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Atomic Data for Heavy Element Impurities in Fusion Reactors

Summary Report of First IAEA Research Co-ordination Meeting

IAEA, Vienna, Austria

14 – 15 November 2005

Prepared by

R.E.H. Clark

January 2006

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Abstract

Twelve international experts discussed in detail the properties of heavy elements relevant to fusion energy research participated at the first Research Coordination Meeting (RCM) of the Coordinated Research Project (CRP) on “Atomic data for heavy element impurities in fusion reactors” at IAEA Headquarters on 14-15 November 2005. The participants summarized all recent relevant developments in their research efforts. Detailed discussions took place to formulate specific objectives for the CRP. From a list of data needs and a review of current research capabilities, a detailed work plan was formulated for the first phase of the CRP. The discussions, conclusions and recommendations of the RCM are briefly described in this report.

January 2006

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1. Introduction

The first Research Coordination Meeting (RCM) of the Coordinated Research Project (CRP) on the topic of "Atomic data for heavy element impurities in fusion reactors" was held on 14-15 November 2005 at IAEA Headquarters, Vienna,. The main purposes of this RCM were to review the current research activities of the participants, identify data needs for heavy element impurities, and formulate a work plan for the initial phase of the CRP.

The twelve participants in the CRP are experts in the study and understanding of the various heavy-element processes that are likely to be important in fusion reactor research. The list of participants is included as Appendix A. Each participant gave a summary of their on-going research activities and areas of expertise. A detailed work plan was subsequently formulated, after detailed discussions of fusion needs for atomic data describing the behaviour and impact of heavy element impurities.

2. Meeting Proceedings

A. Nichols (Section Head, Nuclear Data Section) welcomed the participants on behalf of the IAEA. He noted that fusion research continues to be an important topic within the IAEA Nuclear Data Section. The atomic processes within fusion plasmas can involve heavy element impurities that differ significantly and are somewhat lighter than the heavy elements studied within the fission process. He expressed optimism that the CRP would produce valuable data that would support the ITER project and other fusion devices. R. Clark (Scientific Secretary) reviewed the proposed agenda, which was accepted without change (Appendix B).

2.1 Summary of current research activities

Each participant reviewed their research activities and capabilities through presentations to the group. The complete presentations were collected electronically and distributed on CD and also made available through the Internet on the Atomic and Molecular (A+M) Unit home page. Brief summaries of these various research capabilities are given below.

M. Cornille of the Observatoire de Paris, Section de Meudon, France, reported on her theoretical work on atomic structure and radiative properties. She uses the Superstructure code of the University College London (UCL) for the calculation of energy levels, line strengths and transition probabilities. Data for collisional processes are calculated using the UCL distorted wave (DW) codes JAJOM and JAJOM-CBE. Recently, she has calculated collision strengths for Ne-like ions important for astrophysical and laboratory plasmas. She has also recently calculated ionisation and excitation energies for Xe, Ar and Kr, as well as radiative probabilities for Ar II, Ar III, Xe II and Xe III (data that are necessary to construct a collisional-radiative (CR) model). She will continue to focus on similar types of calculations, especially excitation cross sections for Ar^{q+} and Xe^{q+} .

K. Katsonis of the Laboratoire de Physique des Plasmas at the Université de Paris, France, summarized recent theoretical work undertaken with three computer codes. He described a few-body classical trajectory Monte Carlo (CTMC) code using up to three active electrons and adopting the Coloumb approximation. Next, he summarized his CR model code for cold plasmas up to 50 eV. The third code calculates cross sections for the collision of heavy particles with heavy particles (including atoms, ions or simple molecules) as both target and projectile, as well as electron collisions with any of these species. Calculations of cross

sections for ionization, excitation and charge transfer can be carried out. Furthermore, he is able to calculate transition probabilities for noble gas ions with charges in the range $0 < q < 8$, with significant effort and priority focused on Xe and Ar. Comparisons are made with other theoretical methods and experimental observations

