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I N D C INTERNATIONAL NUCLEAR DATA COMMITTEE

14th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

Summary Report of IAEA Technical Meeting

IAEA, Vienna, Austria

24 – 25 June 2004

Prepared by

R.E.H. Clark
N.J. Peacock

January 2006

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Abstract

The 14th Meeting of the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council was held on 24-25 June 2004, at the IAEA Headquarters in Vienna, Austria. Subcommittee members reviewed the work of the Atomic and Molecular Data Unit over the two-year period from June 2002 to June 2004, and made recommendations that covered the 2005-2006 budget cycle. The proceedings, conclusions and recommendations of the meeting are briefly described in this report, along with a short summary of the activities of the IAEA Atomic and Molecular Data Unit of the Nuclear Data Section from June 2002 to June 2004.

January 2006

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1. Introduction

The 14th Technical Meeting of the Subcommittee on Atomic and Molecular (A+M) Data for Fusion of the International Fusion Research Council was held on 24 and 25 June 2004, at the Agency Headquarters in Vienna, Austria. Primary objectives of the meeting included a detailed review and assessment the Agency activities in the area of atomic and molecular data and plasma-surface interaction data for fusion for the period June 2002 to June 2004, and the formulation of recommendations to the Agency regarding the A+M programme for the years 2006 and 2007.

The Meeting was attended by ten subcommittee members (Appendix 1). Dr. N. J. Peacock (UKAEA) served as Chairman of the meeting, while Dr. R. Clark (Head, Atomic and Molecular Data Unit of the IAEA) served as Scientific Secretary. Nine other members of the subcommittee were in attendance: J. Roth (IPP), E. Menapace (ENEA), T. Kato (NIFS), R. Janev (Macedonian Academy of Sciences), M. Crisp (USDoE), W. P. West (GA), H. Kubo (JAERI), R.Guirlet (CEA) and Yu. V. Martynenko (Kurchatov Institute). The A+M Data Unit was represented by Dr. A. L. Nichols (Head, Nuclear Data Section) and Dr R. E. H. Clark (Head, A+M Data Unit).

2. Meeting Proceedings

Dr. A. Nichols opened the meeting by welcoming all subcommittee members to the IAEA and Vienna. He strongly endorsed the work of the subcommittee, and emphasized the importance of their thoughts and recommendations to the intermediate- and longer-term work programme of the A+M Data Unit, in their advisory role to the IFRC. There are increasingly important long-term needs for A+M data, as a consequence of the exciting developments towards large, internationally-managed fusion devices. Site selection for the ITER project can be expected within the next 12-18 months, and will have a significant, positive impact on fusion research around the world.

The agenda had been distributed before the meeting, and was accepted without any changes. Before the technical business began, Dr. T. Kato delivered an appreciation of the life and work of Dr. T. Shirai (deceased) and his highly valued contributions to the Atomic and Molecular Data Subcommittee.

During the morning session of the first day, staff from the A+M Unit reported in some detail on their activities over the previous two-year period, including a review of the Data Centre Network (DCN) and electronic databases. A demonstration of the electronic databases was presented, and a recent upgrading of the Unit server was described. Specific issues with the DCN were discussed, including the increased possibilities of linking the databases through a common search engine. A+M Co-ordinated Research Projects (CRP), Technical Meetings (TM) and workshops were also reviewed, including descriptions of current CRPs, along with proposed dates for the publication of final results in *Atomic and Plasma-Material Interaction Data for Fusion (APID)*. Topics of highest priority for new CRPS were extensively discussed, with subcommittee members making a number of specific recommendations (Section 3).

An important Technical Meeting had been held in October 2003 at the Institut für Plasmaphysik, Forschungszentrum Jülich, Germany. The A+M Data Subcommittee reviewed the resulting recommendations and concluded that the TM had been highly successful in defining A+M and plasma-surface interaction data needs for the next ten years.

A summary was presented of the workshop on "Atomic and molecular data for fusion energy research", held at the International Centre for Theoretical Physics, Trieste, Italy in September 2003. Members of the subcommittee strongly endorsed the workshop concept, and urged the Unit to plan additional A+M workshops at periodic intervals.

Various data dissemination methods were reviewed, as used by the A+M Unit. The main publications of the A+M Unit were assessed and discussed: *International Bulletin on Atomic and Molecular Data for Fusion* ("Bulletin"), and *Atomic and Plasma-material Interaction Data for Fusion (APID)*. Both publications are fully up to date. Several new electronic tools were also described, including the new search engine to access a number of databases and interfaces to well-known computer codes for the generation of new data.

