 – 12:30 J.W. Davis
Codeposition and Plasma Interaction with Codeposited/Mixed
Materials
- 12:30 – 13:30 *Lunch*
- 13:30 – 14:30 Robert E.H. Clark
Electron Impact Processes in Atomic Ions
- 14:30 – 15:00 *Afternoon Coffee*
- 15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

Thursday, 31 August

- 09:00 – 10:00 All
Discussion
- 10:00 – 11:00 Denis Humbert
Atomic and Molecular Data on the Web
- 11:00 – 11:30 *Morning Coffee*
- 11:30 – 12:30 Thomas Schwarz-Selinger
Plasma Wall Interaction in Magnetic Fusion
- 12:30 – 13:30 *Lunch*

- 13:30 – 14:30 Ronald McCarroll
Photo-fragmentation of Atoms and Molecules
- 14:30 – 15:00 *Afternoon Coffee*
- 15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

Friday, 1 September

- 09:00 – 10:00 All
Discussion
- 10:00 – 11:00 Robert E.H. Clark
Electron Impact Processes in Atomic Ions
- 11:00 – 11:30 *Morning Coffee*
- 11:30 – 12:30 Ronald McCarroll
Photo-fragmentation of Atoms and Molecules
- 12:30 – 13:30 *Lunch*
- 13:30 – 14:30 J.W. Davis
Codeposition and Plasma Interaction with Codeposited/Mixed
Materials
- 14:30 – 15:00 *Afternoon Coffee*
- 15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

Monday, 4 September

- 09:00 – 10:00 All
Discussion
- 10:00 – 11:00 Ronald McCarroll
Charge Exchange in Collisions of Ions with Atoms and Molecules
- 11:00 – 11:30 *Morning Coffee*
- 11:30 – 12:30 Joseph Abdallah, Jr.
Use of Atomic Data in Plasma Modeling
- 12:30 – 13:30 *Lunch*
- 13:30 – 14:30 Robert E.H. Clark
Electron Impact Processes in Atomic Ions

14:30 – 15:00 *Afternoon Coffee*

15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

Tuesday, 5 September

09:00 – 10:00 All
Discussion

10:00 – 11:00 Robert E.H. Clark
Electron Impact Processes in Atomic Ions

11:00 – 11:30 *Morning Coffee*

11:30 – 12:30 Ronald McCarroll
Charge Exchange in Collisions of Ions with Atoms and Molecules

12:30 – 13:30 *Lunch*

13:30 – 14:30 Joseph Abdallah, Jr.
Use of Atomic Data in Plasma Modeling

14:30 – 15:00 *Afternoon Coffee*

15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

Wednesday, 6 September

09:00 – 10:00 All
Discussion

10:00 – 11:00 Tilmann Märk
Fundamental Elementary Process in Plasmas

11:00 – 11:30 *Morning Coffee*

11:30 – 12:30 Detlev Reiter
Atomic and Molecular Data in Fusion Edge Plasmas

12:30 – 13:30 *Lunch*

13:30 – 14:30 Ronald McCarroll
Charge Exchange in Collisions of Ions with Atoms and Molecules

14:30 – 15:00 *Afternoon Coffee*

15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

Thursday, 7 September

09:00 – 10:00 All
Discussion

10:00 – 11:00 Tilmann Märk
Fundamental Elementary Process in Plasmas

11:00 – 11:30 *Morning Coffee*

11:30 – 12:30 Detlev Reiter
Atomic and Molecular Data in Fusion Edge Plasmas

12:30 – 13:30 *Lunch*

13:30 – 14:30 Tilmann Märk
Fundamental Elementary Process in Plasmas

14:30 – 15:00 *Afternoon Coffee*

15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

Friday, 8 September

09:00 – 10:00 All
Discussion

10:00 – 11:00 Detlev Reiter
Atomic and Molecular Data in Fusion Edge Plasmas

11:00 – 11:30 *Morning Coffee*

11:30 – 12:30 Robert E.H. Clark
Electron Impact Processes in Atomic Ions

12:30 – 13:30 *Lunch*

13:30 – 14:30 Joseph Abdallah, Jr.
Use of Atomic Data in Plasma Modeling

14:30 – 15:00 *Afternoon Coffee*

15:00 – 17:30 Workshop Participants
Exercises
(Adriatico Guest House – Eklund Informatics Lab (Lower Level 1))

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