T. Kato reported on research activities at the Atomic and Molecular Data Research Center of the National Institute for Fusion Science in Japan. She reported that EUV spectra of Xe ions were observed from LHD plasmas as well as from charge exchange spectroscopy. These spectra were analyzed by comparing with other experiments and theoretical data. The recombination data for Xe¹⁰⁺ ions were also presented. Plans are being made to evaluate the atomic data for Fe ions for the satellite "SolarB", which will be launched next year. EUV spectra of Fe ions from the Sun will be measured by SolarB. A study will be undertaken of the EUV spectra of Fe ions by comparison with the spectra observed from LHD. Experiments are also underway on the topic of plasma and charge exchange spectroscopy. Theoretical studies include the identification of Xe ion lines, and the development of diagnostics using spectral lines. A CR model for high Z ions is also being studied, and will require new calculations of the excitation, ionisation, recombination (radiative and DR) and satellite lines. Calculations will be carried out using the HULLAC and FAC codes, and extensive data compilations will take place. Fe, Xe and Sn are the elements of primary interest.

M. O'Mullane of the Department of Physics and Applied Physics, University of Strathclyde, UK, attended in place of H. Summers. He reported efforts to model integrated heavy species for ionization states and spectral emissions in plasmas. Verification of the modelling capability in ITER scenarios and experiments is a high priority. Plans are being formulated to contribute to the fundamental database, including dielectronic recombination (DR), ionisation, and R-matrix calculations, especially pseudo-state radiation damped and fully relativistic calculations along iso-electronic sequences. Advanced population calculations will be carried out on the basis of intermediate coupling (IC) unified with charge exchange spectroscopic analysis for medium/heavy species.

I. Bray of Murdoch University in Australia attended in place of D. Fursa. He described recent work on theoretical calculations of cross sections using the close coupling method for electron scattering from atoms and ions. Cross sections can be determined for the processes of elastic scattering, excitation and ionisation from the ground state and between excited metastable states. Differential, integral and total cross sections are calculated. The method can be applied to heavy targets such as Hg, Ba, Cs, Y and Zn. The current approach is a non-relativistic formulation adopted to heavy targets by semi-relativistic methods such as intermediate coupling. Future plans include development of a full relativistic Dirac method to be applied to Hg. Calculations for ion atom scattering can also be carried out, but is computationally expensive. The method uses one or two active electrons with others accounted for by a frozen core.

J. Colgan attended in place of H. Zhang of the Los Alamos National Laboratory (LANL), USA. The LANL group plans to use the RATS relativistic code to look at the structure of Xe I-IV. New theoretical approaches include (a) semi-relativistic DW method starting with Cowan's code, and (b) fully relativistic DW method based on DFS or Grant MCDF codes. Both methods could calculate all processes of interest, including transition probabilities, excitation, ionisation and recombination. The group will also participate in the non-LTE workshop IV, and will calculate basic atomic data and emissivities for many elements of relevance to fusion plasmas, including Ar, Mo, Xe and Au.

Luo Zhengming from the Institute of Nuclear Science and Technology at Sichuan University, China, reported on their experimental measurements of ionization cross sections by electron impact. Work is underway to complete measurements of K-shell ionisation cross sections for Al, Ti, Fe, Ni, Cu and Mo. Similar measurements will also be undertaken to determine the L-shell ionisation cross sections for Mo, W and Au by means of electron impact over the energy range from 5 to 30 keV. Efforts are underway to improve the experimental accuracy. A new thick target method is being developed to measure K-shell ionisation cross sections for C, N and O over the 2 to 30 keV energy range.

A. Müller of the Institut für Atom und Molekülphysik, Justus-Liebig-Universität, Giessen, Germany, reported on experiments to measure the cross sections for ionization and recombination processes. Current work includes measurements of electron impact ionization, photoionization and di-electronic recombination (DR) using crossed and merged beams of electrons or photons with single- and multiple-charged ions. Results for single and multiple ionization cross sections and for DR of several species were reported. Use of the principle of detailed balance yields detailed information on recombination cross sections from the studies of photoionization processes and vice versa. Experiments on electron-ion recombination can be performed for almost any charge state of any element requested provided the case is sufficiently strong to be granted beam time at one of the German heavy-ion storage rings. Fusion-relevant recombination studies are performed at the Heidelberg storage ring on medium-charge Fe ions such as Fe¹³⁺. Energies up to 1 keV are possible for the proposed electron-impact ionization measurements. Preparations to extend this range to 5 keV and higher are underway. Target ion charge states up to $q = 15$ can be studied, depending on the heavy element requested. Measurements of single and multiple ionization of Xe⁹⁺ ions by electron impact are classed as high priority.