Following the A+M Unit presentations, the Subcommittee reviewed the on-going and planned work programmes of the A+M Unit. The Subcommittee acknowledged the efforts of the Unit to address all of the recommendations from the previous meeting, and concluded that the Unit had been remarkably effective in meeting the goals while operating with limited staff numbers. The final session of the meeting was devoted to formulating recommendations for the Unit, and setting priorities for Unit activities (Section 3, below).

3. Recommendations and Conclusions

The Subcommittee spent considerable time analyzing the current data needs in fusion research and establishing priorities. A definitive set of recommendations were formulated from the prioritized list in order to assist the A+M Unit in their work plans. These recommendations are as follow:

1. The CRPs on "Molecular processes in edge plasmas" and "Atomic and molecular data for fusion plasma diagnostics" will finished on schedule in 2004, and two volumes of APID will be produced as outputs from these important activities.

2. A CRP on "Tritium inventory in fusion reactors" was initiated in 2002, and will be extended with a final RCM in 2006. Subcommittee members recommend that dusty plasmas and sticking coefficients for tritium be included as topics in the extension, and that (if needed) additional expertise should be added to the CRP for this purpose.

3. Establish a new CRP in 2005 on "Atomic data for high-Z element impurities in fusion reactors" (there are also on-going studies for ITER). An investigation of data reduction methods should be included in this CRP to make the data usable in a 2D modelling code.

4. Establish a new CRP in 2006 on "Data for surface composition dynamics relevant to erosion processes".

5. Organize and hold a CM in 2005 on diagnostics methods for measuring isotope ratios in burning plasmas (H, He, D, T, Be and Li), possibly leading to a TM in 2007 on this same topic.

6. Organize and hold a TM in 2006 on materials for fusion plasma-facing components, possibly leading to the start of a CRP in 2007 on material properties (consider including liquid walls).

7. A+M Subcommittee is cognizant of the importance of the physics of burning plasmas.

8. Subcommittee members were impressed by the high technical standards, debate and resulting recommendations that emerged from the TM in Jülich. The appendices from this meeting should be given close attention – their list of excellent recommendation is an example of how well the IAEA is able to keep abreast of current trends and data needs in fusion.

9. Subcommittee members were impressed by the increasing efforts by the Unit to use a variety of electronic interconnections among databases and codes. GENIE and DANSE are two Web search engines that allow simultaneous retrieval of data from different Web sites, and are under development. GENIE is dedicated to numerical atomic data, while DANSE is focused on bibliographic atomic and molecular data. The Subcommittee strongly recommends continued development of these two important tools, especially the addition of processes (atomic-ion collisions) and databases to the searches (four out of fifteen DCN members now accessible).

10. Subcommittee members were heartened by the recent progress to access the Los Alamos codes on atomic structure and cross-section calculations, and the ion collision codes of Dubois and Hansen through Internet interfaces. Efforts should continue to extend the capabilities of this rapid and highly-efficient method of data manipulation.

11. Subcommittee members endorse the organization of a TM to investigate the establishment of a code centre network. This proposed network should follow the same general form as the existing DCN, and should also compile a list of codes and their capabilities as well as contact persons for such codes.

12. The issue of directly performing modelling calculations within the A+M Unit was raised – Subcommittee members endorse unanimously the statement that the overall objective of the A+M Unit should be to establish high-quality databases, and not to undertake modelling calculations.

13. Formulation of XML standards was raised - Subcommittee members believe that the use of XML will increase over time, and urge the Unit to remain involved in these developments, although not playing a major role.

14. The efforts of the A+M Unit to address all of the recommendations from the previous meeting were most highly praised – staff have been remarkably effective in meeting the goals while operating with a limited number of professional staff.

Subcommittee members noted the increasingly high level of importance being placed on plasma interactions with the wall; there is a need to increase the expertise of the subcommittee in this area through the introduction of two appropriate new members (proposed by the subcommittee).

4. Concluding Remarks

Following a detailed presentation of the work of the A+M Unit that covered the period from June 2002 to June 2004, the A+M Subcommittee of the IFRC acknowledged the significant level of success of the Unit in achieving the goal of establishing databases focused on A+M and plasma-surface interaction data for fusion research. Following detailed discussions on data needs and priorities, the subcommittee formulated an extensive list of recommendations to assist the A+M Unit over the next two-year period. More extensive recommendations are required to cover plasma-surface and material data issues, and therefore the subcommittee is in the process of identifying two new members with the relevant expertise to consider these topics.

