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Atomic Data for Heavy Element Impurities in Fusion Reactors

Summary Report of the final Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

4–6 March 2009

Prepared by

R.E.H. Clark
International Atomic Energy Agency, Vienna, Austria

April 2009

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Abstract

Eleven experts on the properties of heavy elements of relevance to fusion energy research attended the final Research Coordination Meeting (RCM) on Data for Heavy Element Impurities in Fusion Reactors, held at IAEA Headquarters on 4-6 March 2009. Participants summarized their accomplishments with respect to the revised work plan formulated at the second RCM. The overall work plan for the CRP was assessed and reviewed in detail, and achievements were noted. Discussions, conclusions and recommendations of the RCM are briefly described in this report.

April 2009

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1. Introduction

The final Research Coordination Meeting (RCM) of the Coordinated Research Project (CRP) on atomic data for heavy element impurities in fusion reactors was held on 4-6 March 2009 at IAEA Headquarters, Vienna. The agreed aims of this meeting were to review the work plan formulated at the second RCM, and to report on and assess the results of the CRP.

Ten of the CRP participants and one observer (Ch. Berenguer of Universite de Paris Sud) attended the meeting. The list of participants is given in Appendix 1, while the Agenda is included as Appendix 2. Each participant presented a summary of work performed since the first RCM, and their abstracts are included as Appendix 3. Overall results achieved within the CRP were assessed, and conclusions to the CRP were formulated and agreed.

2. Presentations and Proceedings

D. Abriola (Deputy 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 CRP, the importance of the data for fusion research, and expressed confidence that timely and useful new data would be reported as a consequence of this final RCM.

R. Clark (Scientific Secretary) reviewed the proposed agenda, which was fully adopted (see Appendix 2). Each participant gave a detailed presentation of their research activities carried out during the final phase of the CRP. These presentations were collected and made available for download to memory sticks. Copies of the presentations are also available on the Atomic and Molecular (A+M) Data Unit home page. Accomplishments of the CRP were discussed in detail, and final conclusions were formulated and agreed.

J. Colgan of the Los Alamos National Laboratory (USA) provided an overview of the achievements from the Los Alamos group over the five years of the CRP. He reviewed the calculational tools adopted during these studies, including theoretical methods. Los Alamos now maintains a web interface to the codes, allowing users world wide to carry out calculations. A number of comparisons with experiments and other theoretical calculations within the CRP have been carried out, showing good agreement and providing a high level of confidence in the calculations. Los Alamos data have been used in calculations of radiative cooling losses in the solar corona, with the inclusion of many ions of heavy elements. The results compare favourably with other calculations and reinforce the level of confidence in the current data. Results from Los Alamos are in the process of tabulation for inclusion in the IAEA A+M databases, with preliminary files already sent for verification of format. Data will also be archived at Los Alamos, with accessibility through the web-based interface to the calculational tools.

I. Bray of Curtin University of Technology (Australia) described calculations of cross sections using the convergent close coupling (CCC) method. Such calculations are important in fusion plasma studies and also have applications in astrophysics, the lighting industry and materials research. These research studies also provide a more rigorous foundation for collision theory. The theoretical basis for the CCC method was briefly reviewed, including the extension to relativistic theory. A number of comparisons of the CCC results to experiment and other theory were shown. CCC theory performs extremely well in matching with experiment, even for cases in which other theoretical approaches have difficulties. For regimes in which methods such as distorted wave (DW) are expected to be reasonable, the agreement between DW and CCC is good. Examples were shown for a large number of ions of elements of interest to fusion. Data calculated during the course of the CRP will be made available to the IAEA A+M Unit, and will also be placed on the web site at Curtin University.

A. Müller of the Institut für Atom- und Molekülphysik, Universität Giessen (Germany) presented results from measurements of electron impact ionization and recombination for a number of ions. Colliding beam techniques have been developed and used by Müller and co-workers for over thirty years - beam densities for ions are many orders of magnitude lower compared with targets of neutrals, making such measurements much more challenging. A crossed-beams apparatus with ten years of successful operation was used at Giessen. The method for determining the overlap of the two beams was described, the overlap being crucial in determining the absolute cross sections. Results were compared with DW and CCC calculations. Details of cross-section studies as a function of energy were discussed, including the presence of metastable states and resonances. Total cross sections for single ionization of xenon ions through to the +25 stage were presented, representing an improvement of ten ion stages over what was originally thought to be possible. Multiple ionizations were measured - double ionization is often significant compared with single ionization, and can dominate under certain conditions. The electron-ion recombination data reported at the meeting were obtained at the Heidelberg heavy-ion storage ring. Large discrepancies between theory and experiment at low energies for the more complex ions were noted. Iron ions in high charge states were normally addressed, and the large amount of data from this work will be included in the IAEA A+M databases.