V. Nikulin of the Theoretical Astrophysics Department of the Ioffe Physical Technical Institute, Russia, reported on recent theoretical work on charge transfer between heavy element ions and alpha particles. Cross sections for charge transfer in collisions of alpha particles and Be-like oxygen were calculated using the close coupling method with thirteen four-electron quasi-molecular basis states in the energy range of 20 keV to 2 MeV. Charge-changing collisions between ions within the beams occur at keV energies due to betatron oscillations. A coupling-state molecular treatment of charge transfer in slow collisions between quadruply-charged bismuth ions in ground and metastable states has been performed. New research will provide theoretical data on the electron transfer and excitation processes in collisions of the multiply-charged metallic impurity ions of Ti, Cr, Fe, Ni, Mo and W with helium atoms in ground and excited states. Cross sections for single and double electron capture, transfer excitation and excitation of helium will be carried out. Work will also take place on the inverse reactions of alpha-particle neutralization in collisions with metallic ions through the quasi-resonant double electron capture, which may be important in cooling of plasmas containing alpha particles.

M. Trzhaskovskaya reported on theoretical work at the Petersburg Nuclear Physics Institute within the Russian Federation. A major programme of work is underway to provide new data for radiative recombination (RR) of heavy impurities with electrons, which is the inverse process of photoionisation. The fully relativistic method will be adopted to calculate partial and total RR cross sections for the ground and excited states of heavy element impurities from neutral to highly charged states. These calculations will use the self-consistent Dirac-Fock method. Relativistic and retardation effects can become large for high ion stages of heavy elements and for high photon energies, so that the fully relativistic treatment is required. Previous calculations have involved the use of the non-relativistic Hartree-Fock method.

Plans include the representation of the cross sections by means of fits to simple analytic expressions. Preliminary calculations of partial and total RR cross sections have been carried out for Ar-like iron.

W. Wiese of the National Institute for Standards and Technology (NIST), USA, summarized work in three programme areas embracing the atomic spectroscopy of heavy elements. Experimental studies are under way to produce and analyze spectra of highly-ionized tungsten with an electron beam ion trap (EBIT); excellent spectra in the extreme UV and soft X-ray region have already been obtained for ions in the range W^{40+} to W^{50+} . A new and expanded critical compilation of spectroscopic reference data for Fe I and Fe II is near completion. Finally, ionization cross-sections for neutral and singly-ionized Mo, W and other heavy elements are being calculated with the binary-encounter-Bethe (BEB) model.

B. Den Hartog reported on experimental work at the University of Wisconsin, USA. Techniques and accomplishments were described involving the measurement of transition probabilities in the first and second spectra of many heavy elements. Recent work in the application of new atomic data to astrophysics problems and progress in the construction of a Spatial Heterodyne Spectrometer were presented. Future plans include quantification of the transition probabilities related to divertor physics. Measurements will be made to produce large data sets of the transition probabilities of heavy elements ranging from UV through to IR. These capabilities will be expanded into the VUV region, and targeted species may include W II, Mo II or other species of interest including I-III spectra

3. Data Needs and Specific Objectives

Following the summary presentations of on-going research, a discussion of the specific goals for the CRP took place. During the course of this debate, a detailed work plan was developed, with each participant identifying and agreeing their possible contributions, as noted below.

3.1. Scope of the CRP

Participants agreed that the CRP should consider relevant elements heavier than Mg. Primary elements of interest include the noble gases (Ar, Kr and Xe), Si, Cl, Cr, Fe, Ni, Cu, Mo and W. Two main areas to be addressed are the edge and core regions, because the charge states found in these two regions differ dramatically due to their very different temperatures. Atoms are dominated by neutrals and low ion states in the edge region, while the core region gives rise to highly-charged ion states. Since the atoms found in one region of the machine are likely to migrate throughout the plasma, data will be needed for nearly all stages of ionization.