Appendix 1

IAEA Technical Meeting:
14th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

24-25 June 2004, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA Technical Meeting:
14th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

24-25 June 2004, IAEA Headquarters, Vienna, Austria

Agenda

Thursday, June 24 **Meeting Room: A-04-18**

09:30 - 10:00 Opening. Welcome to Subcommittee members
Adoption of Agenda

Session 1: General Report on Activities since May 2002

10:00 - 11:00 Report on the activities of A+M Data Unit June, 2002 June 2004, *R. Clark*

11:00 - 11:30 *Coffee break*

Session 2: Data Centre Network, database activities and computer issues

11:30 - 12:30 Review of DCN, databases and computing issues, *D. Humbert*

12:30 - 14:00 *Lunch*

Session 3: Review of Current and planned CRPs

14:00 - 15:30 Results from recent CRPs, review of current CRPs and new CRPs to start in 2004-2007 period, *R. Clark*

15:30 - 16:00 *Coffee break*

Session 4: Review of 2002 TM and 2003 Workshop

16:00 - 17:30 Review of activities, *R. Clark*

Friday, June 25

Session 5: Code Interfaces and Publications

09:00 - 10:30 Status of interfaces to codes on the Internet and Unit publications, *R. Clark and D. Humbert*

10:30 - 11:00 C*offee break*

Session 6: Review of Unit status

11:00 - 12:30 Review of status of A+M Unit, *Subcommittee members*

12:30 - 14:00 *Lunch*

Session 7: Recommendations for new projects, setting of priorities

14:00 - 13:30 Recommendations for any new projects as well as setting priorities for Unit activities, *Subcommittee members*

15:30-16:00 *Coffee Break*

Session 8: Formulation of meeting conclusions

16:00 - 17:30 Formulation of meeting conclusions and Executive Summary of the Meeting

17:30 - *Adjournment of Meeting*

Appendix 3

IAEA Technical Meeting:
14th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

24-25 June 2004, IAEA Headquarters, Vienna, Austria

Activities of the Atomic and Molecular Data Unit June 2002 - June 2004

I. Introduction

During the two year period since the last meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion, the Atomic and Molecular (A+M) Data Unit has made significant progress on supplying data relevant to fusion energy research. The Unit has followed the recommendations of the Subcommittee - a detailed summary of progress on these recommendations is given in Section II. Database developments, Data Centre Network activities and computing issues are described in Section III. A summary of current and planned CRPs is given in Section IV, while summaries and outcomes of the 2002 Technical Meeting and the 2003 Workshop are presented in Section V. Methods of data distribution, including interfaces to computer codes and publications, are described in Section VI. Section VII contains an overall summary of the work of the Unit from June 2002 to June 2004.

II. Unit Progress on Subcommittee Recommendations

At the previous meeting, the A+M Subcommittee of the IFRC made a number of recommendations to the A+M Data Unit concerning future activities. These recommendations have resulted in specific actions by the Unit. A detailed summary of each recommendation and the resulting progress on the part of the A+M Unit are outlined below.

1. *Recommendation:* Two specialist meetings should be held to discuss the following:

   (a) characterization of dust - impact on the retention of tritium and edge plasma behaviour;
   (b) organize and co-ordinate a meeting to establish an A+M computer code network.

   Progress:

   (a) Due to a number of constraints on personnel, a new Technical Meeting on dust and tritium retention could not be organized. However, provision has been made for the extension of the CRP on “Tritium inventory in fusion reactors” with the possibility of including this topic in this extension.
   (b) A meeting will be held in 2005 to explore the possibility of forming a computer code network. Much preliminary work has been done with a number of individual consultants. A number of codes for calculation of atomic data relevant to fusion energy research have been made accessible through the Internet. A method of using Perl scripts for such an interface has now been successfully applied to several different codes - authors of these codes have expressed their willingness to

participate in a network to encourage the spread of such capabilities, and to support the continued maintenance of such codes.

2. *Recommendation*: Extend the two existing CRPs on "Data for molecular processes in edge plasmas" and "Atomic and molecular data for fusion plasma diagnostics".

