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Atomic Data for Heavy Element Impurities in Fusion Reactors

Summary Report of the second Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

26 – 28 September 2007

Prepared by

R.E.H. Clark

January 2008

IAEA Nuclear Data Section, Wagramer Strasse 5, A-1400 Vienna, Austria

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Abstract

Ten experts on the properties of heavy elements of relevance to fusion energy research participated in the second Research Coordination Meeting (RCM) on Data for Heavy Element Impurities in Fusion Reactors, held at IAEA Headquarters on 26-28 September 2007. Participants summarized their accomplishments with respect to the work plan formulated at the first RCM. This overall work plan was reviewed in detail, achievements were noted, and the plan was subsequently modified to reflect the current state of research. Discussions, conclusions and recommendations of the RCM are briefly described in this report.

January 2008

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Introduction

A second Research Coordination Meeting (RCM) of the Coordinated Research Project (CRP) on atomic data for heavy element impurities in fusion reactors was held on 26-28 September 2007 at IAEA Headquarters, Vienna. The agreed aims of this RCM were to review the work plan formulated at the first RCM, and modify the contents in the light of recent research studies.

Nine of the CRP participants and one observer (Ch. Berenguer of Universite Paris Sud) attended the RCM. The list of participants is included as Appendix A. Each participant presented a summary of work performed since the first RCM. Progress within the CRP was assessed, and the work plan was extended on the basis of the various achievements.

Meeting Proceedings

A. Nichols (Section Head, Nuclear Data Section) welcomed the participants on behalf of the International Atomic Energy Agency (IAEA). He noted the good progress reported during the course of the previous RCM, the importance of the data for ITER, and expressed confidence that the CRP would produce timely and useful new data.

R. Clark (Scientific Secretary) reviewed the proposed agenda. Due to the inability of Prof. O'Mullane to attend, some of the discussion topics were moved from the third day to the afternoon of the second day. Under these circumstances, the modified agenda was adopted (see Appendix 2). Each participant gave a detailed presentation of their research activities carried out during the second phase of the CRP (see Appendix 3 for the short abstracts). These presentations were collected and distributed on CD. The accomplishments of the first 18 months of the CRP were discussed in detail, and the evolving work plan was modified accordingly. Final conclusions from the RCM were formulated and agreed.

V. Nikulin presented theoretical studies of charge transfer processes in collisions of heavy element ions, helium atoms and alpha particles. New data have been generated by means of close-coupling methods. Results were presented from calculations of the partial and total charge transfer cross sections of the collision of Ti^{3+}, Cr^{6+} and Fe^{8+} with helium atoms in their ground and metastable states. Cross sections for alpha-particle neutralization through quasi-resonant double electron capture were also determined. Detailed results from all calculations were presented in graphical form, and have been published in journals and a series of internal reports.

M. Trzhaskovskaya presented her work on the radiative recombination and photoionization cross sections of heavy elements. These calculations are fully relativistic, and were based on the Dirac-Fock method. Cross sections for thirty-one ions of Fe, Ni, Cu, Mo and W were calculated over an electron kinetic energy range of 4 eV to 50 keV. The important stages of ionization stages included closed shell ions, which persist over wide ranges of temperature. Photoionization cross sections from subshells have been fitted to a simple analytic form that contained five fit parameters. All results have been tabulated and published in journals and internal reports.

W. Wiese summarized work at NIST on the spectroscopic properties of heavy elements. Three topics were covered: results of a new critical compilation of atomic transition probability data for Fe I and Fe II have been graphically compared with previous work; calculations for the ionization and excitation cross sections of neutral and singly-ionized Mo and W have been performed by means of the Binary-Encounter-Bethe(BEB) method (this project has halted due to the recent tragic death of Y.-K. Kim); extensive work has been carried out to observe and analyze important parts of the EUV and soft X-ray spectra of very highly-charged ions of tungsten (charges in the range from 40 to 60) by means of the NIST electron beam ion trap (EBIT). Characteristic features were analyzed and explained on the basis of theoretical atomic structure methods. The possibility of using particular line ratios of highly-charged tungsten ions as a density diagnostic for very hot plasmas was also discussed. Other recently completed NIST work on tungsten include a compilation of structure data for W I and W II, and a new analysis of the ionization energies for all W ions to an accuracy of approximately 0.5 percent.

