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## Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV

Summary Report of the Final Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

6 – 8 October 2014

Prepared by

H.-K. Chung, P. Beiersdorfer, A. Müller, Yu. Ralchenko and B. J. Braams

December 2014

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**ABSTRACT**

The final Research Coordination Meeting of a coordinated research project (CRP) on spectroscopic and collisional data for tungsten ions in fusion plasma was held at IAEA Headquarters with 17 external experts representing 14 research groups and staff from the International Atomic Energy Agency. Participants summarized their research during the CRP and made plans for a final report. The proceedings and conclusions of the meeting are summarized here.

December 2014

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# 1. Introduction

The IAEA Coordinated Research Project (CRP) on "Spectroscopic and Collisional Data for Tungsten in Plasma from 1 eV to 20 keV" has the objective to generate experimental and calculated data for radiative and collisional processes involving tungsten ions in a fusion plasma environment. The first Research Coordination Meeting (RCM) of this CRP was held in Vienna on 13-15 December 2010 and the second RCM took place 29-31 August 2012 in Heidelberg, Germany, hosted by the Stored and Cooled Ions Division of the Max Planck Institute for Nuclear Physics (MPI-K). The third and final RCM was held in Vienna on 6-8 October 2014 and this is the report of that meeting.

The purpose of the final RCM was to summarize the research of the participants during the period of the CRP and to review the current status of theoretical and experimental atomic data for tungsten; 17 experts participated in the meeting. The available presentations are collected on the A+M Data Unit web pages at http://www-amdis.iaea.org/CRP/Tungsten/3RCM/. Section 2 of this report provides a brief summary of presentations at the meeting and Section 3 provides a summary of discussions and conclusions. The list of participants is provided in Appendix 1 and the meeting agenda is provided in Appendix 2. Appendix 3 provides a more detailed and technical summary of presentations and relevant references.

The importance of data for tungsten ions in plasma is due to the use of tungsten as a plasma facing material in fusion experiments including ITER. The entire temperature range from $\simeq$1 eV in the divertor plasma up to $\simeq$20 keV in the ITER plasma core is of interest, and all charge states from neutral up to neon-like and a bit beyond are relevant. Emission from the lowest charge states of tungsten provides a tool for real-time erosion measurements and the use of X-ray lines from highly charged tungsten ions is one approach for temperature measurements in hot core plasma. Processes of interest for the CRP and for the present third RCM are excitation and ionization by electron, photon and proton impact, autoionization, radiative de-excitation and recombination, dielectronic recombination, and charge exchange. Data include cross sections, spectroscopic signatures (line radiation) and integrated power loss.

# 2. Presentations

Dr R. Forrest, Head of the Nuclear Data Section, welcomed the CRP participants. He emphasized the important role of tungsten atomic data for fusion applications and explained what is expected from the final RCM and the conclusion of the CRP. The core objective is to provide recommended data for radiative and collisional processes of tungsten in plasma and to have it documented in a CRP final report.

Participants briefly introduced themselves and the agenda was adopted.

### 2.1 Experimental data on electron and heavy particle collisions with tungsten

#### Experimental data for electron-impact ionization, electron-ion recombination and photoionization of tungsten ions

Dr. Müller started with a brief overview of the needs in fusion research for reliable atomic collision data for tungsten ions and pointed out that during the CRP considerable progress has been achieved in all fields of photonic and electronic collisions involving tungsten ions. Work on electron-impact ionization of tungsten ions has been carried out by his group using crossed-beams facility. Recombination experiments were performed at the heavy-ion storage ring TSR of the Max-Planck-Institute for Nuclear Physics (MPI-K) in Heidelberg, Germany. Photoionization experiments with tungsten ions were carried out at the Advanced Light Source (ALS) in Berkeley, USA.

One of the most important results during the CRP is the measurement of recombination rate coefficients where for ions $W^{18+}$ and $W^{20+}$ plasma rate coefficients for recombination at temperatures below 20 eV were found to be roughly three orders of magnitude higher than the rates implemented in the Atomic Data and Analysis Structure Project ADAS. Photoionization of $W^{q+}$ ions with q = 1, 2, ..., 5 has been investigated primarily in the energy range of about 20 to 100 eV. In specific cases the energy range was extended up to the 300 eV region. Previous cross section data on electron-impact ionization of tungsten ions in charge states up to q = 10 were confirmed by new measurements of Alfred Müller's group (using a different experimental setup). New measurements on electron-impact ionization of $W^{q+}$ ions extended the data base to the charge states q = 11, 12,..., 19.

**Absolute measurements of charge exchange cross sections for $W^{8+}$ with Helium at low energies**

The absolute cross sections for tungsten highly charged ions of $W^{q+}$ are particularly important for edge and divertor plasma in ITER as basic data. However, there are few absolute measurements of charge exchange cross sections for $W^{q+}$. Dr Soejima reported the absolute cross sections for charge exchange processes measured in collisions of tungsten highly charged ions with hydrogen and deuterium atoms at collision energies between 0.1eV to 10 keV. Preliminary data of absolute charge exchange cross sections for $W^{8+}$ with helium at collision energies between 20 to 150 eV/u were shown as well as a charge state dependence of the cross sections for $W^{q+}$ (q=5,8,16,18) with helium at collision energies of 10.9×q eV/u. Semiclassical calculations with hidden curve crossing method agree well with the measured cross sections.

## 2.2 Experimental data on tungsten spectra

**EUV spectrum of highly charged tungsten ions in CoBIT**

An electron beam ion trap is a useful device for the systematic spectroscopic studies of highly charged tungsten ions. Dr Sakaue reported on a compact electron beam ion trap, called CoBIT and observed extreme ultraviolet (EUV) spectra of highly charged tungsten ions. The electron energy dependence of spectra was investigated at electron energy from 540 to 1370 eV. Previously unreported lines were identified by comparing the wavelengths with theoretical spectra using a collisional-radiative (CR) model. From the comparison, the observed lines have been identified as 5f-4d, 5p-4d, 5g-4f transitions of $W^{20\text{-}32+}$, and 4f-4d transitions of $W^{27\text{-}30+}$ . Emission lines from $W^{26+}$ were measured around 100Å with a strong peak observed at 102Å and other emission lines at both sides of this strong peak. These lines are emission lines of $W^{26+}$ 4f5s $\rightarrow$4f$^2$ by electron excitation. Also observed were 5s-4f transition lines of $W^{27+}$ around 90 Å and identified as the E3 transitions (5s $\rightarrow$4f, J=1/2 $\rightarrow$ J=5/2,7/2) by comparing with the CR-model. The two emission lines have strong electron density dependence by comparing with experimental spectra and CR-model calculation spectrum.

**Calculation, analysis, and modelling of E1 and M1 lines from W ions in LHD and EBIT plasmas**

Prof Koike reported on the experimental and theoretical investigation of ultra violet (UV) to visible magnetic dipole (M1) line emissions from highly charged tungsten ions in LHD plasmas. M1 lines of $W^{26+}$ ions were measured in visible range and identified as of the J=5 to J=4 transition of triplet H ground state fine-structure multiplet. CR calculations show that the M1 line intensity ratios are sensitive to electron density. For $W^{27+}$, a $^2F_{7/2}$ to $^2F_{5/2}$ M1 line was observed at 337.84 nm. Extensive measurement and modelling were performed for emission lines in the EUV region. A CR model was constructed using atomic structure data considering the inner-shell excited state as well as the outer shell excited states and electron collision data from HULLAC code. The UTA (Unresolved Transition Array) emission was calculated for spectra of 5 to 7 nm wavelength range.

**Tungsten X-ray data needed for core plasma diagnostics and brief update on our recent data production**

Dr Beiersdorfer reported on the high resolution (resolving power~2000) measurements of the intrashell (n = 3 to n = 3) transitions in $W^{48+}$ through $W^{61+}$ in the 26-44 Å wavelength range. The 3s-3p and 3p-3d lines observed were mostly electric dipole allowed transitions. There were many lines observed and yet not to be identified, indicating that much more modelling and experimental measurements are needed for tungsten spectra. A significant effort went for the collisional-radiative modelling using the Flexible Atomic Code (FAC). Measurement and CR modelling effort was augmented with calculations of specific atomic parameters, especially energy levels, radiative rates, oscillator strengths $f_{ij}$, and autoionization rates.

Finally, summarized was an assessment of the tungsten atomic data that is needed to achieve the diagnostic requirements of ITER's core imaging crystal spectrometer, which is designed to measure the ion temperature and ion rotation velocity profiles across the plasma center. The required measurements include a 25-fivefold increase in the accuracy to which the $W^{64+}$ X-ray resonance is known, experimental calibration of its $W^{64+}$ excitation cross section, the position and intensity of dielectronic satellite lines that may blend with it, and reliable ionization balance calculations for tungsten ionization states between $W^{61+}$ and $W^{66+.}$

**Experimental and theoretical analysis of EUV and X-ray spectra from highly charged ions of tungsten**

Dr Ralchenko presented the recent work performed at the Atomic Spectroscopy Group at the National Institute of Standards and Technology on spectroscopy and collisional-radiative (CR) modelling for highly charged ions of tungsten. The NIST Atomic Spectra Database v.5.2 currently contains data on 2229 energy levels and 14510 spectral lines of W ions including 13277 lines with identifications and 779 lines with transition probabilities. Recently NIST Electron Beam Ion Trap (EBIT) was used to produce extreme ultraviolet spectra from N-shell ions of W and the spectra were then analysed using CR code NOMAD. Super Coster-Kronig rates were measured for O2 and O3 states in tungsten using high-resolution asymmetric diffraction spectrometry and compared with theoretical results. This work demonstrates the ability to simultaneously record high resolution (<1 eV) L and K spectra to determine the line shapes of the heavy elements (e.g. W through Am) by using multiple planes of a single quartz crystal and to accurately measure the non-radiative super Coster–Kronig. Also presented was the first results on calculation of single charge exchange between neutral hydrogen and $W^{64+}$ which is expected to be the most abundant ion in the ITER core were presented.

Finally Dr Ralchenko presented a report on the fusion-related W case considered at the 8th Non-LTE Code Comparison Workshop that was held in Santa Fe, NM, USA in November 2013. Almost twenty codes participated in calculation of plasma population kinetics parameters for W at plasma temperatures typical for fusion devices. The results of code comparisons were presented in detail.

**Spectra of W VIII and W IX in the EUV region**

Dr Ryabtsev reported on the spectrum recorded on a high resolution vacuum spectrograph (resolution ~ 0.01 Å) in the region below 350 Å under excitation in a vacuum spark as well as on the 10 m normal incidence spectrograph (resolving power 150 000). Photographic plates are used for precise wavelength measurement while image plates are used for intensity measurements. The spectrum of W VIII in the VUV region belong to the $4f^{13}5s^25p^6$ - ($4f^{12}5s^25p^65d$ + $4f^{13}5s^25p^5(5d+6s)$) and $4f^{14}5s^25p^5$ - $4f^{14}5s^25p^4(5d+6s)$ transitions. Because of large spin-orbit splitting of the 5p electron, the spectrum of W VIII is roughly divided into three groups located approximately at 170, 200 and 250 Å. For verification of the identifications of such complex spectrum as W VIII the isoelectronic spectra of neighboring chemical elements Hf VI, Ta VII and Re IX were studied. On the other hand, the spectrum of W IX is much more complex than W VIII. A set of the lowest levels consists of three even configurations $4f^{14}5s^25p^4$, $4f^{13}5s^25p^5$ and $4f^{12}5s^25p^6$. Using the behavior of the intensities with a change of the excitation conditions in the spark a list of 483 spectral lines in the region 170 - 199 Å, considered as belonging to W IX, was created (http://das101.isan.troitsk.ru/files/SPECTRA/W/linelist.txt). A current state of the theory of atomic spectra does not give the possibility for calculation of W IX with an accuracy needed for detailed identification of this spectrum and its application for quantitative diagnostics of tokamak plasmas.

