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Assess Data Relevant to Spectral Analysis of Fusion Plasmas

Summary Report of IAEA Technical Meeting

IAEA, Vienna, Austria

13 – 14 June 2005

Prepared by

R.E.H. Clark

January 2006

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

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Summary Report of IAEA Technical Meeting

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Abstract

Twelve international experts on the properties of heavy elements relevant to fusion energy research participated in a Technical Meeting at IAEA Headquarters on 13-14 June 2005. Each participant reviewed the current status of their research activities and areas of expertise. Detailed discussions took place to formulate a specific set of data needs for heavy elements for fusion research which could be addressed through a Coordinated Research Project (CRP) on the subject. All the goals of the meeting were achieved, and every participant indicated a desire to contribute to the generation of data for modelling the behavior of heavy elements in fusion-related plasmas, including collisional and radiative properties. The discussions, conclusions and recommendations of the meeting are briefly described in this report.

January 2006

TABLE OF CONTENTS

1. Introduction

A Technical Meeting (TM) was held on 13-14 June 2005 at IAEA Headquarters, Vienna, to "Assess Data Relevant to Spectral Analysis of Fusion Plasmas". The purpose of this meeting was to review the current status of data for heavy element impurities, and to propose areas needing additional research. These areas of research were used as the basis for specifying detailed work plans to be undertaken within a proposed Coordinated Research Project (CRP) on "Atomic data for heavy element impurities in fusion reactors".

Twelve experts on various processes involving heavy elements likely to be important in fusion reactor research participated in the TM. The list of participants is included as Appendix A. Each participant gave a summary of current work in their field of expertise, as well as their active lines of research. Following a discussion of the fusion needs for data for heavy element impurities, a set of recommendations was formulated and agreed for consideration by the CRP participants.

2. Meeting Proceedings

A. Trkov (Deputy Section Head of the Nuclear Data Section) welcomed the participants on behalf of the IAEA. He noted that fusion research continues to advance, and is an important topic within the IAEA Nuclear Data Section. He expressed optimism that the meeting participants would formulate useful recommendations on the topic of heavy elements, and that the collaborative work with Atomic and Molecular Data Unit staff would continue to produce large amounts of useful data for fusion research. R. Clark (Scientific Secretary) reviewed the proposed agenda, which was accepted without change (see Appendix B).

During the course of the first day and a half, each participant gave a summary presentation of their research activities. All presentations were collected on CD and distributed to the meeting participants during the course of the meeting. At the end of these presentations, the current capabilities of each participant were summarized. The final session was devoted to a review of the most pressing data needs for heavy elements, and the formulation of recommendations for a CRP dedicated to this topic.

2.1. Summary of current relevant research

D. Fursa of Murdoch University in Australia reviewed the theoretical work on close coupling calculations of electron scattering from atoms and ions. Elastic scattering, excitation and ionisation were discussed, including those between excited and metastable states. Differential, integral and total cross sections can be calculated. Specific heavy element targets include Hg, Ba, Cs, Y and Zn. Current work includes a non-relativistic formulation adapted to heavy targets by semi-relativistic methods such as intermediate coupling. There are plans to develop a fully relativistic Dirac approach to be initially applied to Hg. The calculation of scattering cross sections from noble gases can be undertaken. Ion atom scattering calculations can also be performed, although the method does have the drawback of being computationally very intensive - the method uses one or two active electrons while the other electrons are treated as a frozen core, in order to make calculations feasible on existing computational facilities,.

Luo Zhengming from the Institute of Nuclear Science and Technology at Sichuan University, China, reported on current experimental measurements of ionization cross sections by electron impact for elements relevant to fusion research, in which efforts are underway to improve the experimental accuracy. Work is progressing to complete studies of K-shell ionisation cross sections for Al, Ti, Fe, Ni, Cu and Mo, while measurements are being made on L-shell ionisation cross sections for Mo, W and Au by electron impact over the energy range from 5 to 30 keV. Plans are also being made to investigate the use of the thick target method to measure K-shell ionisation cross sections for C, N and O with impact electron energies from 2 to 30 keV.

M. Cornille reported on theoretical studies at the Observatoire de Paris, Section de Meudon, France. The Superstructure code is used to calculate energy levels, line strengths and transition probabilities, and the University College London DW code along with JAJOM and JJOM-CBE are being applied to calculate the cross sections for collisional processes. This latter procedure has been used to calculate collision strengths for Ne-like ions important in the study of astrophysical and laboratory plasmas. In addition, calculations have been carried out to determine the ionisation and excitation energies for Xe, Ar and Kr. Radiative probabilities for Ar II-III and Xe II-III have been calculated in the course of constructing a collisional-radiative model. Future work will focus on similar calculations, and the determination of excitation cross sections for Ar^{q+} and Xe^{q+}.