A. Müller presented measurements of cross sections for the electron impact ionization and recombination of heavy element ions. He described the crossed beam experiments at the Institut für Atom- und Molekülphysik, Giessen in detail. The effect of metastable states on the measured cross sections was demonstrated, and the results of measurements of electron impact ionization cross sections for xenon were shown on one graph for the first 15 stages of ionization. Storage rings minimize the effects of the metastable states. Results for the recombination of Fe^{13+} and Fe^{14+} were presented, while preliminary data for Fe^{7+} and Fe^{8+} are undergoing analysis. Results for Si^{3+} are being prepared for publication.

H. Zhang and co-workers have undertaken distorted wave calculations of cross sections for electron impact excitation and ionization of heavy elements. He gave an overview of the Los Alamos codes for structure and cross section calculations. Cross sections have been calculated for excitations from fine structure levels with n = 1, 2 and 3 to levels with n = 2, 3 and 4 for H-like through to Mg-like silicon, chlorine and argon ions. Calculations of electron impact ionization in the configuration average mode among the same set of n values were also carried out. Time-dependent close-coupling calculations of ionization cross sections for Si^{2+} and Si^{3+} in the ground and first excited configuration were compared with distorted wave calculations and experimental data. Fully relativistic calculations of K-shell ionization cross sections for several elements were compared with the experiments of Luo. Fully relativistic distorted wave calculations were carried out for 16 optically-allowed transitions among levels with n = 2 in Be-like ions with Z = 26–92. Structure properties for all ions were also determined.

I. Bray described convergent close-coupling calculations (CCC) for collisions of electrons, positrons, photons, protons and anti-protons with atoms. He described the main features of the CCC method, along with the procedure for converging to a solution. This method has been applied to a number of extremely challenging cases with impressive results. Long-standing discrepancies between theory and experiment have been solved through these comparisons, and the procedure is being expanded in many ways to become a very robust calculation tool.

K. Katsonis presented recent work from GAPHYOR on collisional radiative (CR) models for rare gases with application to fusion plasmas. Calculations of radiative wavelengths and transition probabilities were carried out by means of several computational tools, and the resulting data compared with available measurements. Electron impact cross sections were also calculated on the basis of both the distorted wave and first-order-many-body theories, and the two resulting sets of data compared. These data were used in a CR model to generate synthetic spectra which were compared with several sets of experimental results. The positions and relative strengths of the dominant lines were in good agreement with experiment, although the experiments were not always in steady state situations.

M. Cornille summarised the findings of a series of extensive comparisons and evaluations of transition probabilities for rare gases. Calculations of energies and transition probabilities were carried out by means of the Superstructure and the Flexible Atomic Codes (FAC). Extensive comparisons were made of Xe I to III for several multiplets in each ionization stage. The main features of the two codes were described, and a number of comparisons were shown. Individual lines in these ionization stages are difficult to identify and characterise. Small errors in the energy levels do occur, and the definition of levels can prove to be problematic due to extensive target state mixing. There are also significant differences between the two codes. Considerable reliance is placed on such calculations for many data used in CR models, and this situation constitutes a significant problem that needs to be addressed.

T. Kato reported on recent work on Xe and Fe spectra, and anticipated data needs for ITER. A small quantity of Xe gas was injected into the Large Helical Device (LHD) and the Xe spectrum was observed during heating, steady plasma conditions and radiative collapse and cooling. Theoretical calculations were carried out by several routes, including the GRASP, HULLAC and Cowan structure codes. Lines from Xe^{23+} to Xe^{25+} were observed during the heating process, while lines appeared to originate from the Xe^{8+} to Xe^{17+} ionisation stages when cooling. New lines were identified for Xe^{16+} and Xe^{17+} in the 12 to 16 nm range. Additional unidentified Xe lines were also observed over the 4 to 16 nm range in JT60U. A theoretical model is planned for the Xe ion emissions of LHD and charge exchange spectroscopy by the ECR source. Considerable work has taken place to characterise the spectral line intensities of Fe XIII, and a large number of cross sections for electron impact excitation and ionization have been compared. Many additional cross sections are needed because the current experimental database is not sufficient for the satisfactory development of a CR model. Atomic data needs for ITER were reviewed in which the edge region was judged to be of high importance, along with seeded impurities.