   Progress: Areas for additional research needs were identified in each of the two existing CRPs. Proposals for extensions were formulated – both CRP proposals for extensions were approved, with final RCMs to be held in 2004. The CRP on "Tritium inventory in fusion reactors" will hold the final RCM in 2006.

3. *Recommendation:* Establish a new CRP on "Establishment of recommended A+M databases for plasma edge modelling". This CRP should include the establishment of as complete as possible database to be recommended for use in computer codes modelling edge plasmas - start in 2004.

   Progress: A TM was held in late 2003 to explore the possibility of establishing such a CRP. After identifying several possible areas in which a comprehensive database could be generated, a consensus was reached on the need to assemble a database on hydrocarbon processes. A detailed proposal for the CRP was written, and subsequently accepted by the IAEA in 2004.

4. *Recommendation:* Establish a new CRP on "Data for surface composition dynamics relevant to erosion processes". This CRP should include data collection of solid state diffusion of components of refractory metals and metal multi-layers of elements such as Be, B, C, Cu and W - start in 2005.

   Progress: A new CRP has been accepted into the Atomic and Nuclear Data budget for 2005. The detailed proposal will be presented to the IAEA Research Contracts Committee in due course.

5. *Recommendation:* Significant efforts are required to respond positively to the requests for data in to model new plasma scenarios and address new materials issues - simultaneous organization of three CRPs is endorsed (and may need to increased to four in the future).

   Progress: Proposed budget for the A+M Data Unit contains three to four active CRPs through the 2006-2007 budget cycle. The Unit has received strong support from the Section and Division, and this support is expected to continue into the future.

6. *Recommendation:* Continued development of the search engine should take place, with the goal being to gain access to all DCN-member databases.

   Progress: Work has continued on the numeric search engine with the addition of the KAERI database. The limitation on continued extension now lies in the databases themselves. Unless a database is searchable through Internet commands, the search engine cannot obtain the data. The Unit is now in the process of formulating methods for categorizing data in a consistent manner that will be proposed to the members of the DCN. Considerable work is now underway on developing schema in XML to give a uniform format for A+M data – to be presented at ICAMDATA in 2004.

7. *Recommendation:* The Bulletin constitutes an important means of publishing valuable work on A+M data. Addition of a newsletter style section at the front of the Bulletin is recommended to publicize new features of the electronic databases.

   Progress: Volume 62 of the Bulletin has been published, and volume 63 is in preparation. A+M Unit staff proposed that publication be limited to one issue per year, and that new data should continue to be added to the on-line database as suitable databases are received. The amount of data is generally such that one issue of the Bulletin per year is judged to be sensible and realistic (particularly since the cost of the Bulletin is a large fraction of the Section's printing budget).

8. *Recommendation:* DCN should consider expansion in new geographic areas. New members should work towards gemerating electronic databases on-line, adopting the English language, and ensuring that their databases are relevant to fusion applications.

   Progress: L.E. Machado from Universidade Federal de Sao Paolo was invited to attend the 2003 DCN meeting and present an overview of A+M capabilities within several Brazilian institutions. Rogério de Moraes Oliveira of the Instituto Nacional de Pesquisas Espaciais in Brazil has contacted Machado with regard to the data capabilities available to support the spherical Tokamak in Brazil.

9. *Recommendation:* More publicity is encouraged to ensure that the fusion community is fully aware of the excellent progress being made with respect to the data network.

   Progress: A newsletter page has been added to the latest issue of the Bulletin, and an e-mail list is in preparation. Updates are also frequently added to the home page of the A+M Unit.

10. *Recommendation:* In view of the number of hits on the network, there should be a major upgrade of computer facilities.

    Progress: A new server has been installed (Compaq Proliant ML530) that came on-line in November 2003. Features include two Intel Xeon processors, 400 MHz system bus, much increased memory, 3 HD, SCSI, RAID 2,high speed IDE RW CD-ROM.

11. *Recommendation:* In light of the importance placed on the assessment of data by users of the databases of the A+M Unit, careful assessments should continue to be the standard for additional entries to the database.

    Progress: New data are carefully assessed before being added to the database. When possible, the accuracies of the data are evaluated and a grading system is applied to new data.

12. *Recommendation:* Informal meetings of DCN representatives should be encouraged at ICAMDATA meetings.