3.2. Fusion plasma processes

The important processes in the modelling of fusion plasmas include collision and radiative data (in which the collision data include both electron and heavy-particle collision processes). Participants agreed that the important processes were as follows:

Collision data: electrons: excitation, ionisation, recombination including DR;
heavy particles: charge exchange and excitation (thermal and beam).
Radiation data: transition probabilities, transition energies and energy levels, ranging from IR to X-rays.

Participants stressed the vital need to assess the accuracy of all of the data. Often the knowledge of the uncertainty of the data is as important as the numerical value. The following were determined to be realistic goals with respect to the accuracy of the data:

Radiative processes: probabilities of 10-20%, and transition energies of 0.1%;
Collision processes: realistically, the general goal should be better than a factor of 2; benchmark data of 10-20%.

3.3. Identification of tasks

With the important elements and processes specified, well-defined goals were matched with the expertise of the participants. The following specific tasks were identified as having a high probability of being achieved by the time of the next RCM.

Radiative processes:

1. Calculation of energy levels and transition probabilities of Ar I-IV for a limited number of multiplets. Cornille can carry out calculations using the SST and FAC codes. Katsonis will carry out similar calculations using the CbA method for comparison. Kato agreed to look into adding comparisons with the results from the HULLAC code. Comparisons with results from the LANL non-relativistic (CATS) and relativistic (RATS) codes will also be included. NIST will critically compile all available energy level and transition probabilities for Ar I-XVII.
2. Katsonis will work on similar calculations for Xe II-IV using the CbA code (non-relativistic), while LANL will make comparisons with the relativistic RATS code (wavelength and transition probability data to be compared). Cornille will compare the FAC and SST results for these ions, and NIST will provide the latest compilation of energy levels and make these data available on their Web site. Kato has spectra for Xe IX-XXVI; some lines cannot be identified from the NIST compilation, but there appear to be insufficient resources at present to address this issue.
3. NIST compilations similar to Xe are under consideration for Ar and Kr, with a time scale of 2-3 years
4. Separate issues include data on W I and II for influx issues, as well as the other ion stages. NIST is in process of compiling structure data for W I and II. Den Hartog will measure W II transition probabilities (relatively extensive data already exist for W I). NIST is undertaking measurements with EBIT of tungsten spectra in high stages of ionisation, roughly from W XXX to W LXXII, and is carrying out a compilation of W spectra. There will be many gaps in the spectra, but this compilation will include new data for ionisation energies at accuracies of better than 1%.
5. Although of some importance, other heavy elements are of lower in priority in this CRP.
6. The Kato group plans to study the EUV spectra for iron ions (mainly Fe IX-XV), as well as some others. They will measure the wavelengths – a model should be developed for these lines to assist in plasma diagnostics.

Collisions:

(a) Electron collisions

1. Colgan and Bray will calculate cross sections for electron impact excitation and direct ionisation for Na- and Mg-like Si, Cl and Ar, using the CCC and TDCC codes for comparison. Estimates of inner core ionizations will be provided as well. Badnell will also contribute in this area.
2. The thick substrate method can be extended to inner shell ionisations of all neutral elements. Important questions to be addressed will include: is there a way to correlate the ionisation from the solid to atoms in gas? is the inner shell ionisation insensitive to this effect?
3. NIST will attempt to calculate total ionisation cross sections for several ion stages of W with the BEB method, but no detailed calculations are foreseen.
4. R-matrix calculations of excitation for several isoelectronic sequences are planned by the ADAS group: H-, He-, Li- and F-like, terminating at Kr. Relativistic structure calculations will also be undertaken to push these studies to higher Z. Decisions will be made concerning the cases for comparison (elemental and transitions).
5. Mueller will measure ionisation cross sections, with single and multiple ionisation of Xe^{1+} to Xe^{15+} as the main priorities. Measurements for tin will also be explored, along with DR and radiative recombination for Fe^{8+} , Fe^{13+} , Fe^{14+} and Fe^{16+} .
6. The Kato group will compile and evaluate atomic data for iron ions, including ionization excitation, recombination and DR. Results will be applied to the CR model (may also prove possible to calculate data by means of the HULLAC and FAC codes).