**Spectra of moderately charged ions of heavy elements around tungsten. Some recent results in W IX sequence: The Yb V spectrum**

Dr Tchang-Brillet and Dr J.-F. Wyart presented VUV spectra of tungsten ions from W V to W IX, and of isoelectronic ions as well as the W VIII spectrum and on the isoelectronic ions Hf VI, Ta VII and Re IX. The analysis of spark spectrum provided 242 new energy levels and 1080 spectral lines in the wavelength range of 460-1865Å, identified as transitions between the even configurations $4f^{12}$ and $4f^{11}6p$ (56 levels) and the odd ones $4f^{11}5d$ and 6s (186 levels). The parametric study of configurations including configuration interactions provided better predictions of energy parameters for the higher charged ions of the isoelectronic sequence, although the opening of the $5p^6$ subshell in W IX needs an extended basis of calculations. For weaker charged ions, an extended analysis of the Yb I isoelectronic sequence spectra, with the 5p-6d and 5p-7s transitions in Ta IV and in W V was carried out based on high resolution spark source emission spectra recorded on the 10m normal incidence spectrograph of the Meudon Observatory.

## 2.3 Theoretical atomic data and collisional-radiative models of tungsten ions

**Collisional-Radiative Modelling of Tungsten at temperatures of 1200-2400 eV**

Dr Colgan discussed calculations of tungsten at moderate temperatures of 1200 to 2400 eV using the Los Alamos National Laboratory (LANL) collisional-radiative modelling ATOMIC code. The presentation was focused on the LANL ATOMIC calculations that were made for NLTE-8 for tungsten and discussed different models that were constructed to predict the tungsten emission. In particular, comparisons between semirelativistic configuration-average and fully relativistic configuration-average calculations were discussed as well as semirelativistic calculations that include fine-structure detail, either including full configuration-interaction or including only intermediate-coupling. The difficulty of ensuring completeness with respect to the number of configurations included in a CR calculation was presented.

**Electron-impact Excitation Cross sections and Polarization of Highly Charged Tungsten Ions**

Prof Srivastava described a number of theoretical and experimental investigations that have been performed to study L-shell tungsten ions X-ray spectroscopy as well as the M-shell spectra of various tungsten ions. Following the previous study of electron-impact excitation cross sections for dipole allowed transitions from M-shell of the Zn-like through Co-like W ions, electron-impact excitations from the L shell *viz.* $n$=2→$n$=3 transitions of the ground state in the Mg-like $W^{62+}$, Na-like $W^{63+}$, Ne-like $W^{64+}$, F-like $W^{65+}$ and O-like $W^{66+}$ ions were carried out. The fully relativistic distorted wave (RDW) theory has been used to calculate the excitation cross sections for electric and magnetic dipole as well as quadrupole transitions in the electron-impact energy range from threshold excitation energy up to 60 keV. Analytic fits to the calculated excitation cross sections have been also done for the plasma modelling purposes. Very recently, we have also studied the M-shell electron excitations *viz* $3p \rightarrow 3d$ transitions in Fe-like $W^{48+}$ through Al-like $W^{61+}$ ions. The electron-impact excitation cross sections as well as linear polarization for all the fourteen tungsten ions in the range of incident electron energies up to 20 keV have been calculated.

**Dielectronic recombination and electron-impact excitation of highly charged tungsten ions**

Mr Wu presented on behalf of Prof Dong, the total and partial EIE (electron-impact excitation) and DR (dielectronic recombination) cross sections of initially highly charged $W^{42+}$ - $W^{45+}$ ions using the multiconfiguration Dirac-Fock (MCDF) method. It has been found that the differences of linear polarization of the same transition lines but formed by the EIE and DR processes are very large. Therefore, one can use these degrees of linear polarization to diagnose the formation mechanism of these relevant X-ray emissions. Also, the specific plasma condition could be further assessed by measuring the linear polarizations of the corresponding spectral lines. By using the flexible atomic code (FAC) that is based on the relativistic configuration interaction method [3], the total and partial DR rate coefficients of initially highly charged $W^{37+}$ - $W^{46+}$ tungsten ions were calculated. A detailed comparison shows that the excitation from the 4*p* subshell dominates the total DR rate coefficients followed by the excitations from the 4*s* and 4*d* subshells, while the contributions of excitations from the 3*l* (*l=s, p, d*) subshells are significant only at high electron temperatures. Apart from the DR rate coefficients, the total radiative recombination (RR) and three-body recombination (TBR) rate coefficients are also estimated semiempirically for an electron number density of $10^{14}$ $cm^{-3}$.

**Electron-impact ionization calculations of tungsten ions**

Dr Kwon presented electron-impact ionization (EII) cross section for $W^{17+}$ and $W^{1+}$ using the flexible atomic code (FAC) based on a distorted wave (DW) approximation and compared available other previous theoretical and experimental results. Our level-to-level DW (LLDW) calculations for ground and excited states of $W^{17+}$ agree well with recent experiment but for ground state of $W^{1+}$ the calculated cross section is still 25% larger than measurement. For a comparative study, R-Matrix calculations for collisional excitation (CE) cross sections for lowly charged $W^{3+}$ and $W^{+}$ were carried out. The FAC R-Matrix calculation agrees with the DARC R-Matrix calculation by Ballance et at. [4] for the most dominant 5p to 5d excitation of $W^{3+}$ while the configuration-average DW (CADW) by Ballance et and LLDW cross sections are about 45% and 13% larger than the R-Matrix cross sections, respectively.

**Statistical Theory for Radiative-Collisional Processes with Heavy Ions in Plasmas**

Dr Lisitsa reported the universal statistical model of the electron-impact ionization of heavy ions and related ionization rates in plasmas, which is based on the notion of collective excitations of atomic electrons as is done in condensed medium. The frequency of collective oscillations is described using the Brandt-Lundquist local plasma frequency model, and the distribution of atomic electron density is assumed to be according to the Thomas-Fermi model. The extend comparison with experimental data as well as other numerical codes was made for many elements from Mendeleev table, namely W, Xe, Kr, Fe, Ar and U. It was shown that statistical models for atomic processes: ionization cross sections and, rates DR rates are in good correspondence with detailed calculations and experiments. Quasi-continuum spectra of heavy ions seem to be affected by the collective plasma effects of atomic shell–envelope of spectral lines arrays.

**Unified database of radiative recombination and photoionization data for tungsten ions in plasmas. Atoms in laser and fusion plasmas**

Dr Trzhaskovskaya and Dr Nikulin presented new relativistic calculations of the photoionization and radiative recombination (RR) data performed by the Dirac-Fock method for 33 tungsten ions from ranges $W^{14+}$ -$W^{23+}$ and $W^{47+}$ - $W^{71+}$. The calculations of the total and differential RR cross sections for the highly charged uranium ions $U^{91+}$,$U^{90+}$, and $U^{89+}$ are in good agreement with experimental data. Their unified database includes the partial photoionization cross sections and the total RR cross sections in the electron energy range from 1 eV to ~80 keV and the partial and total RR rate coefficients and radiated power loss rate coefficients were calculated in the temperature range from $10^4$ K to $10^9$ K. The exact consideration of the electron exchange was shown to be of importance in the RR and photoionization calculations for low-charged ions especially at low energies. Relativistic and multipole effects are of importance for highly charged ions and at high energies. The influence of plasmas temperature and density on the energy spectrum and level occupation numbers of ions in Local Thermodynamic Equilibrium (LTE) plasmas was also studied with the code PLASMASATOM based on the average-atom model using the self-consistent field (SCF) Dirac-Slater method. New calculations were performed for the tungsten dense plasmas at density $3.3\times10^{19}$ cm$^{-3}$ (normal metallic density is $6.3\times10^{22}$ cm$^{-3}$). In addition, the non-linear SCF screening model was employed for calculation of the screening impurity potential for the first time. Results demonstrate that the energy spectrum and level populations for a tungsten ion with regard to temperature differ considerably from those for a free neutral atom.

## 3. Discussions

Three discussion sessions were moderated by A. Müller, P. Beiersdorfer and Yu. Ralchenko on the topics of experimental collisional data for tungsten ions, spectroscopic measurements and theoretical atomic data and modelling.

### 3.1 Experimental collisional data for $W^{q+}$ ions

**I) Dielectronic and radiative recombination**

Work on recombination probably was the most important collision-related topic addressed within the frame of the present CRP and among all collision studies presented during the meeting. It has most likely the highest impact on fusion plasma modelling. The main reason is that theoretical methods previously employed to obtain plasma rate coefficients for recombination of complex many-electron ions were not adequate and were never tested against direct experiments with tungsten ions (because there were none).

During the last several years, recombination rate coefficients and cross sections have been measured at the TSR storage ring in Heidelberg for ions $W^{18+}$, $W^{19+}$, $W^{20+}$, and $W^{21+}$ in the energy range from 0 to several 100 eV. So far, final data are published for $W^{18+}$ and $W^{20+}$. The data for $W^{19+}$ and $W^{20+}$ are still under analysis but will be published within the next few months. The experiments show that the total recombination cross sections, especially at low energies, are orders of magnitude above radiative recombination. New theoretical attempts to describe the experimental data use approaches characterized as “damped and partitioned” (Badnell et al.) and “statistical” (Flambaum et al.). The new calculations make up for most of the previously existing huge discrepancies between theory and experiment, however, substantial deviations remain in the details of cross sections while the plasma rate coefficients obtained by theory and experiment as a function of temperature begin to converge.

It would be good to have more measurements for lower and higher charge states, however, the storage ring TSR has been shut down in Heidelberg and will no longer be available for such measurements. There is some chance that TSR will be transferred to CERN and operate as a ring whose main purpose would be to store and manipulate radioactive beams. However, it will take many years until further measurements with tungsten ions might be possible again at TSR if it is transferred to CERN. Other storage rings capable to store and cool tungsten ions are or will soon be available at the GSI Helmholtz Center for Heavy Ion Research or at the new FAIR facilities in Darmstadt. But beam time in that environment is so oversubscribed that chances are small to ever get time for measurements just producing data without a very strong physics case.

Beside heavy ion storage rings, EBIT devices can provide possibilities to measure recombination cross sections, however, energies below 10 to 20 eV are not accessible while this is the range where there is the largest uncertainty in the existing theoretical work. All in all the perspectives are not very good that further relevant measurements on recombination of tungsten ions in a wider range of charge states can be carried out in the foreseeable future. There is agreement, though, among the participants of the discussion that the investigated ions in charge states around q=20 are probably the most difficult ("the worst") to describe by theory. Calculations for other ions are expected to be easier, especially near closed-shell configurations. Moreover, experiences from systematic studies of dielectronic recombination of a long isonuclear sequence of $Fe^{q+}$ ions in charge states from q=7 to 23 show that even for this relatively light element at charge states off closed shells, theory and experiment typically do not match well in the details of resonance structure, but are close to one another in plasma rate coefficients.

In the context of recombination yet another aspect was extensively discussed: the role of external electromagnetic fields on dielectronic recombination. Müller and his group have measured dependences of cross sections for dielectronic recombination on the presence of electric and magnetic fields. Electric fields mix states with different angular momenta $l$, while perpendicular magnetic field components mix states with different orientation quantum numbers $m_l$. These effects change the autoionization rates of Rydberg states with high principal quantum numbers $n$ and thus influence dielectronic recombination. The thoroughly investigated effects found in the experiments could not be well reproduced by state-of-the-art theory and therefore this area of research went dormant for the last ten years. The experiments and theory had shown however, that big effects on the plasma rate coefficients can result if sufficiently strong electric fields are present. The plasma rate coefficient for dielectronic recombination of $Fe^{15+}$, for example, can change by a factor 3 or higher at temperatures between $10^5$ and $10^6$ K by the presence of electric fields of the order of kV/cm. Field effects mainly influence Rydberg states with high n. These are especially important for ions in low-charge states. A question is, which high Rydberg states can survive in a plasma. The situation is complex already for isolated single ions in external fields.