M. Trzhaskovskaya of the Department of Theoretical Physics, Petersburg Physics Institute (Russia) described calculations of radiative recombination and photoionization cross sections as well as radiative rates. The cross sections have been calculated by means of fully relativistic Dirac-Fock (DF) theory. Such calculations of radiative recombination are normally not fully relativistic and only take into account the dipole effects. The present work takes account of relativistic effects and all important multipoles. Comparisons with the dipole show that these effects can become important at energies of a few keV, depending on the shell and ionization stage. The method has been applied to 68 ions of elements from silicon to tungsten that are of high importance to fusion studies, and comparisons made with other theoretical calculations. These results compare well with other relativistic calculations where available, and show the increasing importance of relativistic corrections at high energies. Data have been fitted to analytic forms for ease of use in calculations. All results have been tabulated and prepared for inclusion in the IAEA A+M databases.

V. Nikulin of the Division of Plasma Physics, Atomic Physics and Astrophysics of the Ioffe Physical Technical Institute (Russia) summarized work accomplished on charge exchange and excitation of heavy elements in collision with helium ions and alpha particles. Close coupling theory was adopted, based on two or many electron quasi-molecular states. The effective potential was defined in terms of screened diatomic molecular orbitals (SDMO). New data important for charge exchange recombination spectroscopy were obtained for collisions between helium atoms in the ground state and a large number of impurity ions up to tungsten. Partial and total cross sections of electron capture for Ti^{3+}, Cr^{5+} and Fe^{7+} in collisions with helium in metastable states were calculated for the first time. Results have been compared with other calculations where possible. Calculations of alpha-particle neutralization through quasi-resonant double electron capture in slow collisions with C^{2+} and Ti^{2+} were carried out for the first time. Cross sections for electron capture and excitation in alpha-particle collisions with Be-like oxygen were determined. Results have been compared with other calculations where possible. Data have been tabulated, and are available for inclusion in the IAEA A+M databases.

Zhu Jingjun of Sichuan University (China) presented work on measurements of electron inner shell ionization cross sections for heavy element impurities. Problems of target fabrication in self-supporting thin targets were noted, and improvements included the adoption of thin targets with a thick substrate. A correction on the re-ionization contribution in the thin target by electrons reflected from the substrate has been performed by means of the bipartition model of analytical electron transport theory. Adjustments for multiple scattering or mean track length were performed by means of the Monte Carlo method. The thickness of the target has been determined by Rutherford backscattering spectroscopy (RBS), and efficiency calibration of the Si(Li) detector was undertaken by comparing the experimental and theoretical (PENELOPE code) thick carbon target bremsstrahlung spectra produced by electron impact. An overall uncertainty for the experiment was estimated to be 10% to 15%. This method has been applied to the measurement of inner shell ionization cross sections of a number of important elements for fusion. The results have been compared with that of other groups and theories for each measured element. Specifically for Mn, Fe, Ni, Cu and W, results have been compared with Los Alamos calculations, and were shown to be in good agreement, giving confidence that the inner shell ionization process can be measured accurately in this experimental arrangement. Thick target studies involved the introduction of the Tikhonov regularization method and classical molecular dynamics (CMD) to resolve the inverse problem. The K-shell ionization cross sections of Ni and Si have been measured and compared with measurements from other groups and theoretical results. The data from this set of experiments have been tabulated, and can be included in the IAEA A+M databases.

W. Wiese of the National Institute of Standards and Technology (NIST) (United States) reviewed the work on spectroscopic data for heavy elements and collision calculations for atoms and molecules. NIST uses an electron beam ion trap (EBIT) for measurements of the properties of highly-charged ions. The EBIT device is able to hold ions in place for long periods of time and reaches very high stages of ionization, currently up to the +68. NIST EBIT has been used to observe spectra for a number of ion stages of heavy elements of interest to fusion research, particularly tungsten for which extensive data tables are now available. Collisional ionization cross sections have been calculated using the binary encounter Bethe (BEB) method developed by Kim (deceased). This method is continuing to be applied to new ions and molecules by co-workers of Kim. Measurements of transition probabilities and wavelengths of many transitions in chlorine have been carried out by means of the wall-stabilized arc. Data from these experiments are in the process of being tabulated for inclusion in the NIST databases.