Review and Update of Work Plan

The work plan from the first RCM was reviewed and re-assessed. Progress and updates were noted for each task. Results of this review are presented below.

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 by means of both the Superstructure (SST) and the Flexible Atomic Codes (FAC). Katsonis will undertake similar calculations with the CbA method for further comparison. Kato agreed to look into the possibility of generating results from the HULLAC code. Equivalent data from the LANL non-relativistic (CATS) and relativistic (RATS) codes will also be included in this exercise. NIST will critically compile all available energy level and transition probabilities for Ar I to XVII.

> **Progress:** Calculations of transition probabilities have been carried out by using experimental energies in the CbA code for Ar I – V; SST calculations have also been made - these results were better for Ar than for Xe. Data from CATS calculations were compared with the experimental energies and transition probabilities and equivalent CbA data and, and were often found to be satisfactory. The RATS code is not expected to give good results for Ar I – V stages, and therefore no calculations have been undertaken for these cases. NIST is close to completing a new comprehensive compilation of all available energy levels and radiative transition probabilities for all stages of ionization, which will contain several thousand transitions.
>
> **Update:** SST and FAC are judged to be inadequate. Therefore, the proposal has been made to carry out additional comparisons of CATS results with GRASP2, as well as all other available data. CATS, CbA and some experimental data exist for many of the ion stages, but results still need to be generated from GRASP2. Katsonis will produce graphs similar to those of the NIST comparison exercise, and Cornille will run some GRASP2 calculations. LANL will also carry out further calculations; data exist for Ar VII – Ar XVIII, and LANL staff will continue to perform CATS calculations down to the neutral species. NIST will complete a critical compilation of energy levels and transition probabilities for all Ar ions.

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 to be made available on their web site. Kato has observed spectra for Xe IX to XXVI; some lines cannot be identified from the NIST compilation, but there appear to be insufficient resources to address this issue at the present time.

Progress: Calculations have been carried out with the CbA code for Xe I – V, along with equivalent studies with GRASP2 for Xe III to VI. Data generated by the CATS code appear to be satisfactory for all the ionization stages considered. SST calculations have been undertaken for all ionization stages, but the results are unsatisfactory; FAC data are also inconsistent for these ions, while the RATS calculations for Xe II and III are in poor agreement with the other studies. NIST staff have finished a compilation of energy levels for these stages of ionization. Kato found many lines are still missing for Xe XVII and XVIII, while other ion stages were satisfactory.

Update: GRASP2 calculations will be carried out by Jun Yan in collaboration with Katsonis for Xe III to VII. Comparison graphs will be prepared for GRASP2 and CATS, as well as other data. Kato is comparing data from GRASP and CATS for Xe XVII. The NIST compilation is completed, and nothing more will be done in this particular area over the next 18-month period of the CRP.

3. NIST compilations are under consideration for Ar and Kr, with a time scale of two to three years.

   Progress: New compilation for Kr has been completed and published.

   Update: NIST compilation will soon be placed on the web.

4. Existing issues include data describing W I, II and other ion stages for influx issues. NIST staff are in the process of compiling structure data for W I and II. Hartog will measure W II transition probabilities (relatively extensive data exist for W I). NIST is undertaking measurements with EBIT of the ionisation energies of W III to LXXII, and is assembling a compilation of W spectra; there will be many gaps in the spectra, but the compilation will include new data for ionisation energies at accuracies of better than 1%.

   Progress: W I – II - NIST has completed a structure compilation based on earlier work with JAERI (now JAEA). Hartog was not able to secure funding for the comparative experimental programme, so no results have been produced yet. NIST has undertaken a new analysis of the ionization energies for all W ions to an accuracy of the order of 0.5%. NIST and JAEA staff have produced a compilation of energy and wavelength data for all available W ions representing approximately 40 ions out of a total of 74.