Diffusion of ions in a plasma complicates the situation further. Transport in a fusion plasma can result in the presence of certain charge states of (tungsten) ions in regions where they are not expected when equilibrium is assumed and equilibrium is not a good approach. It is recommended therefore that the possible influence of macroscopic and collisional microfields on dielectronic recombination should be kept in mind in plasma modelling and that these field effects in plasmas have to be more thoroughly assessed. Further work clarifying field effects in plasma environments is necessary. It is also required that collisional destruction of the intermediate highly excited states populated during dielectronic recombination processes is considered when the plasma density increases.

**II) Electron-impact ionization**

Net ionization of an ion can result from a number of different electron-ion collision processes:

a) Direct knock-off removal of an outer-shell electron, termed direct ionization (DI)

b) Excitation of an inner-shell electron so that an autoionizing intermediate state is produced; by a subsequent Auger decay an electron is released from the atom or ion; the process is termed excitation-autoionization (EA)

c) Dielectronic (radiationless) capture of the incident electron with simultaneous inner-shell excitation reducing the ion charge state by one unit; the resulting highly excited state may then decay by the emission of two electrons (either sequentially or simultaneously) and, thus, an ionized ion with a charge state one unit above that of the parent ion is produced. The whole process is resonant as a result of the first step, the dielectronic capture, which is essentially a time-reversed Auger decay.

By the time of the CRP meeting experimentally determined electron-impact ionization cross sections were available for all ions from $W^{1+}$ to $W^{19+}$ at electron energies from below the ionization thresholds up to 1000 eV. A problem in all measurements with multiply charged ions that cannot be stored prior to the collision is the presence of ions in long-lived excited states in the parent ion beam. Even when ions are stored for several seconds prior to the start of a measurement, metastable ions may still be present. The presence of such states can be detected by the experimental techniques available in Müller's group. Fine energy scans with very good statistics at small energy steps reveal ionization thresholds of different beam components. Theoretical modelling of the resulting apparent cross sections which are typically measured with uncertainties of less than 10% provides information about the fractions of beam components and hence reliable cross sections for the ground state of the investigated ion, which is usually by far the dominant beam component. It was pointed out in the discussion that a plasma of course also contains long lived excited states whose ionization cross sections are needed.

Experience has shown that DI and EA can be fairly well described by distorted-wave calculations. It is necessary, however, that these calculations include all relevant excitations from different inner shells to all excited states that significantly contribute to EA processes. It is also necessary to consider the branching ratios for different decay paths of the intermediate highly excited states. For Auger decay of autoionizing states the branching ratio was usually assumed to be 100% in the past. Recent calculations include the determination of real branching ratios. Comparison of the measurements on electron-impact ionization of tungsten ions (in charge states up to q = 19) with distorted-wave calculations including a sufficient number of excitations shows remarkably good agreement. This is true even for $W^{5+}$ which is the worst case with respect to metastable contaminations. By suitable modelling by theory it was possible to find out that about 25% of a typical $W^{5+}$ ion beam produced in an electron-cyclotron-resonance ion source are in the excited $4f^{13}\,5d^2$ and $5p^5\,4f^{14}\,5d^2$ configurations.

Expectations for the theoretical description of ionization cross sections for ions imply that the distorted-wave calculations become increasingly better with increasing charge state of the parent ion while resonances are of decreasing significance. In the experiments studying electron-impact ionization of tungsten ions, no significant contributions of resonant processes could be found in the range of charge states q from 1 to 19 at energies up to 1 keV. This fact together with the observations that distorted wave calculations for DI and EA are in quite good agreement with the experimental data might lead one to the conclusion that electron-impact ionization cross sections for tungsten ions may be calculated with good accuracy up to the highest charge states without considering resonance contributions. However, measurements by Alfred Müller’s group for highly charged xenon ions in charge states beyond q=18 (up to 25) provided evidence for strong contributions of resonant processes to net single ionization. Considering the predictions by theory groups this finding was quite unexpected for such high charge states. Radiative decay of intermediate highly excited states is strongly increasing with increasing ion charge states and should eventually take over relative to Auger decays. But it is not obvious for which charge states and which intermediate resonances this will happen. The experiments with xenon ions suggest, that resonances might also show up for charge states beyond the presently available experimental data. Charge states of tungsten ions, isoelectronic with $Xe^{19+ \text{ to } 25+}$, are $W^{39+ \text{ to } 45+}$. Calculations of cross sections in this range of charge states using the R-matrix approach should be feasible and might help to clarify if resonances are important for these ions.

It is obviously necessary to explore, for which charge states of tungsten there might be resonant contributions, and to assess the related cross sections. This can, in principle, be done with ion storage ring experiments, however, as pointed out above, beam time will not easily be granted for an experiment with the objective to just explore a fusion-relevant ionization cross section. Combination of a very powerful, state-of-the-art ECR ion source and the crossed-beams technique for the measurement of absolute ionization cross sections available in Alfred Müller’s group might facilitate the extension of the existing measurements of tungsten ions to the region around q=40. However, this would require a substantial investment in hardware and manpower that cannot be easily acquired. Ionization cross sections have been measured at EBIT facilities in the past. Again, funding for systematic measurements at an EBIT of potentially fusion-relevant data, which have to be normalized to theory is hard to get.

### III) Electron-impact excitation

No electron-impact excitation measurements have been carried out on tungsten ions. There have been electron-impact excitation measurements mostly for lighter ions in the past. Dunn and coworkers in Boulder, Colorado, and at Oak Ridge, Tennessee, have measured absolute excitation cross sections in a crossed-beams configuration by looking at fluorescence from the excited state. These experiments were extremely time consuming. A new approach was developed independently by Dunn et al. and Chutijan et al.. Electron and ion beams are merged and the electron energy loss is measured. In order to make sure that all scattered electrons can be collected, these experiments have to be restricted to a very short range of energies just around and above the excitation threshold. Both setups are still in existence. Dunn’s experiment is at Oak Ridge where the atomic physics program has essentially been shut down. Chutijan’s setup has not been used lately. No details are known about its status.

Peter Beiersdorfer pointed out that electron-impact excitation experiments have been carried out at EBIT devices. In particular, measurements and a careful analysis of data have been carried out in his group. Getting absolute cross sections in a device with an inventory of several ion species carrying different electrical charges and the necessity to rely on theory (for radiative recombination) makes a measurement and the analysis of the recorded data very cumbersome. Experiments could be done in principle for tungsten ions, however, the present funding situation makes it very difficult to acquire grants for such work.

An alternative approach is to look at autoionizing excited states instead of monitoring fluorescence or electron energy loss. In electron-ion crossed-beams experiments one can measure the production of ionized ions arising from inner-shell excitation with subsequent Auger decay. Alfred Müller et al. have recently published detailed measurements on electron-impact ionization of $N^{5+}$ ions. From the extremely precise cross section measurements one can infer the contributions arising from direct and resonant excitation processes. These and all other existing measurements provide benchmarks for testing theoretical methods. Calculations for the excitation of tungsten ions carried out in Rajesh Srivastava's group have been tested against such experimental benchmarks.

**IV) Photoionization**

Alfred Müller and colleagues have measured photoionization of tungsten ions. Data are now available for $W^{1+}$, $W^{2+}$, $W^{3+}$, $W^{4+}$, and $W^{5+}$. Single ionization and in some cases also multiple ionization were studied. Absolute cross sections with high energy resolution were determined over wide energy ranges. The idea for these measurements within the context of the present CRP was to exploit, firstly, the time-reversal relation between recombination and photoionization, and secondly, contribute to the exploration of the electronic structure of tungsten ions with respect to the spectroscopy which formed a considerable fraction of all efforts made within this CRP.

It is known that the plasma density in a fusion device is low so that absorption of high-energy photons is unlikely. Thus, cross sections for photoionization are not of prime importance for fusion. It is nice to see, however, that state-of-the-art R-matrix theory can reproduce the main features of the experimental results. This is important since R-matrix calculations can also be used to obtain electron-impact ionization, excitation and recombination cross sections. Thus, photoionization is a good testing area for R-matrix approaches to fusion-relevant processes.

**V) Charge transfer collisions of ions with plasma components: He, $He^+$, H, D, …**

A very substantial body of literature is available on charge transfer cross sections for ions colliding with neutral atoms and molecules. Much less experimental data are in the literature for ion-ion collisions. Scaling rules have been developed for ion-neutral collisions and the question of excited-state population in an electron capture event has been extensively addressed. The most recent revival of this field of research was related to the observation of (soft) X-rays from comets. The explanation of this stunning observation was the interaction of multiply charged ions present in the solar wind with gas in the vicinity of a comet. The short-wavelength spectra observed by X-ray satellite missions could be modeled on the basis of existing knowledge about the highly excited states into which an electron is captured in a charge transfer collision.

In a fusion plasma, charge transfer is an important issue. Many of the required data are available and important basics are known. In a preceding CRP Vladimir Nikulin has calculated cross sections for charge transfer collisions of a variety of ions with neutral and ionized helium. Within the present CRP Makoto Imai had previously reported about a new effort in Japan to obtain charge transfer cross sections for tungsten ions with plasma components. At the present CRP meeting the status of this work was presented by Kouichi Soejima. Particularly interesting, both for the understanding of fusion plasmas and from a fundamental point of view, is the investigation of collisions with H and D targets. While much knowledge is available for this topic in general, the situation at very low energies in the eV/u range is not equally well understood and further investigations are desirable. In the new charge transfer experiments with tungsten ion beams one has to be aware of the possible presence of metastable states as in all collision experiments employing multiply or highly charged (tungsten) ions. An incident $[W^{q+}]^*$ ion in an excited state may capture an electron to an excited level and the resulting $[W^{(q-1)+}]^{**}$ ion may subsequently autoionize and, thus, loose the captured electron again.

EBIT may be used for charge exchange cross section measurement since the charge transfer cross sections are generally very large. For example, an experiment with only 200 ions per second can provide a meaningful result.

### 3.2 Spectroscopic data from experiment and calculation

Various aspects of spectroscopic measurements of tungsten ions have been discussed: atomic data, charge state distribution (CSD) modelling, influence of plasma transport etc.

A comprehensive review of the spectroscopic data available in 2009, at the onset of the CRP, had been provided by Kramida and Shirai, who produced a compilation of all available spectroscopic data for all tungsten ions. The review made it clear that most of the spectroscopic data for tungsten are missing. In fact, many ionization states of tungsten had not even a single entry in their compilation.

Much new spectroscopic data have been produced since the beginning of the CRP, ranging from near-neutral tungsten to $W^{66+}$ ions and from the optical to the X-ray wavelength bands. In an update of the earlier compilation, Kramida in 2011 reported on numerous new theoretical and experimental efforts producing tungsten data, and even more such data are now available at the end of the CRP.

Regretfully, the newer data are not yet available online. Atomic structure and transition probabilities are relatively well documented for low charged ions at the NIST ASD (Atomic Spectroscopy Database). However, it is a rather slow process to populate the standard reference database, as data are evaluated and recommended as a self-consistent set. The time lag is caused by the available resources. In order to compensate, the NIST database provides a bibliography listing that includes the newer papers, and, thus, it is more up to date than the atomic data themselves. The lack of compiled reference data mainly affects computational efforts, where such data are used to test the reliability of a given atomic calculation. For highly charged ions, atomic physics packages such as FAC or HULLAC are often used to handle a massive number of levels and transitions, and even a few experimental reference points can anchor a given calculation.

In absolute terms, the spectra of many tungsten ions are still not investigated at all or are incompletely understood. For example, experimental data between 2 and 25 Å only exist for near 6 Å from a few charge states and are otherwise non-existent. Even many features remain unidentified in the spectra measured under this CRP, which indicates that theory is not yet able to produce synthetic spectra that are reasonably close to the measured data to enable identification. Generally, the unidentified lines are from tungsten ions away from closed shells, which means that open-shell tungsten ions needs much more work.