T. Kato of the National Institute for Fusion Science (NIFS) (Japan) described work on plasma diagnostics by spectra from the large helical device (LHD) and studies of atomic data. Line intensities in carbon ions have been quantified in connection with radiative collapse of plasmas in LHD. CV line intensity ratios are affected by recombination at the end of the plasma. Observations of CV line ratios in non-radiative collapse indicate the existence of an ionizing plasma even after the neutral beam injection (NBI) has ended, which implies the motion of ions towards the centre at the end of the NBI. Some line ratios differ from theoretical predictions for CV, indicating the need for better atomic data even for this system. Iron is an important impurity in many fusion devices, and specific EUV spectral lines were examined for use in density diagnostics. Work on data compilation and evaluation for iron is ongoing at NIFS, and spectra from higher Z elements have been studied. Calculations were carried out using the atomic structure code of Cowan and compared with spectra, allowing identification of a number of lines. Compilation work on data for electron and atom collisions is continuing at NIFS, with a number of new compilations completed and available.

H. Summers of the University of Strathclyde (UK) described the systematic production of baseline heavy element atomic data. Due to the complexity of open shells in heavy elements, most spectral work will most likely focus on ion stages with one or two electrons outside a closed shell. Many states can be lumped together for other ion stages. The main requirement will be to get useful spectral properties for a few ion stages as well as the total radiated power from all ions. Modelling codes are limited in the amount of data that can be used, and a balance must be struck between size and retaining the important physics. The method developed in the ADAS system for an automated method of generating data was described. Baseline sets of data use less sophisticated approximations, but can be upgraded as needed, and the automated system can generate data for many energy states in all stages of ionization. The resulting data could be combined into super stages, lumping energy levels and ion stages together in regimes where only radiated power is important, but retaining detail within spectra to be analysed. Comparisons have been made of the approach with encouraging results. Baseline data can be used to reformulate the combining of states, and the baseline datasets can be upgraded.

K. Katsonis of the Université Paris-Sud (France) discussed work in progress on the calculation of transition probabilities of argon and xenon species for optical diagnostics and modelling of fusion plasmas. Transition probabilities are important in the analysis of spectral lines of plasmas and, together with cross sections for collision processes, are the main determinants of the theoretical spectra calculated using collisional-radiative (CR) models. Atomic energy levels and transition probabilities have been calculated for a number of ion stages of argon and xenon. Calculations were carried out by means of several computer codes including CbA (coulomb approximation code), the Los Alamos CATS code, and the GRASP and SST codes. Results have been compared, and graphs of comparisons were shown. CATS results were found to be reasonably reliable, and could be generated easily through the online interface. CR models were carried out by adopting calculated data – there was generally good agreement between the resulting theoretical spectra and experimental observation. There are plans to connect the CR model to transport calculations, but such an effort would be a long-term project. M. Cornille, who had not been able to attend the meeting, had contributed to these studies and the work on collision cross sections presented by Ch. Berenguer.

Ch. Berenguer of the Université Paris-Sud (France) presented calculations of electron impact excitation cross sections for the lower energy levels of Ar I and Xe I. The resulting cross sections were integrated over a Maxwellian electron distribution to obtain rate coefficients as a function of electron temperature. Rate coefficients are used as input to a CR code, and the results for transitions from the ground p^6 and excited s^1 shells of argon and xenon were presented. Several calculations were carried out for comparison - Los Alamos codes were used in both distorted wave (DW) and first-order many-body theory (FOMBT) mode, as well as adopting different amounts of mixing of basis states. A quasi-classical (QC) evaluation was used following numerical solutions of the few-body problem, as well as the semi-empirical formula of Drawin, as adapted by Katsonis for rare gas atoms. Comparison of the DW and FOMBT was made to assess the effect of the choice of potential in the weak coupling approximation. Calculations using the QC and semi-empirical method were based on experimental energies and transition probabilities with the Coulomb approximation. Experimental data and other calculations were also included when available. The DW and FOMBT calculations were generally in good agreement, and mixing effects converged with relatively few configurations. FOMBT results were found to be preferable, and were calculated by means of the online interface to the Los Alamos codes. Resulting rate coefficients were used in CR calculations and are in the process of being compared to experiment. Large amounts of data are needed for many stages of ionization for a full CR model calculation.