   Update: Results for transition probabilities will depend on funding possibilities. NIST has completed the compilation of structure data for W I and II and ionisation energies for all W spectra to an accuracy of better than 1%. EBIT measurements will continue at NIST on highly-ionized W spectra up to W LXIV.

5. Although of some importance, other heavy elements have been assessed at a lower priority.

   Progress: NIST is compiling transition probabilities for all ionization stages of Cl.

6. The Kato group plans to study the EUV spectra for iron ions (mainly Fe IX – XV), and also some others. Wavelengths will be measured – a model needs to be developed to quantify these lines and assist in plasma diagnostics.

   Progress: Fe UV spectra have been observed for Fe IX – XV charge states in the LHD. A model for Fe XIII plasma diagnostics has been produced. Solar and EBIT data are also available.

   Update: A CR model for Fe XIII has been produced to aid in plasma diagnostics. An evaluation of the atomic data is now in progress. NIFS is collaborating with the EBIT in Tokyo to measure the wavelengths of iron ions.

Collisions

I. Electron collisions

1. Colgan and Bray will calculate the cross sections for electron impact excitation and direct ionisation of Na- and Mg-like Si, Cl and Ar by means of convergent close-coupling (CCC) and time-dependent close-coupling (TDCC) codes for comparison. Estimates will also be made of inner core ionization cross sections. Badnell will contribute in this area.

   Results: Data for CCC have not been completed for these ions, but a major rewrite of the program has been undertaken and a relativistic code produced. LANL staff have completed calculations for electron impact direct excitation and direct ionization for Mg-like through to H-like Si, Cl and Ar by means of CATS/ACE. Benchmark comparisons of Si III and IV with TDCC for ionization from ground level have been carried out. Inner shell ionizations were included for some stages of ionization.

   Update: Depending on the ion, non- relativistic and relativistic CCC calculations will be carried out for Na- and Mg-like ions of a number of elements, including those listed above. The electron Na data are ready to be published in *At. Data Nucl. Data Tables*. LANL will extend the calculations for these three elements to the neutral stage. All data will undergo evaluation.

2. The thick substrate method can be extended to inner shell ionisations of all neutral elements. Important questions to be addressed include: is there a way to correlate the ionisation from the solid to atoms in the gas phase? Is the inner shell ionisation insensitive to this possibility?

   Results: Luo was unable to attend the RCM. LANL did some relativistic calculations of K-shell ionization cross sections of Mn I, Fe I, Ni I and Cu I, and L-shell calculations of W I for comparison with the experimental results of Luo - relatively good agreement was observed.

   Update: LANL calculations indicate that correlation effects are not significant, since the independent atom results agree well with experiments to within the level of accuracy of the measurements. No further calculations are anticipated unless new experiments are performed.

3. NIST will attempt to add total ionisation cross sections for several ion stages of W by means of the BEB method, but no detailed calculations are foreseen.

   Progress: NIST calculated BEB ionization cross sections (and derivatives) for W I and II out of the ground state and some excited metastable states. W II data were compared with Giessen experiments, and good agreement was found. No comparisons were possible for W I.

   Update: W I and II cross section calculations have been completed, and no further work is anticipated.

4. R-matrix calculations of excitation cross sections for several isoelectronic sequences are planned by the ADAS group: H-, He-, Li- and F-like that will terminate at Kr. Relativistic structure calculations will also be undertaken to extend these studies to higher Z. Decisions will be made concerning comparison by element and transition.

   Results: Unfortunately, the ADAS representative was unable to attend the RCM; hopefully, the results will be made available at a later date. The CCC method will be applied to H-, He- and Li-like ions in the near future.

   Update: Await report from ADAS group.

5. Mueller will measure ionisation cross sections, with single and multiple ionisation of Xe^{+} 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+}.

   Progress: Cross sections for single ionization of Xe II – XVI have been measured at Giessen. Selected multiple ionization cross sections are also available. Some results are available for several charge states of Sn, while measurements of recombination are complete for Fe XIV and XV and Si IV.

