



International Atomic Energy Agency      INDC(NDS)-460

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**I N D C** INTERNATIONAL NUCLEAR DATA COMMITTEE

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**IAEA WORKSHOP ON**  
**“Atomic and Molecular Data for Fusion Energy Research”**

**8-12 September 2003**  
**International Centre for Theoretical Physics**  
**Trieste, Italy**

**SUMMARY REPORT**

**Prepared by: R.E.H. Clark**

**May 2004**

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## **Abstract**

On September 8-12 a workshop on Atomic and Molecular (A+M) Data for Fusion Energy Research was hosted by the International Centre for Theoretical Physics in Trieste Italy. The workshop was attended by twelve students representing eleven Member States. A total of five lecturers, including four external to the Agency, made presentations to the workshop. All lecturers provided advance copies of the lecture materials and all 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 by the conclusion of the workshop. During the course of the workshop the students were given the opportunity to describe their backgrounds and research interests. The workshop did arouse interest in A+M processes related to fusion. The workshop was viewed as successful by the students.

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May 2004

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## **1. OVERVIEW**

The Workshop on Atomic and Molecular Data for Fusion Energy Research was hosted on 8-12 September 2003 by the International Centre for Theoretical Physics (ICTP) at Trieste, Italy. The Atomic and Molecular (A+M) Subcommittee of the International Fusion Research Council (IFRC) had recommended holding such a workshop. The workshop was attended by twelve students, four external lecturers and two IAEA staff. Due to the fact that the workshop was hosted by the ICTP, rather than being an official ICTP workshop, the A+M Unit provided the secretarial support for the workshop. However, the ICTP personnel were exceedingly helpful in all aspects of the workshop and gave assistance in many matters during the course of the workshop. The list of participants of the workshop is included in Appendix 1.

## **2. BRIEF WORKSHOP PROCEEDINGS**

### **2.1 Introduction**

Due to the hosted nature of the workshop, most of the preliminary preparations were undertaken by the A+M Data Unit. This included writing of the notice of the workshop, tailoring an application form for workshop attendees, receiving applications and evaluating the applicants, reviewing the budget requirements, etc. It is noted that in all these steps the ICTP co-ordinating person, B. Stewart, was extremely helpful. A detailed checklist of required tasks with a comprehensive timeline was provided. All preparations went smoothly. Four external lecturers were arranged 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 by B. Stewart. R. Clark welcomed the participants on behalf of the IAEA and introduced the lecturers and their fields of expertise. The schedule for the week was introduced and adopted. The schedule is included as Appendix 2. The general outline was to begin each day with one hour of discussion of the material from the previous day, including solutions to the assigned exercises. This 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 large computing room was 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. These are summarized briefly in this section.

Muhammad Salahuddin from the Atomic Energy Commission of Pakistan has a background and interest in theory of plasmas, in particular looking at spectroscopy of magnetized plasmas. Xiangdong Li from the Chinese Academy of Science has an interest in theoretical atomic spectra and spectra from plasmas. He has done some work with dense plasma screening. Ram Prakesh of the Institute for Plasma Research in India has a current interest in collisional radiative models, including impurity transport. He has worked with a

number of A+M databases through the Internet. Natasa Markovska of the Macedonian Academy of Sciences and Arts has an interest in plasmas processes such as particle surface interactions and quantum modelling. Mahmud Vahdat Roshan of the Nuclear Fusion Research Center of Iran has an interest in various tokamak parameters, dense plasma experiments, short pulses and plasma focus. Mykhaylo Koma of the Uzhgorod National University of the Ukraine has an interest in two electron capture processes in slow ion-atom collisions. David Rapisarda Socorro from CIEMAT in Spain is a doctoral student using the TJ-II stellarator in Madrid for studies of ion dynamics. Annarita Larrichiuta of the University of Bari, Italy, has been working on studies of electron molecule collision cross sections, specifically on hydrogen, oxygen and nitrogen molecules. Makoto Imai of Kyoto University in Japan has worked on ion-atom collision processes. He has been involved in absolute cross section measurements for electron capture processes. Kieran McCarthy of CIEMAT in Spain works on the TJ-II stellarator at the Nuclear Fusion Laboratory. Yong-Joo Rhee of Korea Atomic Energy Research Institute has a background in establishing databases for a variety of A+M processes. Raul Barrachina of the Bariloche Atomic Center has an interest in theoretical atomic collision theory.

Each student 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. Some of the discussions have led to continued contacts after the conclusion of the workshop.

## 2.2 Lecturers

There was a total of five lecturers, four 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 three lectures focused on electron impact processes in atoms and ions, as well as using such data in modelling of plasmas in fusion machines. Processes detailed 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 using the online database to look at specific data for some of the processes and to use modelling codes to arrive at some parameters for fusion related plasma conditions.

J. Davis of the Institute for Aerospace Studies presented three lectures on co-deposition and plasma interaction with co-deposited materials. He gave 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. Of particular interest was the description of possible processes in ITER involved in determining tritium inventory.

T. Maerk of the Universitat Innsbruck gave a thorough review of processes involving molecules in fusion plasmas. He gave 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. He explained the theoretical methods for calculations and the difficulties of such calculations. He gave a good overview of the experimental techniques for measuring a number of processes involving molecules. The leading locations of research in these areas were outlined. The students were presented with several exercises giving them a feel for parameters involved in molecular processes.

R. McCarroll of the Universite Pierre et Marie Curie, France, gave three lectures on heavy particle collisions. He summarized the basic processes of 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. He went through 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 gave some realistic estimates.

J. Roth of the Max-Planck Institut fur 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. Roth outlined the major processes that occur when plasma constituents interact with a pure material. He introduced methods for analysing such interactions. He introduced the students to a number of available means of predicting 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.

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 seeing 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 were distributed to the students before the close of the workshop. K. Sheikh of the A+M Data Unit was instrumental in collecting the materials, making the CDs and working with the ICTP staff to ensure the students had working Internet access, as well as taking care of many routine administrative matters.

Materials from the lecturers are available on request by CD.

### **3. RECOMMENDATIONS AND CONCLUSIONS**

This was the first ICTP workshop the A+M Unit was involved with. The workshop was viewed as very successful from the students as well as the lecturers. The students uniformly recommended that additional workshops be planned and that they cover at least a two week period. All the students had favourable comments regarding the lectures. They were all pleased to have the entire set of materials on CD to take with them to their home institutions.

This workshop had been recommended by the A+M Subcommittee of the IFRC. The Subcommittee has also recommended that if it were held successfully, there should be an effort to hold such workshops periodically. Following the successful completion of this first workshop, it is recommended that the A+M Unit follow the advice of the Subcommittee and



hold such workshops periodically. It is believed that this would be of high value in bringing more young researchers into A+M physics in support of nuclear fusion energy.

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**LIST OF PARTICIPANTS**

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**WORKSHOP PROGRAMME**

Slot	Monday	Tuesday	Wednesday	Thursday	Friday
09:00-10:00	Introduction	Discussion	Discussion	Discussion	Discussion
10:00-11:00	Roth (1)	Roth (2)	Clark (2)	Maerk (2)	Maerk (3)
11:30-12:30	McCarroll (1)	Davis (1)	Davis (2)	Roth (3)	Clark (3)
14:00-15:00	Clark (1)	McCarroll (2)	Maerk (1)	McCarroll (3)	Davis (3)
15:00-17:30	Exercises	Exercises	Exercises	Exercises	Exercises

Morning Coffee: 11:00-11:30

Lunch: 12:30-14:00

Afternoon Coffee: 15:30-16:00

<sup>(1),(2),(3)</sup>Lectures

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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.

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