3. Review and Update of Work Plan

The work plan from the second RCM was reviewed, and the outcome from each task identified. All items from the original work plan are listed below with updates from the second RCM, followed by the final outcome in italics.

Radiative Processes

1. Calculation of energy levels and transition probabilities of Ar I to 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 by means of 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 adopting experimental energies in the CbA code for Ar I to V; SST calculations have also been carried out - 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 were often found to be satisfactory. The RATS code is not expected to give good results for Ar I to 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 to 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.

Calculations have been completed as per the above specifications. Comparisons of calculations with GRASP have been made. Results are available for Ar I to V. Non-relativistic calculations were generally satisfactory, relativistic less so.

Results were not as satisfactory for the lower stages of ionisation. At higher energy and higher stages of ionisation, calculations were carried out with both SST and FAC, but need to be completed. A selection will be made of cases to be compared. Calculations have also been carried out for xenon.

2. Katsonis will work on similar calculations for Xe II to 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 to 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.

Results are available for Xe I to V. For 4p – 4d transitions of Xe XVII and XVIII, Kato group have undertaken line identification, and the results were published in JPB (2008).

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.

The work on krypton will be published as an electronic paper – J. Phys. Chem. Ref. Data (JPCRD). Studies involving the argon compilation are nearly complete.

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 and 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.

A complete ionisation energy table for all ions of tungsten to 0.5% precision has been compiled and is also available in JPCRD. There has been no further contribution from the Lawler group due to lack of funding. EBIT measurements have been completed for highly ionised tungsten spectra and published for W+40 to W+63

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.

NIST has nearly finished compilation for all ionisation stages of chlorine. Many gaps in energy levels have been filled. New experiments have been conducted on Cl I and results published in Phys. Rev. A.

6. The Kato group plans to study the EUV spectra for iron ions (mainly Fe IX to 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.

Measurements of iron species have been extended to Fe XXII and XXIII. Collisional radiative models have been carried out spanning the iron species from Fe+12 to Fe+21. Line ratio studies for diagnostic analysis were carried out for carbon ions C III to V and for iron ions Fe XIII and XXII.

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 be made of inner core ionization cross sections. Badnell will also 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.

Extended DWBA calculations (threshold to 100*threshold) to the neutral stages of Si, Cl and Ar. All stages have been published in PRA for ionisation and excitation. Data are being formatted for inclusion in the databases.

Cross-sections were calculated for H-, He-, Li-, Na- and Mg-like ions of the requested elements by means of the CCC method. The relativistic CCC (RCCC) method has been developed and applied to highly-ionised H-like ions. Data for ionisation and excitation are available (see web site) and have been used to compare with DWBA and experiment. Generally good agreement has been found.

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 research coordination meeting. LANL carried out 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.

The measurement of ionisation cross sections on a number of elements has been performed. K-shell data for S, Cl, Ca, Zn, and L shell data for W, Bi, Ba, Gd have been measured by means of the thin target on substrate method. The thick target method was used for measurement of K-shell ionisation of Ni and Si.

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.

A further calculation was carried out for Ar I ionisation and excitation cross sections by means of the BEB and plane wave Born (scaled) methods.

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 research coordination meeting; 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.

Electron impact excitation data for He-, Li- and F-like ions were completed and published (approximately 20 ions in each sequence). Emphasis was placed on the iso-electronic sequence behaviour. Comparative codes were set up under ADAS for detailed examination of outliers, etc.

A new action was taken on providing a comprehensive baseline of data for collisional-radiative modelling of all heavy species, semi-automatically. This capability is being incorporated in ADAS.

5. Müller 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 to 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.

Measurements of single ionisation cross sections of Xe+1 to Xe+22 from threshold to 1000 eV were completed and preliminary data are available on Xe+23 to Xe+25. Multiple ionization data are available for a selection of charge states. A publication is in preparation.

Recombination data are available for Fe^{+7} to Fe^{+10} and Fe^{+13} to Fe^{+16}, and most of the results have been published.

Data for carbon are under analysis and not yet ready for delivery.

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.

Data evaluation of proton impact fine structure redistributive collisions has been made for Fe X to XV and Fe XVII to XXIII. These are published in the NIFS data series (nos. 95 and 99). Data evaluations for electron impact excitation for Fe X, Fe XI and Fe XIII were carried out and published in the NIFS data series (no 104). Data evaluation for electron impact ionization is in progress.

<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 III and Ti III impurity ions. Results will be tabulated for inclusion in electronic databases.