    Progress: Informal meetings of DCN representatives have taken place at ICAMDATA 2002, as well as at the APIP meeting in Santa Fé in 2004. Discussions included better methods of data sharing and development of XML standards for A+M data. A presentation will be made on the XML work at ICAMDATA 2004.

13. *Recommendation:* The A+M Unit should plan to follow up the ICTP workshop of 2003 with a further workshop of similar format in 2005 – two-week duration on a focused topic (e.g., plasma-material interactions), and a larger number of attendees.

    Progress: The A+M Unit has included a two-week workshop in their budget plans for 2006. One aim will be to accommodate a larger number of participants. The 2003 workshop was extremely successful, and the students also recommended a lengthier workshop in the future.

14. *Recommendation:* The concept of a code network was endorsed - codes linked to the A+M Unit should have a level of quality consistent with that of the DCN.

    Progress: A technical meeting is scheduled for 2005 to explore the initiation of a code network. Preliminary work with several authors of codes has taken place in the form of consultancy visits to the IAEA. These consultancies have resulted in significant code resources becoming available through the Internet. Authors were very positive about the idea of a network for mutual continuing support of their codes.

15. *Recommendation:* Modern data needs and computer networking have led to greatly increased needs for large amounts of high quality data, placing increased demands on the A+M Unit. All possibilities should be explored to make additional professional staff support available to the Unit, particularly in the area of plasma-surface interaction physics.

    Progress: Since the IAEA Nuclear Data Section continues on zero budget growth, there is virtually no possibility of increasing staff levels at this time. Exploration for cost-free experts has so far been unsuccessful, with only two or three opportunities arising for the entire Department.

16. *Recommendation:* Each Subcommittee member should inform his/her Member State representative to the IAEA of the importance A+M data to achieving fully controlled fusion.

    Progress: to be discussed among Subcommittee members.

17. *Recommendation:* An additional member should be introduced into the Subcommittee with expertise in the area of plasma-material properties.

    Progress: to be discussed among Subcommittee members.

18. *Recommendation:* From time to time, some Subcommittee members are unable to attend due to financial constraints - some means of offering travel assistance should be investigated.

    Progress: Travel and subsistence costs for IFRC Subcommittee meetings have now been included in the budget.

III. Data and Computing Issues

As mentioned in the previous section, a new server has been purchased and installed, with a total memory of 1 GB. This new server has two processors, each one nearly an order of

magnitude faster than the previous server. The disk system consists of three large drives, each one over an order of magnitude larger in capacity than the previous server. These hot-plugged disks are linked using the RAID system to insure full functionality in the event of a complete failure of any one unit. The new server uses the Linux Redhat 9 operating system, the Apache software for the web server, and PosgreSQL for database management. All functionality of the previous server has been retained. Significant new services can be provided, such as running cross-section calculations on the server that could not be carried out on the previous server.

A meeting of the Data Centre Network took place in 2003. As mentioned in the previous section, an observer from Brazil attended, and this new member has begun co-ordinating Brazilian efforts to apply the capabilities in data generation to fusion applications. During the course of the meeting, the list of priorities was reviewed, and subsequently made available on the homepage of the A+M Unit. The formulation of XML standard formats for A+M data was also raised, and a recommendation was made to await further developments and pursue informal meetings on this topic at conferences. Such meetings have taken place, a presentation will be made at ICAMDATA 2004, and plans are being made to hold a Consultants' Meeting in 2005. Interest has been expressed to invite an ITER representative as an observer to subsequent DCN meetings in order to better facilitate Data Centre priorities.

Considerable work has taken place to develop and improve the Aladdin numerical database system. A new version is being tested that can merge four existing databases into one, and so handle the overlap of similar data types in different databases. Substantial amounts of new data have been entered into the databases, and a large number of entries for charge exchange have been reviewed and entered. Furthermore, significant amounts of data for electron excitation and ionization of a number of elements have been calculated at the Los Alamos National Laboratory, and are now in the system. Work is also underway to establish links between the numerical and bibliographic databases, and to allow conversions between different sets of units in order to facilitate the comparison of data from different sources.

AMBDAS is the interface to bibliographic data, and has undergone extensive updating for easier usage. Thus, the request form has been streamlined and searches are more reliable - for example, in searching for references with two reactants, the ordering of reactants will not exclude any data. New data from DCN have been incorporated into the AMBDAS databases, and can be used to produce volumes 62 and 63 of the Bulletin. Work continues on to form electronic links to available articles.