All of the experimental data so far were produced by collisional excitation. Spectral lines produced by charge exchange also will need to be measured, as charge exchange is expected to play a role in current and future fusion devices.

Model calculations need to include the line formation mechanisms that exist in magnetic fusion devices from the cool plasma edge to the hot core. In order to test model calculations, benchmark spectra are needed with high resolution from plasmas that ideally have a uniform density and electron temperature. As a minimum, the plasmas need to be well characterized. Tungsten spectra exist from optically thin plasma generated by lasers. However, libraries of experimental spectra from fusion machines such as LHD, ASDEX, JET, K-STAR, NSTX, etc. would be most useful for developing model calculations, as those data are taken under the appropriate plasma conditions. Nowadays all magnetic fusion machines have or will have some components made of tungsten in anticipation of ITER, including machines where all plasma-facing components are made of tungsten, and it would be wise to obtain and utilize the spectroscopic information from these machines. Therefore, the interaction between atomic physicists utilizing EBITs or sliding sparks and plasma physicists is very important in tungsten spectroscopy, and in many cases it probably needs to be improved. Examples of an active collaboration between plasma physicists and atomic physicists are the LHD (Large Helical Device, NIFS, Japan) collaboration with the COBIT device (A low-energy EBIT at Tokyo EBIT), where tungsten pellets are injected into the main plasmas for spectroscopic measurement, and the ITER core imaging X-ray crystal spectrometer team and the Livermore EBIT team.

A very relevant question is how well and to what extent the charge state distribution (CSD) can be measured through spectroscopic data. As we mentioned above, closed shell and near-closed shell ions are in a better shape than others in terms of spectroscopic identification; however, it not clear that the relevant excitation rates needed to extract a CSD from observed intensities are reliable. There is even less information for the spectral emission of ions with partially open shells, and in many cases not even line identifications exist.

Spectroscopic data are also needed to describe the tungsten emission in the divertor region. Although the electron density is higher and the temperature cooler in the divertor region than in the main plasma, it is possible that non-LTE (Local thermodynamic equilibrium) modelling is required to describe the emission. It is of interest to know how fast the tungsten on the divertor plates erodes in this region. The charge states in this region may not be higher than $W^{6+, 7+, 8+}$, and much of the atomic data in the optical region has been obtained for the relevant charge states from spark experiments since the beginning of this CRP. LANL had a model to assess the quality of atomic data for highly charged tungsten ions, but there is no reliable NLTE modelling capability for low charged tungsten ions $W^{0+ - 5+}$. It is known that the distorted wave method is not good enough compared with R-matrix calculations but a model with R-matrix calculation is not realistic due to the computational cost. R-matrix calculations exist for ionization cross sections, so do atomic structure information underlying the calculations. Optical spectroscopy is a preferred diagnostics for fusion applications because of the ease with which lenses, mirrors, and light fiber optics can be installed. This is especially true for monitoring W migration in the divertor region. Thus, such emission should be included in NLTE models.

A method to utilize a broad continuum was proposed since the continuum level in fusion machine is relatively high with the existence of intermediate to high Z elements. It is found that a large continuum exist for tungsten in the range of 1 to 9 keV spectral range. The continuum measurement will provide <Z>, an average charge state. Motional Stark effect also measures <Z>.

Plasma transport plays an important role in the shaping of the tungsten charge state distribution. The transport effect may change the average charge state <Z> and broaden the spatial range (equivalently the temperature range) where ions of a given charge state are located. Hence the CSD deviates from the transport-free, equilibrium value. This deviation is something that plasma spectroscopists would like to measure because it can be used to infer the amount of plasma transport, provided adequate ionization balance calculations are available from the atomic physics community. Current tokamaks can use the optical emission from low-Z impurities induced by a diagnostic neutral beam to observe transport. A diagnostic neutral beam is not available on ITER, at least in the beginning, and transport measurements must focus on the ionization balance of tungsten, the calculation of which is much less certain than that of a low-Z element, such as carbon or oxygen. For CSD measurements, one should know a few well characterized lines for the purpose of diagnostics. Sensitivities of line intensities with respect to the electron temperature or electron density should be explored.

Since the CSD may not be in the thermal equilibrium but in a “transport equilibrium,” a given charge state may exist at a much lower temperature than the normal temperature where one otherwise expects to find it. Thus, reliable recombination and ionization rates are required at much lower and much higher temperatures than are typically assumed, if the ions are in thermal equilibrium. If ions are transported close to the plasma edge, then they can undergo charge exchange with neutral hydrogen recycling from the wall, and this recombination mechanism must also be included.

Additional conditions were identified that may influence the CSD determination by spectroscopic measurement. A possibly important aspect is the existence of electromagnetic fields in the machine. Ion microfields can mix internal fields and affect atomic data sensitive to the high-lying states such as Rydberg states or dielectronic recombination (DR) channels. Even with a small electric field, recombination rates can be affected. DR rates are found to increase with an increasing electric field for a certain charge state. In addition to the CSD due to increased recombination rates, the spectra will change due to the different the population cascades through the states heavily altered by the existence of electromagnetic fields.

It was noted that transport coefficients are mostly phenomenological, and plasma theory typically predicts much smaller transport than measured. Combining a transport code with spectroscopic code capabilities was suggested.

### 3.3 Theoretical atomic data and modelling

The atomic data discussed in the previous sections not only provide tests for atomic structure and collision theories for tungsten ions but also serves as an input for collisional-radiative (CR) models used to determine radiative properties of tungsten plasmas. A significant part of the discussions were devoted to development and analysis of CR models for tungsten.

Relation of collisional-radiative modelling to plasma transport simulations was one of the central discussion topics. It was strongly emphasized that CR computer modules are fundamentally important for transport codes as the former provide crucial parameters such as mean ion charge, ionization distribution and radiative power losses. However, the size and speed limitations on such modules make them significantly different from the detailed CR codes that may include hundreds of thousands or even millions of atomic states. Yet the transport CR modules can and should be tested with the detailed codes.

The account of high-multipole radiative transitions was another point of deliberation. Since probabilities of forbidden radiative transitions are known to exhibit a very strong dependence on ion charge, such transitions cannot be ignored for highly charged ions of tungsten and ought to be included in CR simulations. In some cases, even such exotic multipoles as, e.g., magnetic octopole in Ni-like ions, can result in noticeable modification in the observed spectrum.

Validation and verification (V&V) of CR models were also extensively discussed at the meeting. The ongoing activities within the framework of the Non-LTE Code Comparison Workshops on testing the CR codes for tungsten were highly appreciated. It was emphasized that comparisons of different approximations in CR modelling (e.g., configuration-average approach vs. detailed level approximation vs. UTA-type methods) is valuable for a better understanding of population kinetics. In addition, discussions were held on importance of analysis of CR models to variations in the input atomic data. To this end, the participants reiterated the value of experimental verification of basic atomic data for tungsten.

The recent measurements of resonance effects in recombination of $W^{19+}$ produced unexpectedly large values for cross sections and rate coefficients. This result may have wide implications on calculation of ionization balance. So far, most of CR calculations for W ions with Z~40 result in a higher mean ion charge than the measured values, and therefore larger recombination rates may explain the observed difference. One of recommendations put forward during discussions was to initiate an extensive calculation of recombination cross sections for mid-charge ions of tungsten with the most sophisticated atomic structure methods. Finally, the effect of electromagnetic fields on dielectronic recombination rates was brought up in discussions as well.

## 4. Conclusions and Recommendations

In the course of the CRP many new measurements and calculations were carried out for collisional and radiative properties of tungsten ions in plasma. Among these are measurements of electron-impact ionization and recombination rate coefficients for intermediate charge states, EUV and X-ray spectral lines and their evaluations, and collisional-radiative model calculations.

Participants discussed the post CRP activities. The available atomic data sets from the CRP participants must be documented and made available on the IAEA web pages. Currently tungsten data in ALADDIN, the IAEA database, are far from comprehensive. Data for excitation, ionization and recombination normally belong in ALADDIN, but some data, for example the extensive data sets from LANL atomic codes, need to be stored separately. Some spectroscopic data such as microcalorimeter data will also be useful to be available through the IAEA CRP web page to allow comparison with measured spectra.

After 4 years of this CRP, unfortunately, high quality atomic data for tungsten ions are still far from comprehensive. The fusion modelling community needs cross sections and rates for collisional excitation, ionization, recombination and radiative power loss for each ion. The most significant area of uncertainty is in the comprehensive cross sections for dielectronic recombination.

A final report of the CRP is to be published in the form of a special issue of the on-line journal Atoms with individual contributions by the participants in the CRP. There is not planned to be a further meeting of the entire CRP, but a smaller meeting for evaluation and recommendation of data for tungsten ions, especially electron collision data, is likely.

Appendix 1

# List of Participants

Mr Zhongwen WU, Northwest Normal University, CHINA

Ms Wan-Ü Lydia TCHANG-BRILLET, Laboratoire d'étude du rayonnement et de la matière en astrophysique (LERMA), Observatoire de Paris, FRANCE

Mr Jean-Francois WYART, Centre Université Paris Sud, Laboratoire Aimé Cotton, FRANCE

Mr Alfred MUELLER, Justus-Liebig-Universität Giessen, GERMANY

Mr Rajesh SRIVASTAVA, Indian Institute of Technology, INDIA

Mr Fumihiro KOIKE, Department of Materials and Life Sciences, Sophia University, Tokyo, JAPAN

Mr Hiroyuki A.SAKAUE, National Institute for Fusion Science, JAPAN

Mr Kouichi SOEJIMA, Faculty of Science, Niigata University, JAPAN

Ms Duck-Hee KWON, Korea Atomic Energy Research Institute (KAERI), REPUBLIC OF KOREA

Mr Valeriy LISITSA, National Research Center "Kurchatov Institute", Moscow, RUSSIAN FEDERATION

Mr Alexander RYABTSEV, Russian Academy of Sciences, RUSSIAN FEDERATION

Ms Malvina TRZHASKOVSKAYA, Petersburg Nuclear Physics Institute of National Research Center "Kurchatov Institute", Gatchna, RUSSIAN FEDERATION

Mr Vladimir K. NIKULIN, Ioffe Institute of the Russian Academy of Science, St. Petersburg, RUSSIAN FEDERATION

Mr Peter BEIERSDORFER, Lawrence Livermore National Laboratory (LLNL), UNITED STATES OF AMERICA

Mr James COLGAN, Los Alamos National Laboratory (LANL), UNITED STATES OF AMERICA

Mr Yuri RALCHENKO, National Institute of Standards and Technology (NIST), UNITED STATES OF AMERICA

Mr Christopher J. FONTES, Los Alamos National Laboratory (LANL), UNITED STATES OF AMERICA

## IAEA

Mr Bastiaan J. BRAAMS, International Atomic Energy Agency, AUSTRIA

Ms Hyun-Kyung CHUNG, International Atomic Energy Agency, AUSTRIA

Appendix 2

# Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV

6 – 8 October 2014, IAEA Headquarters, Vienna, Austria

Scientific Secretary: Mr B. J. Braams

## Agenda

### Monday, 6 October 2014 — Room C-0739

| | |
|---|---|
| 09:30-09:45 | R. A. FORREST, B. J. BRAAMS: Welcome, adoption of the agenda |
| 09:45-10:30 | Alfred MÜLLER, Justus-Liebig-Universität Giessen: Experimental data for electron-impact ionization, electron-ion recombination and photoionization of tungsten ions. |
| 10:30-11:00 | Discussion: Experimental data on electron collision processes with tungsten. |
| 11:00-11:15 | ***Break*** |
| 11:15-11:45 | Kouichi SOEJIMA, Niigata University, Japan: Measurements using an electron beam ion source of charge transfer cross sections for collisions between tungsten ions and helium atoms. |
| 11:45-12:15 | Discussion: Experimental data on heavy particle collisions. |
| 12:15-13:30 | ***Lunch*** |
| 13:30-14:00 | Hiroyuki SAKAUE, National Institute for Fusion Science, Toki, Japan: EUV spectra of highly charged tungsten ions in CoBIT and LHD. |
| 14:00-14:30 | Fumihiro KOIKE, Sophia University, Tokyo, Japan: Calculation, analysis, and modelling of E1 and M1 lines from W ions in LHD and EBIT plasmas. |
| 14:30-15:00 | Peter BEIERSDORFER, Lawrence Livermore National Laboratory: Tungsten X-ray data needed for core plasma diagnostics and brief update on our recent data production. |

15:00-15:30 ***Break***

15:30-16:00 Yuri RALCHENKO, National Institute of Standards and Technology: Experimental and theoretical analysis of EUV and X-ray spectra from highly charged ions of tungsten.