New data for partial and total cross-sections for single and double electron capture, transfer excitation and target helium excitation in collisions of impurity ions Ti+4, Si+4, Ni+6, Cu+6, Mo+6, W+6 with helium atoms in the ground state were obtained in the energy range of impurity ions from 4 to 800 keV.

Cross-sections of alpha particle neutralization through the quasi-resonant double electron capture into metastable 1snl states of helium in slow collisions with Ti+2 ions were completed. Study of alpha particle collisions with Si+2 ions is in progress.

An electronic database for cross-sections has been prepared for fifteen collision systems.

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 to LXXIV, Mo VII to XLII, Cu XII to XXIX, Ni XI to XXVIII and Fe IX to 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.

Relativistic calculations in the Dirac-Fock method of the radiative recombination and photo-ionisation cross-sections for thirty six ions of Si, Cl, Ar, Ti, Cr, Kr and Xe were completed. Photo-ionisation cross-sections were fitted to an analytical expression and the fitting parameters are included in the database.

Radiative recombination rate coefficients for nine W ions from Pd-like to bare nucleus were calculated in a wide temperature range (from 10^3 -10^{10} K).

Relativistic and multipole effects were shown to be important in calculations of radiative recombination cross sections and rates at high energies. A new relativistic expression for rate coefficients was found on the basis of the relativistic Maxwell-Juettner distribution. This correction is very important at high temperatures. The results obtained in 2008 were published in five papers.

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.

<u>IV. CR model comparisons</u>

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 modelling codes.

Clark and Katsonis comparisons were made for Ar.

4. Recommendations and Conclusions

The work plan for the coordinated research project has been substantially completed. Large quantities of data were measured and calculated, and have been tabulated in electronic form – these data are already available on several databases, and will be included in the IAEA A+M database. A number of very important comparisons were made between experiment and theory and among different theories in order to assess the validity of the different techniques. Data have been applied to collisional-radiative models and used in analysis of spectra observed in different plasma devices. As planned, the overall result of the CRP is a significant increase in the available data for heavy element impurities in fusion devices.

Much more data are needed for the modelling of fusion plasmas, and a single coordinated research project cannot be expected to completely fulfill all such data needs. Significant additional data are needed for many ionization stages of elements such as the inert gases and tungsten. The participants agree that additional benefit would be gained from initiating another CRP at a future date to concentrate on tungsten, in light of the importance of this element in future fusion devices and the extreme complexity of the energy levels of the numerous tungsten ions.

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

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Appendix 2

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

Agenda

Wednesday, 4 March **Meeting Room: A-27-74**

09:30 – 10:00 Opening, Adoption of Agenda: D. Abriola, R. Clark

Session 1: Progress Reports I

Chairman: H. Summers

10:00 – 10:45 J. Colgan
Atomic data for heavy elements relevant to magnetic fusion and astrophysics using the Los Alamos atomic physics codes

10:45 – 11:15 *Coffee Break*

11:15 – 12:00 I. Bray
Convergent Close-Coupling calculations of electron-impact ionisation of intermediate and highly charged ions

12:00 – 14:00 *Lunch*

Session 2: Progress Reports II

Chairman: T. Kato

14:00 – 14:45 A. Müller
Experimental cross sections for electron-impact ionization and electron-ion recombination

14:45 – 15:30 M. Trzhaskovskaya
Radiative recombination and photoionization cross sections for heavy element impurities in plasmas

15:30 – 16:00 *Coffee Break*

16:00 – 16:45 V Nikulin
Charge exchange and excitation in collisions of heavy-element impurity ions with helium atoms and alpha particles in fusion reactors

16:45 – 17:30 Zhu Jingjun
Electron-impact inner shell ionization cross section measurements for heavy element impurities in fusion reactors

Thursday, 5 March

Session 3: Progress Reports III

Chairman: I. Bray

09:30 – 10:15 W. Wiese
Three highlights of the recent NIST spectroscopic research on heavy elements

10:15 – 10:45 *Coffee Break*

10:45 – 11:30 T. Kato
Plasma diagnostics by spectra from LHD and Atomic data

11:30 – 12:15 H. Summers
Systematic heavy element atomic data production for fusion applications

12:15 – 14:00 *Lunch*

Session 4: Progress Reports IV

Chairman: A. Müller

14:00 – 14:45 K. Katsonis
Transition Probabilities of Ar and Xe Species for Optical Diagnostics and Modelling of Fusion Plasmas

14:45 – 15:15 *Coffee Break*

15:15 – 16:00 C. Berenguer
Electron Collision Excitation of the Lower Ar I and Xe I Levels