GENIE is the numerical search engine, and can now accesses seven databases for oscillator strengths, transition probabilities and energy levels, and two databases for collision processes. The main problem in adding new databases is that most Web sites are not fully searchable through the Internet. As this inadequacy is rectified, the databases will be added to the list searched by GENIE.

The bibliographic search engine (DANSE) can access three databases, and permits searches on A+M processes, structure and spectral data, and particle-material interactions.

IV. Co-ordinated Research Projects

There are three active CRPs, and another will begin in 2004. Two of the existing CRPs will end in 2004, and one new CRP will be initiated per year in 2005, 2006 and 2007.

The CRP on "Data for molecular processes in edge plasmas" was extended for an additional year, and the final RCM will take place in 2004. This one-year extension has the specific goals of accruing additional data from measurements and calculations of ionisation cross sections for hydrocarbons, calculations for charge exchange and recombination cross sections, measurements and calculations of cross sections for attachment and detachment, measurements of cross sections for excitation and de-excitation, and detailed comparisons of collisional-radiative models. Results from the CRP will also be published in APID.

The CRP on "Atomic and molecular data for fusion plasma diagnostics" was also extended for an additional year, with the final RCM in 2004. Specific goals within the one-year extension include measurements and calculations of cross sections of excitation, ionization and charge exchange for atoms and molecules, expanding energy ranges for these data, and measurements for radiative processes to support spectral line diagnostics.

The first RCM for the CRP on "Tritium inventory in fusion reactors" was held in 2002 to formulate a detailed work plan. Specific topics to be addressed include carbon issues such as erosion processes, sources and sinks, and hydrocarbon processes; mixed materials pose significant uncertainties identified with chemical erosion, Be-seeded plasmas, NERD profiles of samples and dust sampling; the processes of deposition and co-deposition, and various aspects of an all metal machine. The second RCM is planned for October 2004, with the third and final CRP in 2006.

V. Technical Meeting and Workshop

A large Technical Meeting was held in October 2003 at the Institut für Plasmaphysik, Forschungszentrum Jülich, Germany, to review the current status of A+M and plasma-interaction data for fusion and to make recommendations concerning data needs and priorities. Over fifty specialists in the A+M data field attended this meeting.

Leading researchers presented invited talks on the following topics:

Current Status of Fusion Research;
A+M Data Needs in Fusion Reactors;
Plasma-Surface Interaction and Material Properties Data Needs in Fusion Reactors and Data Generation Activities.

A poster session addressed current research activities as well as modelling and diagnostic needs in fusion energy research. The resulting mixture of invited and contributed talks resulted in a very thorough overview of the current status of A+M data generation and databases.

Participants formed themselves into three working groups to discuss the following major topics:

atomic and molecular data,
plasma-material interaction, and
material properties.

These three working groups met separately to formulate specific recommendations within each of these three areas. During the last session of the meeting, representatives from each working group reported on their agreed findings and results.

The Atomic and Molecular Working Group noted the impressive body of A+M data relevant to fusion research that has been accumulated over the years and implemented within the fusion plasma application codes. As a result, the breadth of fusion-relevant data generated has been extensive and adequately addresses the developing needs of fusion research. However, gaps in A+M data continue to appear, and the main priorities at the present time are as follows:

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

The Plasma-material Interaction Working Group noted the need to address the physics of the erosion mechanisms and the transportation and redeposition of eroded material, and to demonstrate tritium removal from a Tokamak. These important issues will require more laboratory work on wall diagnostics, with the need to dedicate operational time on a Tokamak to such experiments. Successful modelling of the results is an essential requirement to develop our understanding of wall physics. Topics of highest priority can be identified by dividing the data requirements into those involving carbon as the first wall material and those associated with an all-metal machine. Carbon issues include the 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. More information is also needed on techniques for the removal of tritium from deposited layers - techniques developed from laboratory experiments (oxidation, laser de-sorbtion) need to be tested and validated in existing fusion devices. All-metal machine require quantitative studies of the erosion of high-Z target plates by seed impurities, including confirmation that a reduction in divertor temperature offsets the increased erosion by seed impurities. Furthermore, the high heat flux performance of high-Z components needs to be investigated by means of laboratory experiments, and through the use of high-Z divertor plates in studies of relevance to ELM scenarios.