16:00-16:30 Alexander RYABTSEV, Russian Academy of Sciences, Institute of Spectroscopy, Troitsk: Spectra of W VIII and W IX in the EUV region.

16:30-17:00 Wan-Ü Lydia TCHANG-BRILLET, Observatoire de Paris, LERMA, and Jean-François WYART, Université Paris Sud: Spectroscopic Properties of Moderately Charged Ions of Tungsten.

17:00-17:30 Discussion: Experimental data on tungsten spectra. (to be continued).

19:00 Social dinner.

## Tuesday, 7 October 2014 Room C-0739

09:00-09:30 James COLGAN and Chris FONTES, Los Alamos National Laboratory: Collisional-Radiative Modelling of Tungsten at temperatures of 1200-2400 eV.

09:30-10:00 Rajesh SRIVASTAVA, Indian Institute of Technology at Roorkee: Electron-impact excitation cross sections and polarization of highly charged tungsten ions.

10:00-10:30 Zhongwen WU (for Chenzhong DONG), Northwest Normal University, Lanzhou, China: Theoretical study on electron-impact excitation and dielectronic recombination of highly charged tungsten ions.

10:30-11:00 ***Break***

11:00-11:30 Duck-Hee KWON, Korea Atomic Energy Reseach Institute: Electron-impact ionization calculations for tungsten ions.

11:30-12:00 Valeriy LISITSA, National Research Center "Kurchatov Institute", Moscow, Russian Federation: Statistical theory for radiative-collisional processes with heavy ions in plasmas.

12:00-12:30 Malvina TRZHASKOVSKAYA, Petersburg Nuclear Physics Institute and Vladimir K. NIKULIN, Ioffe Physical Technical Institute: Unified database of radiative recombination and photoionization data for low-charged tungsten ions in plasmas. Atoms in laser and fusion plasmas.

12:30-14:00 ***Lunch***

14:00-15:30 Review: Spectroscopic data from experiment and calculation.

15:30-16:00 ***Break***

16:00-17:00 Review: Collisional data from experiment and calculation.

## Wednesday, 8 October 2014 Room C-0739

| | |
|---|---|
| 09:00-12:00 | Discussion. Data quality, data uncertainties, priorities for further experiments and calculations. Outline of meeting report. |
| 12:00-13:30 | ***Lunch*** |
| 13:30-16:00 | Plans for CRP final report, any remaining business. |
| 16:00 | Close of meeting. |

# Author Summaries

## Experimental data for electron-impact ionization, electron-ion recombination and photoionization of tungsten ions

ALFRED MÜLLER

Justus-Liebig-Universität Giessen, Germany

Dr. Müller started with a brief overview of the needs in fusion research for reliable atomic collision data for tungsten ions and pointed out that theoretical results on complex ions, particularly for electron-ion recombination, have been very unreliable in the past. He highlighted the situation before the start of the present CRP. The only reliable (experimental) results were available for electron-impact ionization of $W^{q+}$ ions with q = 1, 2, ...,10. But the experiments are sometimes difficult to interpret because of the presence of metastable ions in the experiments. No experimental results had been available prior to the present CRP for electron-ion recombination or photoionization of tungsten ions.

During the CRP considerable progress has been achieved in all fields of photonic and electronic collisions involving tungsten ions. Work on electron-impact ionization of tungsten ions has been carried out by Alfred Müller's group at the Institute for Atomic and Molecular Physics in Giessen, Germany, using their home-built crossed-beams facility. Recombination experiments were performed at the heavy-ion storage ring TSR of the Max-Planck-Institute for Nuclear Physics (MPIK) in Heidelberg, Germany. Collaborators of the Giessen team on the subject of recombination included members of Andreas Wolf's group based at the MPIK and of Daniel Savin's group from the Columbia Astrophysics Laboratory in New York. Photoionization experiments with tungsten ions were carried out at the Advanced Light Source (ALS) in Berkeley, USA, by the Giessen team in collaboration with David Kilcoyne from the ALS with help by Ron Phaneuf and David Esteves from the University of Nevada, Reno, USA.

Most important for the objectives of the CRP was the demonstration of huge deviations between the expected and the measured recombination rates for tungsten ions in an intermediate range of charge states, where the 4f subshell is opened. For the ions $W^{18+}$ and $W^{20+}$ plasma rate coefficients for recombination at temperatures below 20 eV were found to be roughly three orders of magnitude higher than the rates implemented in the Atomic Data and Analysis Structure Project ADAS that addresses the atomic requirements for (fusion) plasma modelling. Even at temperatures around 200 eV where these ions are most abundant in a collisionally ionized plasma, the measured rate coefficients are about a factor of 4 above the ADAS assumptions. The results on recombination of $W^{18+}$ and $W^{20+}$ have been published [1,2]. The ion charge states $W^{19+}$ and $W^{21+}$ were also investigated [3] but the analysis of the experimental data is not yet finalized. By the experiments, new developments in theory (Nigel Badnell et al.; Victor Flambaum, Gleb Gribakin et al.) were initiated. With the new approaches, theory is now becoming capable of accounting for much of the low-energy recombination observed in the experiments.

Photoionization of $W^{q+}$ ions with q = 1, 2, ..., 5 has been investigated primarily in the energy range of about 20 to 100 eV [4]. In specific cases the energy range was extended up to the 300 eV region. Absolute cross sections and detailed energy scans at a typical resolution of 100 meV were measured. Relativistic Dirac R-matrix calculations by Brendan McLaughlin and Connor Ballance are in quite fair agreement with the experimental findings for q = 2, 3, and 4. For $W^{5+}$ ions, cross sections were measured to be extremely rich in resonance structures. Publications of the joint results of experiment and theory are in preparation.

Previous cross section data on electron-impact ionization of tungsten ions in charge states up to q = 10, obtained by Erhard Salzborn's group (also in Giessen), were confirmed by new measurements of Alfred Müller's group (using a different experimental setup). The new data include detailed energy scans measured with very good statistics and small energy steps. By observing fine-structures in the cross sections and especially in the threshold region, the role of metastable ions in the primary ion beam used in the crossed-beams experiments could be elucidated. This, in turn, supports new theoretical attempts to model the experimental observations by accounting for contributions of metastable ions (V. Jonauskas et al., publication in preparation). New measurements on electron-impact ionization of $W^{q+}$ ions extended the data base to the charge states q = 11, 12,..., 19. Work on $W^{17+}$ has been published [5]. Configuration average distorted wave calculations carried out in Müller's group for the investigated charge states are in remarkable agreement with the experimental data. On this basis accurate plasma rate coefficients could be determined for the ground levels of the investigated tungsten ions. The results will be published in due time.

**References**

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**Absolute measurements of charge exchange cross sections for $W^{8+}$ with Helium at low energies**

K. SOEJIMA

Niigata University, JAPAN

The absolute cross sections for tungsten highly charged ions of $W^{q+}$ are particularly important for edge and divertor plasma in the ITER as a basic data. However, there are few absolute measurements of charge exchange cross sections for $W^{q+}$. In our project, the absolute cross sections for charge exchange processes are measured in collisions of tungsten highly charged ions with hydrogen and deuterium atoms at collision energies between 0.1eV to 10 keV. In this summary, we show preliminary data of absolute charge exchange cross sections for $W^{8+}$ with helium at collision energies between 20 to 150 eV/u. And a charge state dependence of the cross sections for $W^{q+}$ (q=5,8,16,18) with helium at collision energies of 10.9×q eV/u. The main features of the experimental apparatus are only summarized here. The apparatus was composed of a tandem mass spectrometer and compact EBIS type highly charged ion source named mini-EBIS. An ion beam guide named OPIG within a collision cell is a key technique for low energy collision experiments. Supplying a high frequency electronic field to OPIG enable us to measure the cross section down to 0.1 eV/u collision energy. Projectile tungsten ions were produced in mini-EBIS using $W(CO)_6$. Stable producing of $W^{q+}$ (q=5～20) is succeeded under sever temperature control on a sample gas handling system with the mini-EBIS. Projectile ions were injected to the collision cell with OPIG. In the collision cell, the charge exchanged ions of $W^{(q-1)+}$ and $W^{(q-2)+}$ were produced as followed reactions;

$$W^{q+} + He \rightarrow W^{(q-1)+} + He^{+} \text{ single charge exchange } \sigma_{q,q-1},$$

$$\rightarrow W^{(q-2)+} + He^{2+} \text{ double charge exchange } \sigma_{q,q-2}.$$

Projectile and product ions were extracted from the collision cell and mass selected then detected with a channeltron multiplier. The absolute cross sections were estimated using initial growth rate method. Collision energy was determined from a voltage difference between ion source and center of collision cell. The results of collision energy dependences of the absolute charge exchange cross sections for $W^{8+}$ with helium are as follows; $\sigma_{8,7}$ is about $5\times10^{-15}$ cm$^2$ , $\sigma_{8,6}$ is about $1.5\times10^{-15}$ cm$^2$ and both the cross sections are almost independent of the collision energy. The overall uncertainty in the measured cross sections was estimated to be approximately 20%.

The calculated result using semiclassical approximation with hidden curve crossing method by Inga et al. is well reproduced the cross sections in the energy range measured. Below the lowest energy measured of 20 eV/u, the cross sections become drastically decreasing in the calculation. The energy dependence of the calculated cross sections is responsible for getting weak rotational coupling. Then, we should measure the cross sections below 20eV/u to confirm whether the calculated energy dependence is true or not since the confirmation lead to the existence of an isotope effect. The results of charge state dependences of the cross sections for $W^{q+}$ (q=5,8,16,18) with helium are as follows; less steep increasing of $\sigma_{q,q-1}$ is consistent with the well-known nature of highly charged ions, as for the $\sigma_{q,q-2}$ the charge state dependence is almost flat, which is off of a characteristic of highly charged ions. The charge state dependences for experimental and calculated, using scaling law proposed by Selberg et al., cross sections do not correspond well. The absolute measurements for charge exchange processes of $W^{q+}$ will be continued to investigate the unique property.

**EUV spectrum of highly charged tungsten ions in CoBIT**

H.A. SAKAUE

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Tungsten is planned to use as material for the divertor plates in ITER because of higher sputtering threshold energy for light ion bombardment, the highest melting point among all the elements, and less tritium retention compared with carbon-based materials. However impurity tungsten enters the high-temperature plasma and is ionized to highly charged ions, and then highly charged ions emit very strong photons of EUV and/or X-ray. This emitted photon has very important information on plasma diagnostics; information on electron and ion temperature, electron density, impurity ion abundance and impurity transportation. Nevertheless, it is the present conditions that those emission spectra are very complicated and those spectral data are very poor. Therefore, we observed spectra of highly charged tungsten ions in the extreme ultra-violet (EUV) by using electron beam ion traps.

An electron beam ion trap is a useful device for the systematic spectroscopic studies of highly charged tungsten ions. We have constructed a compact electron beam ion trap, called CoBIT [1,2,3], and observed extreme ultraviolet (EUV) spectra of highly charged tungsten ions. The electron energy dependence of spectra was investigated of electron energy from 540 to 1370 *eV*. Previously unreported lines were presented in the EUV range, and some of them were identified by comparing the wavelengths with theoretical calculations. To identify the observed lines, we have calculated the spectra using a collisional-radiative (CR) model. From the comparison, the observed lines have been identified as 5f-4d, 5p-4d, 5g-4f transitions of $W^{20\text{-}32+}$, and 4f-4d transitions of $W^{27\text{-}30+}$ .