Friday, 6 March

Session 5: Review of Results of CRP

Chairman: W. Wiese

09:00 – 12:30 All
Comprehensive review of results from the CRP

12:30 – 14:00 *Lunch*

Session 6: Summary and Conclusion of CRP

Chairman: J. Colgan

14:00 – 17:00 All
Formulation of CRP summary and conclusion, data collection and APID reports

17:00 *Adjourn*

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

4–6 March 2009, IAEA Headquarters, Vienna, Austria

Abstracts of Presentations

Atomic Data for Heavy Elements Relevant to Magnetic Fusion and Astrophysics Using the Los Alamos Atomic Physics Codes

J. Colgan, H.L. Zhang and C.J. Fontes

Los Alamos National Laboratory, USA

An overview will be given of the recent progress made in computing atomic data for elements relevant to magnetic fusion and astrophysics using the Los Alamos suite of atomic physics codes. A recent paper has described the electron-impact excitation and ionization cross sections that were computed for all ion stages of Si, Cl, and Ar [1]. Another recent study computed all excitation and ionization processes (in the configuration-average approximation) for all ion stages of fifteen elements that are found in the solar corona [2]. These data were used to compute the radiative losses of the Sun for a range of astrophysical conditions. Both of these projects will be discussed at the meeting.

[1] J. Colgan, C. J. Fontes and H. L. Zhang, *Phys. Rev. A* **77**, 062704 (2008).
[2] J. Colgan, J. Abdallah, Jr., M. E. Sherrill, M. Foster, C. J. Fontes and U. Feldman, *Astrophysical Journal* **689**, 585 (2008).

Convergent Close-Coupling Calculations of Electron-impact Ionisation of Intermediate and Highly Charged Ions

I. Bray

Curtain University of Technology, Australia

The Convergent Close-Coupling (CCC) method is applied to the calculation of electron-impact total ionisation cross sections for H-, He-, Na- and Mg-like ions. For low to intermediate charges the non-relativistic CCC method is used. For higher charges a relativistic CCC implementation has been applied with a Breit or Moller correction. Comparisons with the distorted wave Born approximations (DWBA) are often very good, even when electron exchange is very important.

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

Alfred Müller

Institut für Atom- und Molekülphysik, Universität Giessen, Germany

The talk reports on colliding-beams measurements of cross sections for electron-impact single and multiple ionization of Li^{+} and Xe^{q+} ions and of rate coefficients for electron-ion recombination of Si^{3+} and Fe^{q+} ions. Investigated charge states, q, are between 7 and 22 for recombination at the heavy-ion storage ring in Heidelberg and between 1 and 25 for ionization at our crossed-beams apparatus in Giessen. The energy ranges of the measurements vary from threshold up to 1000 eV in the ionization experiments and cover the most important di-electronic resonances above 0 eV in the recombination measurements. The latter comprise data up to several hundred eV depending on the system and the core transitions investigated.

The experimental data will be compared with theoretical calculations. Agreement between predictions and observations is not always satisfying. Problems in the interpretation of experiments often arise from unknown fractions of metastable ions in the primary beams, even at storage rings, where the ions have at least several seconds of time to decay before a measurement starts. Problems in the theoretical treatment often arise from the complexity of ionic structures and the multiplicity of intermediate states that can contribute to the final observation channel. Resonances apparently play an important role not only in recombination but also in the ionization channels.

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

M.B. Trzhaskovskaya[1], V.K. Nikulin[2] and R.E.H. Clark[3]

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[2]*Division of Plasma Physics, Atomic Physics and Astrophysics,*
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[3]*Nuclear Data Section, International Atomic Energy Agency, Austria*

We present calculations and studies performed in the framework of CRP. First, the unified database of the radiative recombination cross sections and photoionization cross sections for the heavy element impurity ions has been supplemented with 36 ions of Si, Cl, Ar, Ti, Cr, Kr, and Xe which are of importance in fusion studies. The fully relativistic calculations have been performed within the Dirac-Fock method taking into account all multipoles of the radiative field. Second, we have studied the impact of multipole and a number of relativistic effects on photoionization and recombination cross sections as well as the radiative recombination rate coefficients. For the first time, the relativistic expression for the rate coefficient has been found on the basis of the relativistic Maxwell-Boltzmann distribution instead of the commonly used non-relativistic distribution. This decreases the recombination rate coefficient considerably in hot plasmas. Third, with this expression, we have calculated partial and total rate coefficients in a wide temperature range for highly-charged tungsten ions which are of great current interest while the relevant data are not available.