   Update: A series of studies of the single ionization of Xe ions in different charge states will be completed. All accessible multiple ionizations for Xe ions will be measured, and recombination data will be finalized for Fe VIII, IX and XVII. As a general test of the procedure, an attempt will be made to measure the ionization of C IV and V in a storage ring from threshold to several keV; if successful, further data will be measured, especially for Fe ions. Use of the storage ring would eliminate the problem of metastable ions in the beam.

6. The Kato group will compile and evaluate atomic data for iron ions, including ionisation, excitation, recombination and DR. Results will be applied to the C-R model (may also be possible to calculate data by means of the HULLAC and FAC codes).

   Progress: A compilation has been completed of the ionization and recombination data for all ionization stages of Fe, as far as they are available. Work has focused on Fe XIII excitation during this phase of the project, although the group plans to extend the study to other charge states.

   Update: Comparisons are being made between the ionization, recombination and excitation data. Detailed data evaluations will be carried out for Fe XIII, along with proton excitation of the fine structure levels of M-shell Fe ions.

<u>II. Heavy particle collisions</u>

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 plasma edge and neutral helium beam diagnostics.

   Progress: Close-coupling calculations have been carried out for electron transfer cross sections in collisions of Ti^{4+}, Cr^{6+} and Fe^{8+} ions with the helium atom in the ground and metastable states.

   Update: Close-coupling calculations will be performed for state-selective electron transfer, transfer excitation and helium excitation cross sections in slow collisions of He atoms in the ground state with Si V, Ni V, Cu VI, Mo VII and W VII ions. An investigation will be completed of alpha-particle neutralization through quasi-resonant double electron capture in the metastable states of He atoms in slow collisions with Si V and Ti V impurity ions. Results will be tabulated for inclusion in electronic databases.

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.

   Results: Cross sections have been obtained for alpha-particle neutralization in slow collisions through quasi resonant double electron capture into the $1s^2$ ground state of helium in slow collisions with C III and Ti III ions. Electron capture and excitation cross sections were calculated for collisions of alpha particles with Be-like oxygen ions in the energy range from 0.2 to 2 MeV. Cross sections were also determined for charge transfer and excitation in slow collisions between Bi V ions in the ground and metastable states.

III. 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 to highly-charged states (to be determined). The Dirac-Fock method will be used, and computed subshell cross sections will be fitted by a simple analytical expression that adopts few fitting parameters.

    Progress: Results have been obtained over an electron energy range of 4 eV to 50 keV for most ion stages of W VII – LXXIV, Mo VII – XLII, Cu XII – XXIX, Ni XI – XXVIII and Fe IX – XXVI. Results were obtained for the ground state and excited states up to n = 20 and for all angular momentum states that make significant contributions (> 0.1%) to the total radiative recombination. The approach used in these calculations was analyzed with models and results from other sources. Computed subshell photoionization cross sections were fitted as a function of energy with an analytical expression that used five fitting parameters.

    Update: Calculations of the radiative recombination and photoionization cross sections will be carried out for closed shell ions of several elements with Z < 13 as well as for Si, Cl, Ar, Ti, Cr, Kr and Xe. The fitting of partial photoionization cross sections will be performed. Calculations of RR rate coefficients for a number of elements of the significant interest to fusion research will be undertaken. An investigation will be made of the impact of specific relativistic and multipole effects on photoionization and RR cross sections and recombination rate coefficients.

2. If necessary, photoionization cross sections could be calculated by Bray for selected examples. Mg-like Si cross sections could be compared as a test case.

    Progress: Photoionization cross section calculations have not been carried out for ions. Is there a need for these cross sections for fusion applications?

    Update: CCC calculations will be undertaken in response to requests for data comparisons and benchmarks.

IV. CR model comparisons

As an additional task, CR model calculations will be carried out using different data sets for radiative and collisional data, as taken from LANL, GAPHYOR, NIST and other sources, to compare with experimental measurements of spectra and radiated power. A comparison will be made between the LANL and Katsonis CR modeling codes.