We observed an unidentified emission lines which are expected from theoretical calculations from $W^{26+}$ around 100Å in CoBIT. As electron energy of CoBIT is increased across the ionization energy (*Ip(25+)*=786.3eV) of $W^{25+}$ from 770eV to 800eV, new emission lines appeared in this emission spectrum. These emission lines are identified as emission lines from $W^{26+}$. Strong peak was observed at 102Å and other emission lines were also observed at both ends of this strong peak. These lines are emission lines of $W^{26+}$ 4f5s $\rightarrow 4f^2$ by electron excitation. And these lines were observed at LHD plasma too. In the same way, we observed 5s-4f transition lines of $W^{27+}$ around 90 Å. The two strong peaks were confirmed at CoBIT. These two lines were identified as the E3 transitions (5s $\rightarrow$4f, J=1/2 $\rightarrow$J=5/2,7/2) by comparing with the CR-model. However, these lines were not confirmed at LHD plasma. It became clear that these two emission lines have strong electron density dependence by comparing with experimental spectra and CR-model calculation spectrum.

In future, we will promote detailed studies for the spectroscopic diagnostics of plasma, such as electron energy dependence and electron density dependence of these tungsten highly charged ions.

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**Calculation, analysis, and modelling of E1 and M1 lines from W ions in LHD and EBIT plasmas**

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Ultra violet (UV) to visible magnetic dipole (M1) line emissions from highly charged tungsten ions in LHD plasmas have been investigated both experimentally and theoretically. Measurements of UV to visible M1 lines have been performed and analyzed. Evaluation of ionization and recombination rate coefficients of W ions has been carried out for further study on ion transport. For several of the observed M1 lines, we have made elaborate theoretical calculations by means of multi-configuration Dirac-Fock method using GRASP family of codes: GRASP2K and GRASP92+RATIP.

For $W^{26+}$, we observed an M1 line at 389.404(6) nm in LHD plasmas and has been identified as of the J=5 to J=4 transition of triplet H ground state fine-structure multiplet by comparing the data with those of CoBIT experiment and the results of theoretical calculation. We further have performed a CR-model calculation on the four major $W^{26+}$ M1 optical emission lines, and have pointed out that the intensity ratios vary as functions of electron density. Especially, the intensities of J=6 to 5 and J=5 to 4 lines exceed the J=3 to 2 intensity with the increase of electron density in the range from $5 \times 10^9$ $cm^{-3}$ to $5 \times 10^{12}$ $cm^{-3}$ suggesting that the intensity ratios of those M1 lines can be the measure of the diagnostics of the electron densities in LHD plasmas. For $W^{27+}$, we observed a $^2F_{7/2}$ to $^2F_{5/2}$ M1 line at 337.84 nm, which is in reasonable agreement with the values of EBIT experiment and of present and existing theoretical calculations. Because this line is isolated and free from the cascading effect, we have proposed a $W^{27+}$ ion distribution evaluation using this line.

We have made an extensive measurement and spectroscopy modelling for emission lines in the EUV region. We have tried to construct detailed tungsten atomic radiative spectroscopy model for LHD and CoBIT plasmas. With atomic structure calculations considering the inner-shell excited state as well as the outer shell excited states and electron-impact excitation calculation by means of relativistic distorted wave approximations (HULLAC), we prepared the detailed atomic data and built up a collisional-radiative (CR) model. The UTA at 5 to 7 nm wavelength range has been reproduced. Ion charge state distribution in LHD plasmas has been evaluated using the group of spectral lines of n = 5 to 6, and n = 6 to 4 transitions at 2 to 4 nm wavelength region.

**Tungsten X-ray data needed for core plasma diagnostics and brief update on our recent data production**

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During the past two years our project has focused on spectral measurements of the intrashell (n = 3 to n = 3) transitions in $W^{48+}$ through $W^{61+}$. The measurements were made with a high-resolution (resolving power ~2000) grating spectrometer in the 26-44 Å wavelength range. The 3s-3p and 3p-3d lines we observed were mostly electric dipole allowed transitions.

However, they included also four electric dipole forbidden transitions [1]. It is interesting to note that there were many lines observed that we were not yet able to identify, which illustrates that tungsten spectra are far from understood and that much more modelling and experimental measurements are needed.

Our effort included a significant collisional-radiative modelling effort using atomic data we generated with the Flexible Atomic Code (FAC). For example, we have published results from our modelling efforts regarding the n=3 to n=2 X-ray transitions of near neonlike tungsten ions ($W^{56+}$ - $W^{71+}$) [2]. In addition, we have presented very detailed modelling calculations on the n=4 to n=3 spectral emission of $W^{42+}$ through $W^{51+}$, which falls into the 1000 to 4000 eV X-ray range [3].

Our measurement and collisional-radiative modelling effort was augmented with calculations of specific atomic parameters, especially energy levels, radiative rates, oscillator strengths $f_{ij}$, and autoionization rates. For example, we published a list of the ionization energies of all tungsten ions [4]. Our collaborators at the University of Reno used their highly accurate atomic codes based on many-body perturbation theory to make highly accurate calculations of atomic parameters for $W^{27+}$ [5] and $W^{4+}$ [6], which also included dielectronic recombination rates, for $W^{12+}$ [7] and $W^{13+}$ [8].

Finally, we have made an assessment of the tungsten atomic data that is needed to achieve the diagnostic requirements of ITER's core imaging crystal spectrometer, which is designed to measure the ion temperature and ion rotation velocity profiles across the plasma center [9]. The required measurements include a 25-Five-fold increase in the accuracy to which the $W^{64+}$ X-ray resonance is known, experimental calibration of its $W^{64+}$ excitation cross section, the position and intensity of dielectronic satellite lines that may blend with it, and reliable ionization balance calculations for tungsten ionization states between $W^{61+}$ and $W^{66+}$.

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**Experimental and theoretical analysis of EUV and X-ray spectra from highly charged ions of tungsten**

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Yuri Ralchenko (USA) presented the recent work performed at the Atomic Spectroscopy Group at the National Institute of Standards and Technology on spectroscopy and collisional-radiative (CR) modelling for highly charged ions of tungsten. The NIST Atomic Spectra Database v.5.2 currently contains data on 2229 energy levels and 14,510 spectral line of W ions including 13,277 line with identifications and 779 lines with transition probabilities. Recently NIST Electron Beam Ion Trap (EBIT) was used to produced extreme ultraviolet spectra from N-shell ions of W at the beam energy between 1.79 and 2.00 keV. The spectra were then analysed using CR code NOMAD and several dozen lines including about a dozen new lines were identified.

In a different work, super Coster-Kronig rates were measured for O2 and O3 states in tungsten using high-resolution asymmetric diffraction spectrometry. The rates were then compared with the already available calculations and the new theoretical results obtained with the flexible atomic code. This work demonstrates the ability to simultaneously record high resolution (<1 eV) L and K spectra to determine the line shapes of the heavy elements (e.g. W through Am) by using multiple planes of a single quartz crystal and to accurately measure the non-radiative super Coster–Kronig rates which are closely related to the energy level structure of the outer shells of the heavy elements.

Also the first results on calculation of single charge exchange between neutral hydrogen and W64+ which is expected to be the most abundant ion in the ITER core were presented. This process will originate due to injection of fast diagnostic and/or heating hydrogen beams into fusion plasma. The calculations were performed using the Classical Trajectory Monte-Carlo method and the obtained results will then be used in CR modelling of tungsten emission.

Finally, Yu. Ralchenko presented a report on the fusion-related W case considered at the 8$^{th}$ Non-LTE Code Comparison Workshop that was held in Santa Fe, NM, USA in November 2013. Almost twenty codes participated in calculation of plasma population kinetics parameters for W at plasma temperatures typical for fusion devices. The results of code comparisons were presented in detail.

**Spectra of W VIII and W IX in the EUV region**

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The spectrum of tungsten was recorded on a high resolution vacuum spectrograph (resolution ~ 0.01 Å) in the region below 350 Å under excitation in a vacuum spark working with discharge currents from 3 to 50 kA in Troitsk as well as on the 10 m normal incidence spectrograph (resolving power 150 000) of the Meudon Observatory. Photographic plates are used for precise wavelength measurement while image plates are used for intensity measurements.

**W VIII.** Intense lines in the spectrum of W VIII in the VUV region belong to the $4f^{13}5s^25p^6$ - $(4f^{12}5s^25p^65d + 4f^{13}5s^25p^5(5d+6s))$ and $4f^{14}5s^25p^5$ - $4f^{14}5s^25p^4(5d+6s)$ transitions. Because the low-lying configurations $4f^{13}5s^25p^6$ and $4f^{14}5s^25p^5$ coincide in energy, all these transitions are resonance transitions. Because of large spin-orbit splitting of the 5p electron, the spectrum of W VIII is roughly divided into three groups located approximately at 170, 200 and 250 Å. The lines around 170 Å are identified as the $4f^{13}5s^25p^6$ - $4f^{13}5s^25p^5_{j=1/2}6s$ [1] and $4f^{14}5s^25p^5$ - $4f^{14}5s^25p^46s$ transitions. The lines of the group at 200 Å are mostly identified as $4f^{13}5s^25p^6$ - $(4f^{13}5s^25p^5_{j=1/2}5d + 4f^{13}5s^25p^5_{j=3/2}6s)$ transitions. Intense lines in the 250 Å region belong mostly to the $4f^{13}5s^25p^6$ - $4f^{13}5s^25p^5_{j=3/2}5d$ transitions. A total of 187 lines in the region 160–271Å were identified and 102 levels were found, transition probabilities were calculated [2].

For verification of the identifications of such complex spectrum as W VIII the isoelectronic spectra of neighboring chemical elements Hf VI [3], Ta VII [4] and Re IX [5] were studied. In each spectrum the resonance transitions were analyzed and respectively from 144 to 90 energy levels were found. Parametric calculations of the spectra were performed with the aid of the Cowan code leading to fitted energy parameters, together with their ratios to the corresponding *ab initio* values (scaling factors). It was established that in spite of large change in the intensities and relative line positions as a result of a change of relative positions of strongly interacting configurations in the Hf VI – Re IX spectra the scaling factors are generally regular in the sequence. The isoelectronic regularities of the scaling factors for the energy parameters along the sequence Hf VI – Ta VII - W VIII – Re IX can be considered as a proof for reliability of our atomic data for W VIII.

**W IX.** This spectrum is much more complex than W VIII. A set of the lowest levels now consists of three even configurations $4f^{14}5s^25p^4$, $4f^{13}5s^25p^5$ и $4f^{12}5s^25p^6$. A number of interacting excited configurations decaying as the resonance transitions is now 9 (6 in W VIII) with the number of levels 1544 (339 in W VIII). Using a behavior of the intensities with a change of the excitation conditions in the spark a list of 483 spectral lines in the region 170 - 199 Å, considered as belonging to W IX, was created (http://das101.isan.troitsk.ru/files/SPECTRA/W/linelist.txt). According to the calculations the most intense lines of W IX should be located in the region 192 - 197 Å and should belong to the $(4f^{14}5p^4 + 4f^{13}5p^5)$ - $4f^{13}5p^45d$ transitions. The most intense line 193.830 Å can be identified as the $4f^{13}5p^5\ ^3G_6$ - $4f^{13}5p^45d\ (^3P)\ ^3H_6$ transition. A current state of the theory of atomic spectra does not give the possibility for calculation of W IX with an accuracy needed for detailed identification of this spectrum and its application for quantitative diagnostics of tokamak plasmas.

