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

Summary Report of the Second Research Coordination Meeting

Max-Planck-Institute for Nuclear Physics, Heidelberg, Germany
29-31 August 2012

Report prepared by
Bastiaan J. Braams
IAEA Nuclear Data Section

August 2014
Selected INDC documents may be downloaded in electronic form from

http://www-nds.iaea.org/publications

or sent as an e-mail attachment.

Requests for hardcopy or e-mail transmittal should be directed to

NDS.Contact-Point@iaea.org

or to:

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100, A-1400 Vienna Austria

Produced by the IAEA in Austria
August 2014
Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV

Summary Report of the Second Research Coordination Meeting

Max-Planck-Institute for Nuclear Physics, Heidelberg, Germany

29-31 August 2012

Report prepared by
Bastiaan J. Braams
IAEA Nuclear Data Section

Abstract
The second Research Coordination Meeting of a coordinated research project (CRP) on spectroscopic and collisional data for tungsten ions in fusion plasma was held 29-31 August 2012 at Max-Planck-Institute for Nuclear Physics, Heidelberg, Germany. Thirteen projects participate in the CRP and were represented at the meeting together with 8 further experts and 2 IAEA scientific staff. Participants presented their research following which outstanding data needs were identified and a work plan was developed for the remainder of the CRP. The proceedings and conclusions of the meeting are summarized here.

August 2014
# Table of Contents

1. Introduction .......................................................................................................................... 7

2. Presentations .......................................................................................................................... 7
   Opening .................................................................................................................................... 7
   Alfred Müller: Experimental Data for Electron-Impact Ionization, Electron-Ion Recombination and Photoionization of Tungsten Ions. .......................................................... 7
   Peter Beiersdorfer: Tungsten data for current and future uses in fusion and plasma science produced at Livermore. ................................................................. 8
   Hiroyuki A. Sakaue: EUV Spectroscopy of highly charged tungsten ions with electron beam ion traps...................................................... 8
   Yuri Ralchenko: Magnetic-dipole lines from 3d
   ions of tungsten and other high-Z elements. ................................................................. 9
   Fumihiro Koike: MCDF calculation and analysis of E1 and M1 lines from tungsten ions in LHD and EBIT plasmas. ................................................................................... 10
   Chihiro Suzuki: Interpretation of EUV spectra from tungsten ions observed in the Large Helical Device. ......................................................................................... 10
   Thomas Pütterich: Tungsten spectroscopy in fusion plasmas. ........................................... 10
   Sebastijan Brezinsek: Tungsten source spectroscopy for the ITER-Like Wall on JET. ........ 11
   V. S. Lisitsa, V. A. Astapenko and V. A. Shurygin: Ionization balance and polarization radiation emission of tungsten ions in plasmas. ................................................................. 12
   Duck-Hee Kwon, Young-Sik Cho, Yong-Joo Rhee, Young-Ouk Lee: Theoretical cross section for electron impact ionization of W+ forming W2+. .................................................................................... 13
   Xiaoyun Ma, Zhongwen Wu, Chengzhong Dong and Jun Jiang: Electron impact excitation and dielectronic recombination of highly charged tungsten ions. ........................................... 13
   Rajeev Srivastava: Electron excitation of highly charged tungsten ions. ................................ 14
   M. (Alex) Imai: Charge exchange cross sections for Wq+ ions at high energy. ..................... 14

3. Discussion and Work Plan ..................................................................................................... 15
   Review of data needs .............................................................................................................. 15
   Review of experiments and data sources .............................................................................. 15
   Plans for experimental work .................................................................................................. 18
   Plans for theoretical work ...................................................................................................... 22

Appendix I: List of Participants ............................................................................................... 26

Appendix II: Meeting Agenda .................................................................................................. 28
   Wednesday 29 August – Central Seminar Room ................................................................. 28
   Thursday 30 August – Central Seminar Room ................................................................. 28
   Friday 31 August – Central Seminar Room ........................................................................ 29
1. Introduction

Tungsten (atomic symbol W, charge number Z=74) is planned to be used as a plasma facing material in regions of highest heat load (the divertor) in ITER because of its excellent thermal conductivity, high melting temperature and low affinity for tritium. Tungsten is also used on present-day tokamaks in preparation for ITER. Therefore it is important to know the atomic properties of tungsten as a plasma impurity for conditions ranging from those in cold (≃1 eV) divertor plasma to the ≃20 keV electron temperature expected in the plasma core. The entire temperature range and all charge states up to neonlike and a bit beyond are of interest. 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. While tungsten is by far the most important heavy ion impurity in fusion plasma research, it is also one of the most difficult for theoretical calculations. Calculations for near neutral charge states are difficult for any ion, but even in core plasma conditions (T_e~20 keV) tungsten is a (predominantly neonlike) many-electron system.

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. Processes of interest are excitation and ionization by electron, photon and proton impact, auto-ionization, radiative de-excitation and recombination, dielectronic recombination, and charge exchange. Data include cross sections, spectroscopic signatures (line radiation) and integrated power loss.

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 at the Max Planck Institute for Nuclear Physics (MPI-K). The hospitality of the Division and of MPI-K was much appreciated. The 16th International Conference on Physics of Highly Charged Ions (HCI 2012) took place the next week in Heidelberg and many participants of the CRP also attended HCI 2012 while on the other hand some HCI participants joined as expert guests in the meeting of the CRP.