Recommendations and Conclusion

Considerable progress has been made in all elements of the work plan adopted at the first RCM. Modifications have been made to this work plan on the basis of the work undertaken and the progress achieved in addressing the agreed data needs. The CRP is well on the way to fulfilling the goals as set forth in the original proposal. Communications from several ITER representatives indicate that the work plan of the CRP is of high importance to ITER at their current stage of development.

Data generated from the CRP are already being published in the appropriate leading journals, and have been assembled in convenient forms for use in modelling tools. The participants of the CRP have formed good working collaborations, and have communicated their results to the A+M Data Unit. Thus, a successful conclusion to the CRP is anticipated and envisaged by mid-2009.

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Scientific Secretary: R.E.H. Clark

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Appendix 2

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

26–28 September 2007, IAEA Headquarters, Vienna, Austria

Scientific Secretary: R.E.H. Clark

Meeting Agenda

Wednesday, 26 September **Meeting Room: ACV U1 U 636 0**

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

Session 1: Progress Reports I

Chairman: K. Katsonis

10:00 – 10:45 V. Nikulin
Electron Transfer and Excitation in Collisions between Heavy Element Impurity Ions and Helium Atoms

10:45 – 11:15 *Coffee Break*

11:15 – 12:00 M. Trzhaskovskaya
Radiative Recombination and Photoionization Cross Sections for Heavy Element Impurities in Plasmas

12:00 – 14:00 *Lunch*

Session 2: Progress Reports II

Chairman: V. Nikulin

14:00 – 14:45 W. Wiese
Spectroscopic Research Projects on Heavy Elements at NIST

14:45 – 15:30 A. Müller
Experimental Cross Sections for Electron-impact Ionization and Electron-ion Recombination

15:30 – 16:00 *Coffee Break*

16:00 – 16:45 H. Zhang
Distorted-wave Cross Sections of Electron-impact Excitation and Ionization for Heavy-element Impurities in Fusion Reactors

Thursday, 27 September

Session 3: Progress Reports III

Chairman: **T. Kato**

09:30 – 10:15 I. Bray
Convergent Close-coupling Approach to Atomic Collisions

10:15 – 10:45 *Coffee Break*

10:45 – 11:30 K. Katsonis
Application of Rare Gases Collisional-Radiative Models to Fusion Plasmas Optical Diagnostics and Modeling

11:30 – 12:15 M. Cornille
Evaluation of Rare Gas Transition Probabilities

12:15 – 14:00 *Lunch*

Session 4: Progress Reports IV

Chairman: **M. Trzhaskovskaya**

14:00 – 14:45 T. Kato
EUV Spectroscopy from LHD and Atomic Data

14:45 – 15:15 *Coffee Break*

Session 5: Review of Current Status

Chairman: **A. Müller**

15:15 – 17:00 All
Comprehensive Review of Current Status, Including Proposed Areas of Data Needs

Friday, 28 September

Session 6: Review and update of Work Plan for CRP

Chairman: **W. Wiese**

09:30 – 12:30 All
Evaluation and Modification of Work Plan for Final Two Years If CRP

12:30 – 14:00 *Lunch*

Session 6: (Continued)

14:00 – 17:00 All

17:00 Adjourn

Appendix 3

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Scientific Secretary: R.E.H. Clark

SUMMARIES OF THE WORK PERFORMED

Electron Transfer and Excitation in Collisions between Heavy Element Impurity Ions and Helium Atoms

V. Nikulin

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New theoretical data on the partial and total cross sections for electron transfer, transfer excitation and excitation for collisions of Ti^{4+}, Cr^{6+} and Fe^{8+} ions with helium atoms in the ground states were obtained by using the close-coupling method with thirteen (Ti^{4+}) and eleven (Cr^{6+}, Fe^{8+}) two-electron quasi-molecular states in the energy range of impurity ions from 4 to 400 keV. The partial and total cross sections of electron transfer into n-shells of Ti^{3+} (n = 5–8), Cr^{6+} (n = 6–9), and Fe^{8+} (n = 8–11) ions were calculated for the first time for collisions of the impurity ions with helium atoms in metastable states based on seventeen (Ti^{4+}) and ten (Cr^{6+}, Fe^{8+}) one-electron quasi-molecular states.