K. Katsonis of the Laboratiore de Physique des Plasmas at the Universite de Paris, France reported on theoretical work involving three programs. A few-body CTMC code has been developed that uses at least three active electrons. The Coloumb approximation is used to generate large amounts of data for modelling purposes. A CR model code for cold plasmas up to 50 eV has also been developed. Cross sections for the collisions between heavy particles can be calculated, in which either atoms, ions or simple molecules can be used as both the target and projectile. Calculations of the cross sections for electron collision can be carried out with any of the above species, along with cross sections for ionization, excitation and charge transfer. Work on transition probabilities includes calculations for noble gases with charge states in the range $0 < q < 8$. with priority for Xe and Ar. Results are compared with data from other methods and experiments.

M. Trzhaskovskaya reported on theoretical work at the Petersburg Nuclear Physics Institute in Russia. Relativistic calculations of atomic structure and processes such as photoionization, photoexcitation, and radiative recombination are being performed. Furthermore, X-ray and other transition probabilities can be determined. Calculational methods include Dirac-Fock-Slater (DFS), Dirac-Fock (DF) and multi-configuration Dirac-Fock (MCDF); Breit and quantum electrodynamic (QED) corrections are taken into account. Relativistic as well as multipole and retardation effects are of importance in calculations for heavy element ions and ions from low to high charge states. Comparisons of the data generated for photo-ionization and radiative recombination by different methods show good agreement with relevant experimental data. Photoionization cross sections have been approximated with high accuracy by simple fitting formulae that involve 5 fitting parameters in the photon energy range from the ionization threshold up to 50 keV. Cases considered include U ions and neutral Ba, as well as many ions of the light elements from He through to Zn.

E. Salzborn of the Institute für Atom-und Molekuelphysik, Justus-Liebig-Universität, Germany, reported on extensive measurements of the cross sections for single and multiple ionization of multiply-charged ions by electron impact in crossed beam experiments. Measurements have been carried out for electron energies up to 1 keV, and charge states up to $q = 10$ for heavy elements. These experiments will continue with new staff, and can be performed for requested elements.

T. Kato reported on research activities at the Atomic and Molecular Data Research Center of the National Institute for Fusion Science in Japan. Experimental activities include plasma spectroscopy and charge exchange spectroscopy, while theory is being applied to the identification of Xe ion lines. Diagnostics are being developed on the basis of observed spectral lines. A CR model for high Z ions will require new calculations of excitation, ionisation, recombination (radiative and DR) and satellite lines. These calculations will be carried out using the HULLAC and FAC codes, and will include data compilations that concentrate on Fe, Xe and Sn.

V. Nikulin reported on work at the Theoretical Astrophysics Department of the Ioffe Physical Technical Institute, Russia. Semi-classical close coupling (CC) equation methods with 2-, 3- and 4-electron quasi-molecular states are used to study the charge transfer and excitation processes. The modelled processes include transfer and excitation in slow collisions of alpha particles with neutral helium and Li-like C^{3+} ions, and neutralization of alpha particles in slow collisions with Be-like C^{2+} ions. Calculations include differential scattering in the above reactions. A theoretical electronic database has been produced that gives the cross sections for single and double electronic capture in collisions of alpha particles in the energy range from 0.2 to 4 MeV with He-like ions C^{4+}, N^{5+} and O^{6+}, and in collisions of He^{+} ions with H-like B^{4+}, C^{5+}, N^{6+} and O^{7+}. Work is underway to obtain data on cross sections in collision of alpha particles with Li- and Be-like ions of oxygen.

B. Den Hartog reported on experimental work at the University of Wisconsin, USA. Measurements have been made of radiative lifetimes and branching fractions in the first and second spectra of many heavy elements. These are combined to yield large data sets of transition probabilities for lines in the UV through to the IR. There will be an expansion of capabilities into the vacuum ultraviolet (VUV) in the near future. Targeted species may include W II, Mo II and Cu I and II, or other species of interest in diagnosing and modelling the divertor region. These would mainly include the first and second spectra of elements of interest, but could extend to the third spectrum in some cases.