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**Spectra of moderately charged ions of heavy elements around tungsten. Some recent results in W IX sequence: The Yb V spectrum**

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Experimental studies of VUV spectra of tungsten ions from W V to W IX, and of isoelectronic ions are being carried on in the Paris-Meudon Observatory, in collaboration with the Institute of Spectroscopy of Troitsk. Results on the W VIII spectrum [1, 2] and on the isoelectronic ions Hf VI [3], Ta VII [4] and Re IX have been completed for publication.

As for the W IX spectrum, we tried to improve the knowledge of its isoelectronic sequence, by investigating the previously unknown Yb V spectrum. The analysis of spark spectrum led to a publication [5] containing 242 new energy levels and 1080 spectral lines in the wavelength range of 460-1865Å, identified as transitions between the even configurations $4f^{12}$ and $4f^{11}6p$ (56 levels) and the odd ones $4f^{11}5d$ and 6s (186 levels). The parametric study of configurations including configuration interactions provided better predictions of energy parameters for the higher charged ions of the isoelectronic sequence, although the opening of the $5p^6$ subshell in W IX needs an extended basis of calculations.

For weaker charged ions, we report an extended analysis of the Yb I isoelectronic sequence spectra, with the 5p-6d and 5p-7s transitions in Ta IV and in W V, based on high resolution spark source emission spectra recorded on the 10m normal incidence spectrograph of the Meudon Observatory.

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**Collisional-Radiative Modelling of Tungsten at temperatures of 1200-2400 eV**

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We discuss new collisional-radiative modelling calculations of tungsten at moderate temperatures of 1200 to 2400 eV. Such plasma conditions are relevant to ongoing experimental work at ASDEX Upgrade [1] and are expected to be relevant for ITER. Our calculations are made using the Los Alamos National Laboratory (LANL) collisional-radiative modelling ATOMIC code. These calculations formed part of a submission to the recent NLTE-8 workshop that was held in November 2013. This series of workshops [2] provides a forum for detailed comparison of plasma and spectral quantities from NLTE collisional-radiative modelling codes.

This talk will focus on the LANL ATOMIC calculations that were made for NLTE-8 for tungsten and discuss different models that were constructed to predict the tungsten emission. In particular, we discuss comparisons between semirelativistic configuration-average and fully relativistic configuration-average calculations. We also present semirelativistic calculations that include fine-structure detail, either including full configuration-interaction or including only intermediate-coupling. We discuss the difficult problem of ensuring completeness with respect to the number of configurations included in a CR calculation. We conclude with a summary and an outlook for future work.

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**Electron-impact Excitation Cross sections and Polarization of Highly Charged Tungsten Ions**

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Atomic data of tungsten ions are of great significance in order to identify and interpret the spectroscopic data of these ions because of the applications in the plasma-facing magnetic confinement devices. A number of theoretical and experimental investigations have been performed to study L-shell tungsten ions X-ray spectroscopy as well as the M-shell spectra of various tungsten ions present in large abundances for understanding the radiative emission for ITER plasmas [1-4].

In our previous study we considered electron-impact excitation cross sections for dipole allowed transitions from M-shell of the Zn-like through Co-like W ions which were identified as most intense lines in the M-shell spectra [5]. We have now carried out electron-impact excitations from the L shell *viz.* $n$=2→$n$=3 transitions of the ground state in the Mg-like $W^{62+}$, Na-like $W^{63+}$, Ne-like $W^{64+}$, F-like $W^{65+}$ and O-like $W^{66+}$ ions [6]. Fully relativistic distorted wave (RDW) [7] theory has been used to calculate the excitation cross sections for electric and magnetic dipole as well as quadrupole transitions for these ions which were observed recently in the measurements from electron-beam-ion trap (EBIT-I) at Lawrence Livermore National Laboratory [2]. We have performed calculations in the electron-impact energy range from threshold excitation energy up to 60 keV. Analytic fits to our calculated excitation cross sections have been also done for the plasma modelling purposes. Our results where possible have been compared with the few available previous theoretical calculations. Decay of the anisotropic excited states emit polarized radiation and the degree of polarization is directly related to magnetic sublevel excitation cross sections. The expressions for polarization of different transitions are obtained in terms of the magnetic sub-level cross sections using the density matrix theory. Our calculated magnetic sublevel cross sections have been further employed to obtain the linear polarization of the photon emissions for dipole allowed transitions after electron-impact excitation for all the five tungsten ions. All these results can be found in [6].

Very recently, we have also studied the M-shell electron excitations *viz*. 3$p$→3$d$ transitions in Fe-like $W^{48+}$ through Al-like $W^{61+}$ ions. This was in the light of measurements of Lennartsson *et al* [4] who reported the experimental spectra in the 27-41 Å range for these ions. We have calculated the electron-impact excitation cross sections as well as linear polarization for all the fourteen tungsten ions in the range of incident electron energies up to 20 keV.

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**Dielectronic recombination and electron-impact excitation of highly charged tungsten ions**

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Dielectronic recombination (DR) and electron-impact excitation (EIE) of tungsten ions are the most basic atomic processes in nuclear fusion plasmas of the International Thermonuclear Experimental Reactor (ITER) tokamak. A much detailed investigation on these processes is essential for modelling and diagnosing future fusion experiments performed on the ITER. In the present work presented by us, we have studied in much details the total and partial EIE and DR cross sections of initially highly charged $W^{42+}$ - $W^{45+}$ ions using the multiconfiguration Dirac-Fock (MCDF) method [1]. The degrees of linear polarization of the subsequent X-ray emissions from the unequally populated magnetic sublevels of these tungsten ions are also estimated [2]. It has been found that the differences of linear polarization of the same transition lines but formed by the EIE and DR processes are very large. Therefore, one can use these degrees of linear polarization to diagnose the formation mechanism of these relevant X-ray emissions. Also, the specific plasma condition could be further assessed by measuring the linear polarizations of the corresponding spectral lines. For example, the EIE process would dominate in hot and dense plasmas and the DR would dominate in low density plasmas that are cooled and recombining by the capture of free electrons.

In addition, by using the flexible atomic code (FAC) that is based on the relativistic configuration interaction method [3], we have also studied the total and partial DR rate coefficients of initially highly charged $W^{37+}$ - $W^{46+}$ tungsten ions [4-7] that play a very important role in the ionization equilibrium of tungsten plasmas under the running conditions of the ITER. A detailed comparison shows that the excitation from the 4p subshell dominates the total DR rate coefficients followed by the excitations from the 4s and 4d subshells, while the contributions of excitations from the 3l (l=s, p, d) subshells are significant only at high electron temperatures. Apart from the DR rate coefficients, the total radiative recombination (RR) and three-body recombination (TBR) rate coefficients are also estimated semiempirically for an electron number density of $10^{14}$ $cm^{-3}$.

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## Electron-impact ionization calculations of tungsten ions

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We have calculated electron-impact ionization (EII) cross section for $W^{17+}$ [1] and $W^{+}$ [2] using the flexible atomic code (FAC) based on a distorted wave (DW) approximation and compared available other previous theoretical and experimental results. Our level-to-level DW (LLDW) calculations for ground and excited states of $W^{17+}$ [3] agree well with recent experiment but for ground state of $W^{+}$ our calculated cross section is still 25% larger than experiments. Therefore a comparative study between DW and more sophisticated R-Matrix theories for lowly charged tungsten ions is needed. We have carried out R-Matrix calculations for collisional excitation (CE) cross sections for lowly charged $W^{3+}$ and $W^{+}$ by debugging and parallelizing the original FAC R-Matrix routines to be suitable for the large size computations of the complex systems. Our FAC R-Matrix calculation agrees with the DARC R-Matrix calculation by Ballance et at. [4] for the most dominant 5p to 5d excitation of $W^{3+}$ while the configuration-average DW (CADW) by Ballance et at. [4] and our LLDW cross sections are about 45% and 13% larger than the R-Matrix cross sections, respectively. Our FAC R-Matrix calculation for $W^{+}$ still remains ongoing due to computation complexity much more than for $W^{3+}$ and the results will be reported in the near future.

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## Statistical Theory for Radiative-Collisional Processes with Heavy Ions in Plasmas

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The universal statistical model of the electron-impact ionization of heavy ions and related ionization rates in plasmas is developed. The model is based on the notion of collective excitations of atomic electrons alike in condensed medium. The frequency of collective oscillations is described using the Brandt-Lundquist local plasma frequency model, and the distribution of atomic electron density is assumed to be according to the Thomas-Fermi model. The results of calculations according with the statistical approach of the electron-impact cross sections and ionization rates of heavy ions of the various ionization stages for the whole set of different heavy elements are compared with the available experimental and numerical codes data, demonstrating quite satisfactory correspondence.

Oscillator strength $f_{ij}$ is expressed in terms of atomic electron density. Local Plasma frequency method (LPF) – Brandt-Lundquist (1966) as a method for atom response calculation on external actions: atomic transition frequencies are equal to local plasma frequencies. Electron-impact ionization is expressed in terms of the cross section $\sigma(\omega)$.

The oscillator strength $f_{ij}$ is connected with atomic electron density by the relationship

$$f_{if} = 4\pi \cdot n(r) \cdot r^2 \cdot dr$$

It satisfies the sum rule.

The plasma frequency has the standard form:

$$\omega_p(r) = \sqrt{4\pi n(r)}$$

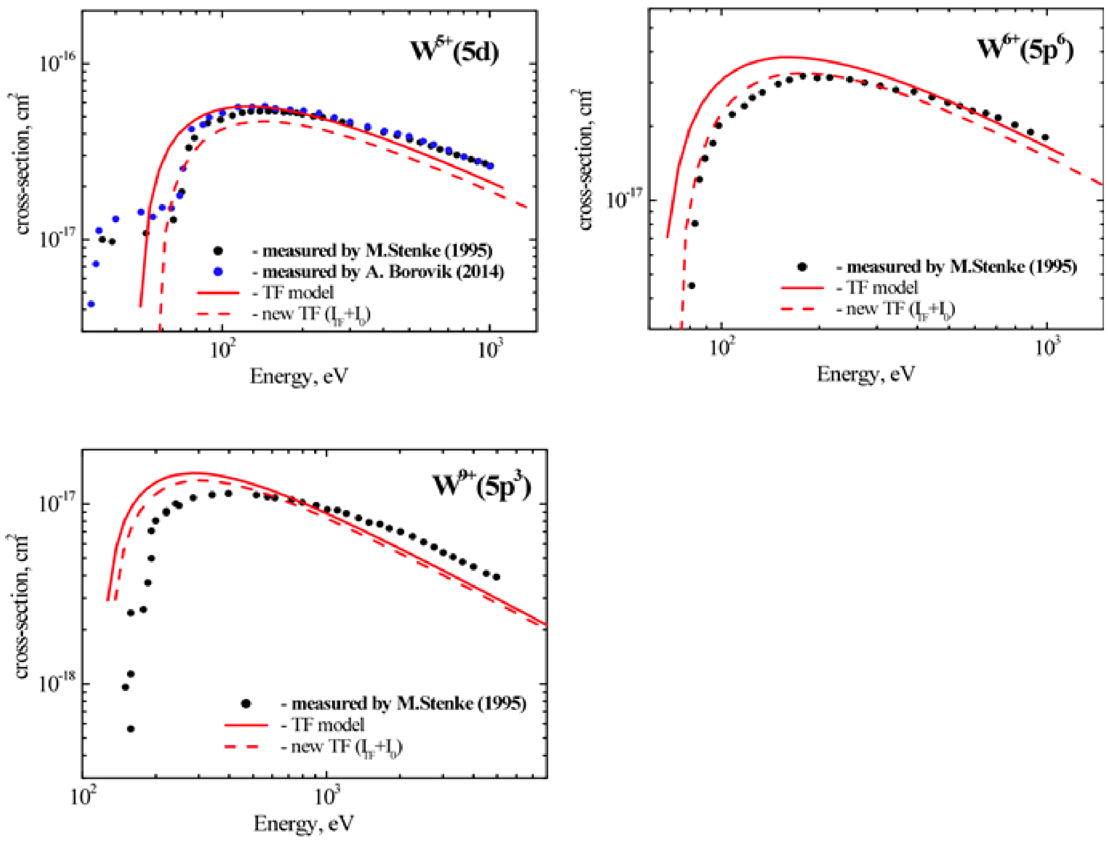
Photoabsorption cross section $\sigma(\omega)$ is a **functional from electron density.**

$$\sigma_{abs}(\omega) = \frac{2\pi^2 e^2}{mc} \int d^3 r\, n(r)\, \delta\left(\omega - \omega_p(r)\right) = \frac{2\pi^2 e^2}{mc} \cdot 4\pi \left( r_\omega^{\ 2} \cdot \frac{n(r_\omega)}{\left| \frac{d\omega_p(r)}{dr} \right|_{r=r_\omega}} \right)$$