Charge Exchange and Excitation in Collisions of Heavy-element Impurity Ions with Helium Atoms and Alpha Particles in Fusion Reactors

V. Nikulin

Division of Plasma Physics, Atomic Physics and Astrophysics of the Ioffe Physical Technical Institute, Russia

Theoretical data for heavy-element impurities obtained in accordance with the Coordinated Research Project will be discussed. New data on the partial and total cross sections of single and double electron capture, transfer excitation and excitation in collisions of impurity ions Si^{4+}, Ti^{4+}, Cr^{6+}, Fe^{8+}, Ni^{6+}, Cu^{6+}, Mo^{6+} and W^{6+} with helium atoms in the ground state were obtained in the energy range of impurity ions 4 ÷ 800 keV. The partial and total cross sections of electron capture into n-shells of Ti^{3+} (n = 5–8), Cr^{5+} (n = 6–9), and Fe^{7+} (n = 8–11) were calculated for the first time in collisions of the impurity ions with helium atoms in metastable states.

The cross sections of the alpha particle neutralization through the quasi-resonant double electron capture into ground ($1s^2$) and metastable (1snl) states of He atoms in their slow collisions with Ti^{2+} ions were calculated for the first time. Data on the partial and total cross sections for the single electron capture and target excitation in collisions of alpha particles with the Be-like oxygen ions were obtained in the high energy range 0.2 ÷ 2 MeV.

Data for charge exchange and excitations in collisions due to betatron oscillations in the ion beams between the Bi^{4+} ions in the ground (6s) and metastable (6p) states were obtained. The fraction of metastable ions in the beams was estimated by comparison of our theoretical data with Giessen experimental results for the total charge exchange cross sections. Gaining insight into charge exchange between identical heavy ions at their collisions due to betatron oscillations is vital to designing accelerators with the aim to generate the intense ion beams.

All calculations of the charge exchange and excitation cross sections in ion-atom collisions were carried out in the framework of the close-coupling equation method involving basis of the many-electron quasi-molecular states.

Electron-impact Inner Shell Ionization Cross Section Measurements for Heavy Element Impurities in Fusion Reactors

Zhu Jingjun

Sichuan University, China

By using the method for thin targets on a thick substrate, we have measured the electron-impact inner-shell ionization cross sections near the threshold energies for the following elements and shells: S-K, Cl-K, Ca-K, Zn-K, W-Lα, Lβ, Bi-Lα, Lβ, Ba-Lα and Gd-Lα. The total uncertainties are estimated to be ~10% to 15%. By using the thick-target method, we measured the K-shell ionization cross sections near the threshold energies for Ni and Si element. The estimated total error is about 10%. The effect of surface roughness on the measurement of lepton impact inner-shell ionization cross sections in the thick-target method has also been studied by using Monte Carlo simulations.

Recent NIST Spectroscopic Research on Heavy Elements

W. Wiese

National Institute for Standards and Technology, Gaithersburg, USA

Three highlights of the recent NIST spectroscopic research on heavy elements will be presented, which are: the experimental work with our Electron Beam Ion Trap on very highly charged tungsten ions of charge states 54 to 63, with accompanying theoretical analysis; measurements of the transition probabilities of numerous lines of neutral chlorine with a wall-stabilized arc; and calculations of ionization and excitation cross sections for some noble gases. Also, I will give a summary of all pertinent NIST spectroscopic compilation work during the duration of this CRP.

Plasma Diagnostics by Spectra from LHD and Atomic Data

T. Kato

National Institute for Fusion Science, Toki, Japan

We have observed EUV spectra from the Large Helical Device (LHD) at the National Institute for Fusion Science (NIFS). We measured spectra of impurity ions; carbon, iron, xenon, tin and tungsten ions. In some cases, the plasma evolution was stable and a steady discharge was obtained, but sometimes the plasma underwent radiation collapse and rapid cooling. For carbon and iron spectra, we studied plasma diagnostics by intensity ratios of spectral lines. For other spectra of higher Z element, xenon, tin and tungsten, we studied mainly on line identifications comparing with theoretical calculations and experimental data. Related atomic data for these researches will be also discussed.