W. Wiese of the National Institute for Standards and Technology, USA, summarized work in three programme areas. First, some measurements of highly-charged W and other heavy elements of relevance to fusion are being undertaken with an electron beam ion trap (EBIT). High-resolution Fourier-transform spectroscopic (FTS) measurements of heavy elements in the visible and IR range are also being carried out. There is the flexibility to include first and second spectra of heavy elements of fusion interest in the course of these measurements. Secondly, calculations of ionisation and excitation cross sections with the BEB method of Kim are continuing. Calculations are underway or planned that use the MCHF and MDHF methods to compile large sets of transition probabilities for some lighter elements and their isoelectronic ions, as are calculations using fully relativistic and QED methods for H-like spectra. Thirdly, critical compilations of spectroscopic reference data are continuing, specifically H through B, Na through Ar, all noble gases, various spectra of W and heavy alkalis. The maintenance of annotated bibliographies of spectra also continues.

H. Zhang of the Los Alamos National Laboratory, USA, reported on their relevant theoretical studies. There are two main approaches to cross-section work: a semi-relativistic distorted wave (DW) method starting with atomic structure from Cowans code, and a fully relativistic DW method starting with DFS or the Grant MCDF codes. All processes including transition probabilities, excitation, ionization and recombination data can be calculated. Future work plans of relevance to the study of fusion plasmas include calculations of basic atomic data and emissivity results for many elements, such as Ar, Mo, Xe and Au.

H. Summers reported on work taking place at the Department of Physics and Applied Physics, University of Strathclyde, United Kingdom. Studies are underway on integrated heavy species modelling for ionization states and spectral emissions in plasmas, in which the verification of the modelling in ITER scenarios and current experiments is an important aspect. Contributions to the fundamental database include di-electronic recombination (DR), ionisation, R-matrix calculations, especially pseudo-state radiation damped and fully relativistic calculations along iso-electronic sequences. Advanced population calculations are being carried out in which intermediate coupling (IC) has been unified with charge exchange spectroscopic analysis for medium/heavy species.

3. Data Needs and Recommendations

There will be a variety of impurity elements present in current and future fusion devices. Some elements will enter the plasma through erosion of plasma-facing components, others will enter through injection of material for diagnostic purposes, and some will be introduced through unavoidable contamination. These materials will have specific spectral signatures and, in come cases, will be very efficient radiators of energy (leading to a cooling of the plasma). The theoretical modelling of such behaviour covers an enormous range of elements, ionization stages and processes. Thus, significant efforts were made during the course of the meeting to make reasonable and practical recommendations concerning the scope of work that could be satisfactorily accomplished by an appropriate CRP.

The initial recommendation concerns the specific elements to be considered. Some question arose as to the meaning of “heavy” element, for in some situations anything above helium could be considered heavy. However, for the purposes of a CRP dedicated to impurity elements in fusion, the concept of “heavy” was judged to begin with elements around aluminium or magnesium. Furthermore, through the use of iso-electronic sequences, not all possible elements need be considered in detail if high-quality data are available for nearby elements. The heavy noble gases (Ar, Kr and Xe) were agreed to be of high importance, along with Si, Cl, Cr, Fe, Ni, Cu, Mo and W. While there is also the possibility of using other heavy materials as dopants in wall materials, their identification is not yet known. Furthermore, the meeting participants agreed that it was probably not feasible to include an extremely large list of such elements for detailed consideration by the CRP.

Considerable discussion took place on the possible final product of the proposed CRP. One single CRP cannot produce a complete and comprehensive data set to satisfy all of the modelling needs for heavy elements. However, one extremely valuable activity would be the production of benchmark data for important processes such as transition probabilities, excitation and ionization cross sections, charge transfer processes and recombination processes. Judgement of the validity of modelling calculations depends on comparisons with such benchmarks in order to assess the accuracy of semi-empirical methods and other approximations used in such models. The CRP should focus on using the expertise available to drive such benchmark calculations and measurements, with comparisons made among independent investigations to assess the accuracy of high priority processes for selected ions.

A question arose concerning the charge states for which data would be needed. The two main areas to be considered are the core and edge regions. Edge regions are at relatively low temperatures, and will be dominated by neutral and low-charged ion states. On the other hand, the core will be at a very high temperature, and heavy elements will exist in highly-charged states. Therefore, a very broad range of charged states will need to be considered. However, most of the prominent lines observed in spectral analyses will arise from a few ion stages near the closed shell ions, for example the Li- and Na-like stages. Participants noted the impracticality of modelling transitions from shells such as d^5 due to the enormous number of levels that arise from the coupling of angular momentum. However, there is no requirement to model such shells as they give rise to extreme blending of spectral lines that are not useful in any diagnosis of the plasma. Therefore, work should concentrate on the ion stages that give rise to the most distinct spectral lines.