(b) Heavy-particle collisions

1. Nikulin will undertake a theoretical study of state-selective single and double electron capture, transfer excitation and excitation in collisions of closed shell Ti^{4+} , Cr^{6+} and Fe^{8+} ions with helium atoms in the ground and excited states. The relative collision energies will be in the keV range, which is important for the plasma edge and neutral helium beam diagnostics.
2. Nikulin agreed to study alpha-particle neutralization in slow collisions with C^{2+} and Ti^{2+} through double electron capture and alpha-particle collisions with O^{4+} ions in the MeV energy range.

(c) Photoionization and recombination

1. Trzhaskovskaya will carry out extensive relativistic calculations for partial and total radiative recombination and photoionization cross sections for many elements, including Fe, Ni, Cu, Mo and W, from neutral through highly-charged states (to be determined). The Dirac-Fock method will be used, and computed sub-shell cross sections will be fitted by a simple analytical expression that uses a few fitting parameters.
2. Photoionization cross sections could be calculated by Bray for select examples, if necessary. Mg-like Si cross sections could be compared as a test case.

4. Concluding Remarks

Extensive discussions during the course of the first RCM on “Atomic data for heavy element impurities in fusion reactors” resulted in the formulation of detailed work plans for the initial activities of the participants and co-workers. The important elements and their processes were identified, and quantification of these data through experimental and theoretical studies were matched with the expertise of the CRP members (see section 3). Specific objectives were agreed for the overall CRP programme, and in preparation for the second RCM in approximately 18 months.

**First IAEA Research Co-ordination Meeting on
Atomic Data for Heavy Element Impurities in Fusion Reactors**

14-15 November 2005, IAEA Headquarters, Vienna, Austria

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**First IAEA Research Co-ordination Meeting on
Atomic Data for Heavy Element Impurities in Fusion Reactors**

14-15 November 2005, IAEA Headquarters, Vienna, Austria

Agenda

Monday, 14 November

Meeting Room: A-26-43

09:30-10:00 Opening, Adoption of Agenda, A. Nichols, R. Clark

Session 1: Progress Reports I

Chairman: J. Colgan

10:00-10:30 M. Cornille
Application of detailed quantum codes in the evaluation of rare gas ions
radiative transition probabilities

10:30-11:00 K. Katsonis
Transition probabilities for low ionization stages of Ar and Xe

11:00-11:30 *Coffee Break*

11:30-12:00 T. Kato
EUV spectra of Xe ions and atomic data for Fe ions

12:00-12:30 M. O'Mullane
Atomic data and modelling for analysis of heavy impurity behaviour in
fusion plasmas

12:30-13:00 I. Bray
Convergent close-coupling approach to atomic collisions

13:00-14:00 *Lunch*

Session 2: Progress Reports II

Chairman: M. Cornille

14:00-14:30 J. Colgan
Calculation of atomic collision data for heavy elements using perturbative
and non-perturbative techniques

14:30-15:00 Z. Luo
L-shell ionization cross section measurements for some heavy elements by
low-energy electron impact

- 15:00-15:30 A. Müller
Absolute cross sections for ionization, excitation and recombination from interacting-beams experiments
- 15:30-16:00 *Coffee Break*
- 16:00-16:30 V. Nikulin
Electron transfer in collisions between heavy element ions, alpha particles, and helium atoms in plasma and in beams
- 16:30-17:00 M. Trzhaskovskaya
Radiative recombination and photoionization processes involving heavy element impurities in plasma
- 17:00-17:30 W. Wiese
Spectroscopy projects at NIST on heavy elements
- 17:30-18:00 B. Den Hartog
Heavy element transition probability data of interest in astrophysics and divertor physics

Tuesday, 15 November

Session 3: Review of Current Status

Chairman: I. Bray

- 09:00-12:30 All
Comprehensive review of current status, including proposed areas of data needs
- 12:30-14:00 *Lunch*

Session 4: Formulation of Work Plan for CRP

Chairman: M. O'Mullane

- 14:00-17:00 All
Formulation of work plan for first two years if CRP.
- 17:30 - *Adjournment of Meeting*

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