Systematic Heavy Element Atomic Data Production for Fusion Applications

Hugh Summers

University of Strathclyde, Glasgow, Scotland, UK

The presentation summarises and illustrates a series of steps which have been implemented for handling heavy elements in magnetic confinement fusion plasma models and spectroscopic diagnostics. The primary objective of establishing an adequate complete baseline of data, within the constraints of available computer systems, has been achieved by semi-automatic scripted operation of atomic structure codes, making use of promotional rules and exploiting resolution levels. The whole is optimised for available distributed computer resources with respect to total radiated power. These methods are used for the three key production steps of specific ion data for emissivity calculation, electron impact ionisation data and di-electronic recombination data, the delivery being to standard ADAS data formats. Assembly in terms of emissivity coefficients, feature emissivity coefficients, effective recombination and ionisation coefficients follows, enabling the ionisation state and radiation emission characteristics of any heavy element in fusion plasma to be generated. In a further step, techniques using superstages, combined with extension of collisional-radiative coefficient types, deliver atomic data in a compressed form which is allowing progress with current generation 2-D plasma transport models.

Transition Probabilities of Ar and Xe Species for Optical Diagnostics and Modelling of Fusion Plasmas

K. Katsonis[1], Ch. Berenguer[1], R.E.H. Clark[2], M. Cornille[3], Bin Duan[4] and Jun Yan[4]

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Transition probabilities ($\mathbf{A_{ij}}$) are important in optical diagnostics of emission lines of plasmas. The transition probabilities along with electron collision excitation cross sections (σ_{ji}) are the main determinants of the theoretical spectra calculated using detailed **C**ollisional-**R**adiative (**C**-**R**) models. Such models are necessary for diagnostics and modelling of plasmas when they cannot be assumed to be in **L**ocal **T**hermodynamic **E**quilibrium (**LTE**). Here we are specifically interested in the evaluation of A_{ij} pertaining to Ar and Xe atoms and their low ionization stages, with application to C-R models for diagnostics and modelling of plasmas of fusion interest. The evaluations of σ_{ji} are addressed separately.

C-R models including spectra up to Ar IX and Xe IX have been developed, covering the entire range of population of the outer p^6 and s^2 shells of the rare gases. Work is in progress on validation of these models and application to rare gas plasmas encountered in fusion research. In the validation process the spectra from several laboratory devices were acquired and studied, including a new series of spectral measurements in the WEGA Stellarator in Greifswald, optical diagnostics of the DIVA plasma reactor in LPGP, a study of Xe ions in the VUV region in IPNAS and dedicated experiments specifically for the validation of these models.

Generation of a huge number of A_{ij} is necessary for complete C-R models. These are based calculations from various theoretical methods and are often the result of a collaborative effort supported by the present CRP.

Finally, an extension of the applicability of our 'zero-dimension' codes to treat the bulk of the plasma state and properties calls for their coupling with detailed kinetic codes as EIRENE.

Electron Collision Excitation of the Lower Ar I and Xe I Levels

Ch. Berenguer[1], K Katsonis[1] and R.E.H. Clark[2]

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Electron collision excitation cross sections (σ_e) and calculations of the corresponding rate coefficients α_{ji} for various distribution functions have been calculated in a collaborative effort and were used in our **C**ollisional-**R**adiative (**C-R**) models. Special care was given to the α_{ji} values because the overall shape of the theoretical spectra obtained by C-R models depends strongly on the accuracies of both transition probabilities and electron collision excitation data.

In this paper we focus on the special case of electron impact excitation cross sections from the ground 3*p* (5*p*) and 4*s* (6*s*) shells of the neutral Ar (Xe) to the lowly excited levels of the atom. Calculations of cross sections for excitation from the ground state of argon and from the metastable states of the 4s and 6s configurations of argon and xenon respectively have recently been completed. Calculations have also been carried out for the excitation from the transitory 4*s* levels of argon. Similar work is underway for xenon.

In evaluating these σ_e we compare results calculated using the following theoretical methods:

I. Distorted Wave (DW) approximation using the Los Alamos ACE codes.
II. First Order Many Body Theory (FOMBT), also with the ACE code, especially near the threshold.
III. Quasi-classical evaluations following numerical solutions of the few-body problem.
IV. The semi-empirical formula introduced by Drawin, as adapted by Katsonis for the rare gas atoms.

We have carried out calculations I and II using different sets of configurations and compared the resulting cross sections. The comparisons with III and IV which are based on experimental energies and on transition probabilities calculated with the Coulomb approximation and NIST values when available are often very satisfactory in the whole energy range and especially in the near threshold energies which are of interest for fusion applications. Comparisons with the small number of available experimental data have also been made.

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