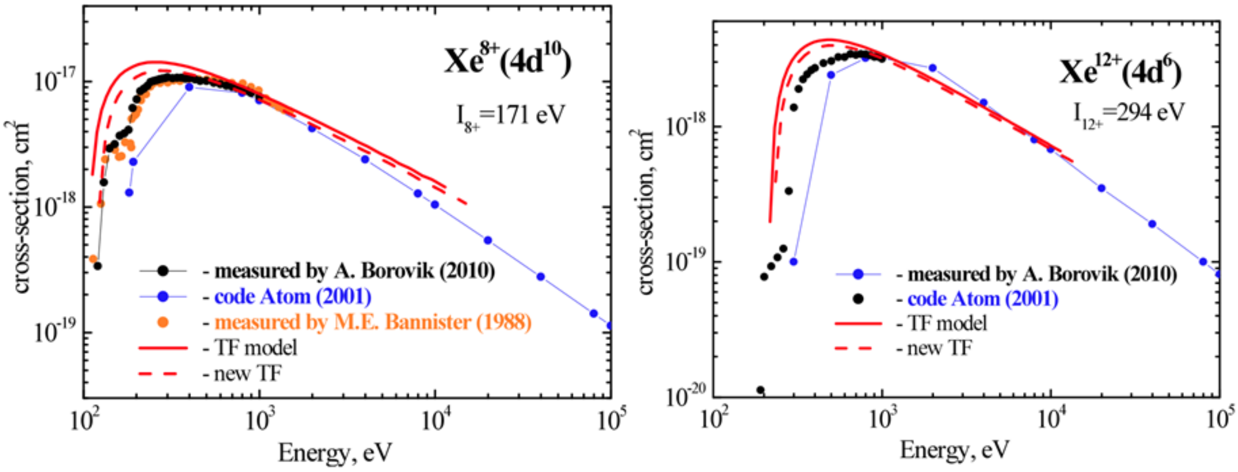
Electron-impact ionization is expressed in terms of the cross section $\sigma(\omega)$.

The extend comparison with experimental data as well as other numerical codes was made for many elements from Mendeleev table, namely W, Xe, Kr, Fe, Ar and U. Some examples of the comparison are presented on figs. below.

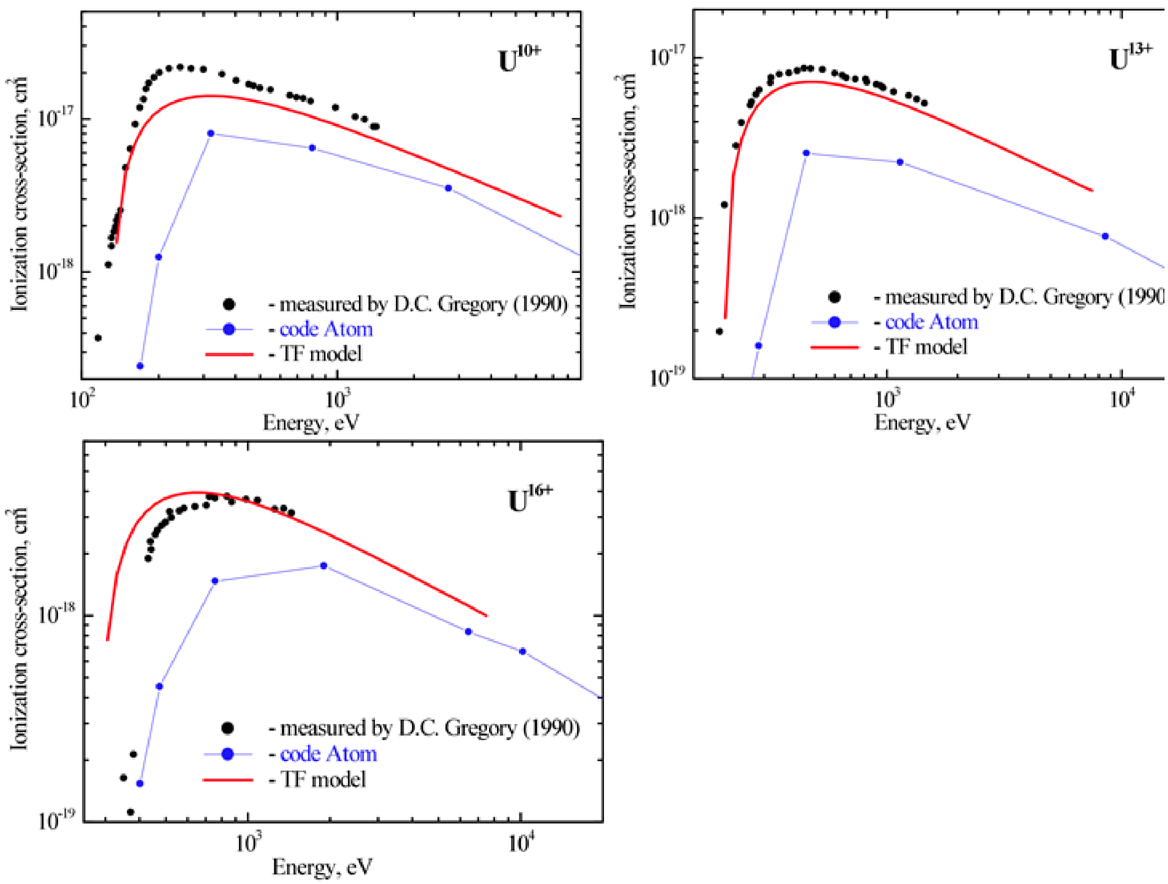
**Electron-impact ionization cross sections of Tungsten ions**



**Electron-impact ionization cross sections of Xe ions**




**Electron-impact ionization cross sections of U ions**



**Conclusions**

- 1. Statistical models for atomic processes: ionization *cross sections and, rates DR rates are in good correspondence with detail calculations and experiments*
- *2. Quasi-continuum spectra of heavy ions seems to be collective plasma effects of atomic shell – envelope of spectral lines arrays*
- *3. Resume: the precision of statistical model for atomic processes and radiative losses of plasma with heavy ions is of the same magnitude as in detail calculations*

**Unified database of radiative recombination and photoionization data for tungsten ions in plasmas. Atoms in laser and fusion plasmas**

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New relativistic calculations of the photoionization and radiative recombination (RR) data were performed by the Dirac-Fock method for 33 tungsten ions from ranges $W^{14+}$ -$W^{23+}$ and $W^{47+}$ - $W^{71+}$ . It should be noted that our calculations of the total and differential RR cross sections for the highly charged uranium ions $U^{91+}$,$U^{90+}$, and $U^{89+}$ are in good agreement with experimental data obtained in GSI [M.B. Trzhaskovskaya, V.K. Nikulin, Optics and Spectroscopy, 95 (2003) 537]. Our unified database includes the partial photoionization cross sections and the total RR cross sections in the electron energy range from 1 eV to ~80 keV. Partial and total RR rate coefficients (RR rates) and radiated power loss rate coefficients (RPL rates) were calculated in the temperature range from $10^4$ K to $10^9$ K.

Peculiarities of the data are discussed [M.B. Trzhaskovskaya, V.K. Nikulin, R.E.H. Clark, Chapter “Accurate Data on Radiative Recombination and Photoionization for Highly charged Tungsten Ions in Plasmas” in book “Horizons in World Physics”, Ed. A. Reimer, vol.277 (Nova, N.-Y., 2012)]. The exact consideration of the electron exchange was shown to be of importance in the RR and photoionization calculations for low-charged ions especially at low energies. Relativistic and multipole effects are of importance for highly charged ions and at high energies. For example, the relativistic Maxwell-Jüttner distribution used for the first time by us in the RR/RPL rate calculations, decreases the rates considerably at a high temperature as compared with the commonly used non-relativistic Maxwell-Boltzmann distribution, the decreasing being ∼ 25% at the temperature kT = $10^9$ K.

The influence of plasmas temperature and density on the energy spectrum and level occupation numbers of ions in Local Thermodynamic Equilibrium (LTE) plasmas was studied. The code PLASMASATOM was created on the basis of the average-atom model using the self-consistent field (SCF) Dirac-Slater method. The average atom model was employed in INFERNO code

[D. A. Liberman, J. Quant. Spectrosc. Rad. Transfer. 27 (1982) 35], PURGATORIO code [B. Wilson et al., J. Quant. Spectrosc. Rad. Transfer. 99 (2006) 658] and in the recent more advanced PARADISIO code [M. Penicaud, CEA-France (2009)].

Our results for the iron, aluminium, and uranium dense plasmas are shown to be in a good agreement with previous calculations by other authors using the above codes, for example, by W.R. Johnson (2001) for iron plasmas at normal metallic density as well as by M. P´enicaud (2009) for uranium plasmas at the ion density Ni =$2.5 \times 10^{19}$ $cm^{-3}$ .

New calculations were performed for the tungsten dense plasmas at Ni $=3.3\times10^{19}$ $cm^{-3}$ (normal metallic density is $6.3\times10^{22}$ $cm^{-3}$). For the first time, the temperature dependence of the energy spectrum and level occupation numbers was determined in the temperature range from 0.1 eV to 10 keV.

In addition, we compared our results with those obtained by a large theoretical collaboration OPAC [D. Gilles et al. (2011)] which was formed to analyse experiments on the opacity of the LULI 2010 campaign useful for astrophysics. In particular, ionization stages q for iron ions in three plasmas with the electron density Ne = $3.16\times10^{20}$ $cm^{-3}$ and temperature 15 eV$\leq$ kT $\leq$ 39 eV were compared with mean ionization stages <q> derived by OPAC collaboration with different eleven codes. Our values of q correlate well with these calculations and are in excellent agreement with the best values of <q> from Opacity Project

[M. J. Seaton, R. M. Badnell, MNRAS 354 (2004) 457] for all three cases, the difference being ∼ 4% at kT =15.3 eV and 0.2% at kT =38.5 eV.

To study tungsten impurities in fusion plasmas, we used for the first time the non-linear SCF screening model for calculation of the screening impurity potential. The well-known Debye model is appropriate only in the case of classical plasmas (high temperature and low density). In our calculations, the chemical potential μ is found before the SCF calculations using the plasmas electron density Ne = $10^{14}$ $cm^{-3}$ and low temperature 1 eV$\leq$ kT $\leq$5 eV. Results demonstrate that the energy spectrum and level populations for a tungsten ion with regard to a temperature differ considerably from those for a free neutral atom. However it was just calculations for a free neutral tungsten atom which were adopted in paper [J. Abdallah Jr. et al., J. Phys. B: At. Mol. Opt. Phys 44 (2011) 075701] as initial data in the collisional radiative model. The average ionization stage <q>=2.07 was obtained for tungsten ion at Ne = $10^{14}cm^{-3}$ and kT = 2 eV. The configurations $5d^3\,6s^1$ , $5d^3\,6p^1$, and $5d^4$ are of the first importance in the radiated power calculations. We obtained the value q =3.45 and the configuration $5d^{2.4}\,6s^{0.1}$ . So we believe that our results could be used as initial data in more sophisticated non-LTE calculations instead data for a free neutral atom. This may drastically change results of these calculations.

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