New data on the partial and total cross sections for electron transfer and target excitation in collisions of alpha particles with the Be-like oxygen ions were obtained for the first time in the energy range of 0.2 to 2 MeV. The cross sections of alpha particle neutralization through quasi-resonant double electron capture at their slow collisions with C^{2+} and Ti^{2+} were calculated. The above calculations were performed by solving the close-coupling equations on the basis of thirteen (O^{4+}) and nine (C^{2+}) four-electron and thirteen (Ti^{2+}) two-electron quasi-molecular states.

Data on the cross sections are needed both to simulate the behaviour of alpha particles in plasma and for plasma core spectroscopic diagnostics. The emission from the excited metallic impurities and helium ions produced in the collisions are of interest for plasma edge diagnostics.

Pioneering theoretical data for single-electron charge transfer and excitations due to collisions between Bi^{4+} ions in the ground (6s) and metastable (6p) states were obtained in the collision energy interval 5 to 75 keV in the centre-of-mass frame. Gaining insight into charge transfer between identical low-charged heavy ions at their collisions due to betatron oscillations is vital to design of accelerators and storage rings to generate intense ion beams. Such beams can also find application in heavy-ion-driven inertial fusion.

Radiative Recombination and Photoionization Cross Sections for Heavy Element Impurities in Plasmas

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We have performed fully relativistic calculations of total cross sections for the radiative recombination of heavy element impurities with electrons, and subshell photoionization cross sections for 31 ions of Fe, Ni, Cu, Mo and W, as important elements in plasma studies. The electron wave functions were determined by means of the Dirac-Fock method, with exact consideration of the exchange interaction between electrons. Adequacy of the model and accuracy of the calculations were analyzed and assessed. Electron kinetic energy range is 4 eV to 50 keV. The total radiative recombination cross section was obtained by calculation of the subshell cross sections for ground and all excited electron states up to states with principal quantum number n = 20. Subshell photoionization cross sections for excited states with $n \leq 12$ and orbital momenta $\ell \leq 6$ were fitted by a simple analytical expression with five fitting parameters. Fits were produced in the photon energy range from 4 eV above the ionization threshold E_{th} to the k_{max} energy where the photoionization cross section falls by five orders of magnitude as compared with the maximum value. Usually, $k_{max} \leq 100E_{th}$ for the s, p, d and f shells, and $k_{max} \leq 10E_{th}$ for the g, h and i shells. As a rule, fitting was carried out with good accuracy when the relative root-mean-square uncertainty was ≤ 2%. The total radiative recombination cross sections and the fit parameters for the subshell photoionization cross sections were presented in tabular form.

Spectroscopic Research Projects on Heavy Elements at NIST

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Three spectroscopic research projects of the NIST Atomic Spectroscopy Group will be discussed: (1) an updated and somewhat expanded critical compilation of spectroscopic reference data for Fe I and Fe II, mainly on improved transition probabilities, will be reviewed; (2) calculations of ionization and excitation cross sections of neutral and singly ionized Mo and W with the Binary-Encounter-Bethe (BEB) model will be reported; (3) extensive efforts have been made by several members of our group to observe and analyze the important parts of the spectra of numerous highly charged ions of tungsten, using the NIST Electron Beam Ion Trap (EBIT) as our principal experimental instrument.

Experimental Cross Sections for Electron-impact Ionization and Electron-ion Recombination

A. Müller

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Recombination of highly charged ions with free electrons has extensively been studied in experiments at heavy-ion storage rings. Dielectronic recombination of highly charged iron ions is a special topic within the recombination study programme, and is the subject of a long-standing research collaboration project between groups from Giessen University, Max-Planck-Institute for Nuclear Physics in Heidelberg, and Columbia University. The Heidelberg heavy ion storage ring TSR has been employed to measure absolute high resolution cross sections and rate coefficients with uncertainties of the order of 20%. The talk will provide an overview of these experiments, particularly the data on Fe^{13+} and Fe^{14+}.