The important processes to be considered are well known:

- electron collisions - excitation, ionisation and recombination processes that include DR;
- heavy-particle collisions - charge exchange and excitation (for both thermal and beam situations);
- radiative processes - transition probabilities, transition energies and energy levels.

These processes have a spectral range that extends from the infrared (IR) to X-rays. The ideal situation would be for the selected processes of specified ion stages to be measured and calculated with the best experimental and calculational techniques for comparison purposes.

An assessment of the accuracy of all data is a vital requirement in the work - often knowledge of the uncertainties in the data is as important as the numerical values. Modellers need to have the best possible determination of the likely accuracy of the data, so that the model can correctly account for ranges of outcomes likely to occur from the possible uncertainties in the data. Based on the experience of the participants, the best measurements or calculations should strive for an accuracy of 10-20% for the transition probabilities and 0.1% for the transition energies of the radiative processes. However, the cross sections for collision processes are not known to better than a factor of two in many cases. Benchmark measurements and calculations need to be undertaken within the CRP to determine selected important cross sections to within 10-20%, and participants agreed that this was an achievable goal.

All data from the measurements and calculations should be made as widely available as possible through electronic means. Progress continues to be made in the interrogation of multiple databases by means of a continually developing search engine. Participants noted that there is a need for a uniform format for data transfer, and that this issue is being addressed through the evolution of XML standards.

The recommendations concerning the scope of the proposed CRP are outlined in the previous paragraphs of this section. Participants developed and agreed upon these various recommendations during the course of their debate within the technical meeting, and advocated the formation of an appropriate IAEA Coordinated Research Project to achieve the desired database objectives. Thus, the meeting was adjourned on completion of the discussions, and on the understanding that NDS staff would pursue the creation of a well-defined CRP on “Atomic data for heavy element impurities in fusion reactors”.

Appendix 1

IAEA Technical Meeting:
Assess Data Relevant to Spectral Analysis of Fusion Plasmas

13-14 June 2005, IAEA Headquarters, Vienna, Austria

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IAEA Technical Meeting:
Assess Data Relevant to Spectral Analysis of Fusion Plasmas

13-14 June 2005, IAEA Headquarters, Vienna, Austria

Agenda

Monday, 13 June   Meeting Room: ACV - F-01-23

09:30 - 09:50 Opening R.E.H. Clark (Head, A+M Data Unit), A. Trkov (Deputy Head, Nuclear Data Section)
Adoption of Agenda

Session 1:.Current Research

Chairman: K. Katsonis

09:50 - 10:30 B. Den Hartog
Heavy Element Spectroscopic Data for the Plasma Edge

10:30 - 11:10 W. Wiese
The Current Spectroscopic Data Situation for the Heavy Elements

11:10 - 11:30 *Coffee Break*

11:30 - 12:10 M. Trzhaskovskaya
Relativistic Study of Photoionization and Radiative Recombination for Atoms and Heavy Highly Charged Ions

12:10 - 12:50 V. Nikulin
Theoretical Studies of Electron Transfer and Excitation in Atom–Ion and Ion–Ion Collisions

12:50 - 14:00 *Lunch*

Session 2: Current Research (Continued)

Chairman: T. Kato

14:00 - 14:40 E. Salzborn
Electron Impact Ionization of Multiply Charged Ions

14:40 - 15:20 Z. Luo
Experimental Study on Inner Shell Ionization Cross Sections by Electron Impact

15:20 - 15:50 *Coffee Break*

15:50 - 16:30 H. Zhang
Relativistic Distorted-wave Calculations of Atomic Data for Heavy Elements

16:30 - 17:10 D. Fursa
The CCC Method: Current Results and Future Directions

17:10 - 17:50 H. Summers
Heavy Species Modelling in Support of EFDA Planning for ITER Spectroscopy and Spectral Analysis

Tuesday, 14 June

Session 3: Current Research (Continued)

Chairman: H. Summers

09:00 - 09:40 T. Kato
EUV Line Emission Spectra of Xe Ions from Low Density Plasmas

09:40 - 10:20 K. Katsonis
Atomic and Molecular Data for Diagnostics and Modeling

10:20 - 11:00 M. Cornille
Atomic Data for Astrophysics and Plasma Applications

11:00 - 11:30 *Coffee Break*

11:30 – 12:30 All
Summary of Current Research

12:30 - 14:00 *Lunch*

Session 4: Formulation of Specific Objectives for Future Research

Chairman: W. Wiese

14:00 - 15:30 Discussion and Formulation of Objectives (All participants)

15:30 - 16:00 *Coffee Break*

16:00 - 17:30 Summary and Conclusion

17:30 - *Adjournment of Meeting*

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