The Material Properties Working Group identified several important areas in need of study. One of the remaining issues for armor materials is their behavior during transient events (ELMs, disruptions, VDEs, etc.) Effects due to neutron irradiation have been considered (up to approximately 1 dpa), and the resulting material degradation was shown to remain within acceptable limits. Material data obtained so far are mainly limited to the operation regime of ITER, and little consideration has been given to devices beyond ITER with neutron fluences. There is a requirement for data defining the high-temperature properties of armour materials, physical properties of mixed and doped materials, and neutron effects. The PSI community should study the proposed candidate materials, and data should be collected in the form of databases with as much detailed information included as possible.

In summary, the TM undertook a comprehensive overview of the current status of databases relevant to fusion energy research. Extensive priority lists were produced, and the suggested

areas for new data generation were found to be in good alignment with the various recommendations from the A+M Subcommittee of the IFRC.

An international workshop on "Atomic and molecular data for fusion energy research" was held at the International Centre for Theoretical Physics, Trieste, Italy, in September 2003. The major goals were to present an overview of A+M data needs in fusion energy research to potential new researchers in the field. Key data areas were covered (lecturers are indicated in parentheses):

plasma-material interaction data for pure materials (J. Roth),
co-deposition of materials and interaction of mixed materials with the plasma (J. Davis),
electron collision processes in atoms and molecules and their ions (R. Clark),
molecular formation and dissociation (T. Maerk), and
charge transfer processes (R. McCarroll).

Twelve students participated in the workshop from eleven Member States. All students were given the opportunity to give a short presentation on their backgrounds and research interests. Time was always taken to review the previous day of lectures and the exercises assigned by the lecturers. Lecture materials and the various exercises were collected on CDs for distribution to all participants. Student reactions were extremely positive, and many suggested that the workshop should be extended to two weeks (as being planned for the 2006 ICTP workshop).

VI. Data Distribution

The main methods of data distribution are the on-line databases (already covered in Section III), publications, and on-line access to computational tools.

The main publications of the Unit are the *International Bulletin on Atomic and Molecular Data for Fusion* (Bulletin) and *Atomic and Plasma-material Interaction Data for Fusion (APID)*. These two publications have continued over the previous two years, with the preparation of Volume 63 of the Bulletin in progress, and Volume 11 of APID submitted to the Agency printers.

A new method of data distribution has been developed and introduced: on-line interface to computational tools. The interface to the average approximation method for calculation of electron impact excitation cross sections of atomic ions represents an earlier version of this approach – allowed a user to obtain an approximate cross section for transitions between non-relativistic electron configurations for a range of energies using an approximation to distorted wave theory ("average approximation" of Peek and Mann). This earlier interface averaged five to ten users per week over the previous two years, indicating a continuing need for such a capability. Therefore, the software has been extended significantly to two new areas through collaboration with A. Dubois and J.P. Hansen - calculation of cross sections for excitation and charge transfer in heavy-particle collisions. The interface underwent significant modification to incorporate a number of checks on the input parameters and to identify any possible problems with the calculation. After significant testing, the interface has reached a point of maturity for use by selected people – potential users have to request a user name and password in order to access the code on the A+M Unit server.

J. Abdallah, Jr. (Los Alamos National Laboratory) has collaborated with the Unit to improve the availability of three of the Los Alamos codes through a similar interface. These codes

allow the calculation of atomic structure (including oscillator strengths), electron impact excitation using two variations of distorted wave theory, and ionization cross sections for electron and photon impact as well as autoionization. Full LSJ fine structure levels are used, and allowance is made for configuration as well as spin-orbit mixing of target states. Users can view the mixing coefficients as well as the oscillator strengths, and most of the data can be presented in both tabular and graphical form. A preliminary version of the interface has undergone extensive testing, and was demonstrated at the Conference on "Atomic Processes in Plasmas" in Santa Fé, April 2004. The codes and interface are located on a server at Los Alamos, with links to the server homepage of the A+M Unit.

VII. Summary

The A+M Data Unit continues to work towards the goal of establishing the necessary databases of atomic, molecular and plasma-material interaction data for fusion energy. These databases continue to expand to meet the needs of the fusion community. Appropriate meetings are held to determine A+M data priorities, and CRPs are regularly established to act as focal points for the development of data in the various recommended areas. The Unit continues to explore new means of disseminating data as new tools become available. Recommendations of the A+M Subcommittee of the IFRC remain an invaluable tool in the work of the Unit to focus A+M data needs and priorities. As seen in this report, the A+M Data Unit follows those recommendations closely.

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