Electron-impact ionization experiments are carried out at Giessen using a crossed-beams technique. Single and multiple ionization has been investigated for numerous singly and multiply charged ions. Absolute cross sections are being measured for ions in the xenon and tin isonuclear sequences and high-resolution energy scans of normalized ion yields have been recorded to provide the detailed energy dependences of electron-impact ionization cross sections. Both single and multiple ionization processes are addressed. The present status of these experiments will be discussed, particularly the cross section measurements for single ionization of Xe^{+} through to Xe^{15+}.

Distorted-wave Cross Sections of Electron-impact Excitation and Ionization for Heavy-element Impurities in Fusion Reactors

Hong Lin Zhang, J. Colgan, C. Fontes and J. Abdallah Jr.

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We present calculations performed for heavy element impurities in fusion energy. Most calculations for electron-impact excitation and ionization were undertaken by means of both the semi-relativistic and the fully relativistic distorted-wave approaches. The semi-relativistic method was used to calculate: (1) excitation transitions from $n = 1$, 2 and 3 levels to $n = 2$, 3 and 4 levels in H-like through Mg-like silicon, chlorine and argon ions; (2) collisional ionization for the ground levels in these ions; (3) configuration-average collisional ionization among all configurations included in the targets; and (4) energy levels and electric-dipole transition probabilities or oscillator strengths. The time-dependent close-coupling method was also used to compute electron-impact ionization cross sections for Si^{2+} and Si^{3+} from both the ground and first excited configurations. Some comparison of these data with the distorted-wave results, as well as with experiments where available, will be shown. The fully relativistic method was used to calculate K-shell ionization of neutral Mn, Fe, Ni and Cu, and L-shell ionization of neutral W for comparison with experiment. Finally, we will present the fully relativistic distorted-wave collision strength results for 16 optically allowed $\Delta n = 0$ transitions with $n = 2$ in Be-like ions with Z = 26–92. This new calculation uses the fully-relativistic Kummer transformation in place of the earlier semi-relativistic Coulomb-Bethe approximation for the "top-up" contribution, and yields more accurate results for high energies. These results will replace the corresponding data published earlier.

Convergent close-coupling approach to atomic collisions

Igor Bray

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Our interest is in the collision of electrons, positrons, photons, and (anti)protons with atoms. The convergent close-coupling (CCC) method formulates the problem as coupled Lippmann-Schwinger equations in momentum space for both the non-relativistic and relativistic cases. This formulation relies on a complete Laguerre basis which ensures that convergence may be studied systematically by simply increasing the basis size. An outline of the CCC method will be given, and extensive comparison with experiment will be presented.

Application of Rare Gases Collisional-radiative Models to Fusion Plasma Optical Diagnostics and Modelling

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Radiation emitted from various plasmas, along with detailed Collisional-Radiative (C-R) models, must be used in the development of the optical diagnostics of plasmas that cannot be assumed to be in Local Thermodynamic Equilibrium (LTE). We are specifically interested in the application of C-R models for diagnostics and modelling of fusion plasmas. Previously, we have developed C-R models for Ar and Xe plasmas of relatively low temperature which were applied to the study of various devices, including the WEGA Stellarator, two SPT-50 prototype plasma thrusters and some dedicated experiments conceived for their validation. As an extension to our earlier models, we have developed C-R models that include spectra of orders IV to IX; these models cover the entire range of population of the outer p^6 and s^2 shells of the rare gases. We are working to validate these models and to apply them to various rare gas plasmas encountered in fusion research.

Evaluation of Rare Gas Transition Probabilities

M. Cornille[1], C. Berenguer[2], K. Katsonis[2] and R.E.H. Clark[3]

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Transition probabilities together with the cross sections of excitation by electron collisions are the main parameters in the definition of the line intensity within each ionization stage. Our interest is in the Ar and Xe ions. Energy levels, wavelengths and radiative transitions probabilities have been calculated using two different numerical codes: SuperSTructure (SST) developed by Eissner and collaborators, and the Flexible Atomic Code (FAC) developed by Gu. The multiplet spectra of Xe II are presented as an example (5p-5d, 5p-6s, 6s-6p), and are compared with the results obtained by the CbA code based on the Coulomb Approximation developed by Katsonis, and with the equivalent data obtained by the Cowan Atomic Code (CATS).

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