The purpose of the second RCM was to exchange information about ongoing research of the participants and to review the status of work on atomic data for tungsten. The available presentations are collected on the A+M Data Unit web pages at http://www-amdis.iaea.org/CRP/. Section 2 of this report provides a 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.

2. Presentations

Opening

Professor Klaus Blaum, Director of the Stored and Cooled Ions Division at the Max Planck Institute for Nuclear Physics welcomed the participants to Heidelberg. The division is concerned with precision experiments on stored and cooled atomic and simple molecular ions and with related theory. The division operates the heavy ion Test Storage Ring (TSR), which is due to shut down at the end of 2012 to be replaced by the Cryogenic Electrostatic Storage Ring (CSR) that is under construction. The division also has a Penning trap for precision measurements and they work with GSI in Darmstadt for new traps on the Facility for Antiproton and Ion Research (FAIR). The supporting theoretical program in the division is focussed on atomic and molecular quantum dynamics.

Dr José Ramón Crespo López-Urrutia (José Crespo), Team Leader for the EBIT project in the Division for Quantum Dynamics and Control and local host (together with Prof Alfred Müller) for the meeting added his welcome. There will be an opportunity in the afternoon to see the TSR, CSR and EBIT facilities.

Dr Müller opened the presentations with an outline of the data situation for tungsten ions as far as they are relevant for charge state distributions in a plasma and then described new experimental work for electron-ion recombination, photoionization and electron-impact ionization. Theoretical predictions for ionization and recombination of near-neutral complex ions have been unreliable in the past. On the experimental side, before this CRP there were data for electron-impact ionization of \( \text{W}^q^+ \): single ionization for \( q=1..10 \), double ionization for \( q=1..6 \) and triple ionization for \( q=1..4 \). For photoionization of \( \text{W}^q^+ \) the only data were for single ionization of the neutral atom, \( q=0 \), and for electron-ion recombination no absolute cross section measurements are available.

New experimental work was reported on electron-ion recombination. This work was done at the TSR ion storage ring at MPI-K in Heidelberg by a group including S. Schippers from the Institute for Atomic and Molecular Physics (IAMP) at University of Giessen and with contributions from Columbia University and GSI Darmstadt. TSR is a unique facility for electron-ion merged beam experiments, offering excellent energy resolution down to \( 10^{-4} \) eV. Measurements are reported for ions in the range \( \text{W}^{17+} \) to \( \text{W}^{21+} \). The measured recombination rate coefficients are up to 3 orders of magnitude larger than hydrogenic radiative recombination rate coefficients and are also significantly larger than some theoretical calculations based on a hydrogenic model. A correct theoretical treatment needs to include fine structure and internal conversion together with a full mixing statistical approach [V. A. Dzuba et al., PRA 86 (2012), 022714; N. R. Badnell et al., PRA 85 (2012), 052716].

Photoionization is studied in experiments done by the team at IAMP, Giessen, working with R. A. Phaneuf et al., University of Nevada, at the Advanced Light Source (ALS) in Berkeley. Measurements are reported of single and double photoionization of \( \text{W}^{1+} \) and \( \text{W}^{2+} \) and of photoionization of \( \text{W}^{4+} \), for photon energy up to about 100 eV. The photoionization data for \( \text{W}^{4+} \) are compared with close coupling Dirac-Coulomb R-Matrix calculations [C. P. Ballance and B. M. McLaughlin]. The peak of the measured cross section, at \( \approx 54 \) eV, is located about 2.5 eV below the peak of the calculated cross section; the absolute cross sections appear to be in reasonable agreement.

Electron impact ionization is studied using a crossed beams setup at IAMP in Giessen. The present work provides data for single ionization of charge states \( \text{W}^{5+} \), \( \text{W}^{8+} \), \( \text{W}^{11+} \) and \( \text{W}^{12+} \) and total ionization of \( \text{W}^{17+} \) for impact energy up to 1 keV.

The outlook for future work within the CRP is to analyze existing data on recombination, measure absolute data for photoionization of ions up to \( \text{W}^{5+} \), and complete the measurements for electron impact ionization for charge states up to \( \text{W}^{17+} \) in an extended energy range, up to 5 keV if possible.

In discussion the question was raised if it is possible to measure state-selective recombination. In general one tries to identify it from resonances, but it is very difficult for tungsten.

Peter Beiersdorfer: Tungsten data for current and future uses in fusion and plasma science produced at Livermore.

Dr Beiersdorfer explained the need of X-ray spectroscopy for ITER and described the development of the Core Imaging X-ray Spectrometer (CIXS) for ITER, which is the responsibility of the USA. Atomic physics has played a very important role throughout the history of experimental plasma physics and has been crucial for understanding the plasma energy balance and for diagnostic development. Already, ITER diagnostics are being developed based on using tungsten radiation. In particular, CIXS is designed to measure the core ion temperature and bulk plasma motion based on the X-ray emission of neonlike tungsten ions (\( \text{W}^{64+} \)). Ionization balance calculations predict that neonlike tungsten will be abundant for electron temperature between 10 keV and 35 keV and it will be the dominant charge state at 20 keV; experiments on the Princeton Large Torus (PLT) suggest that it will be detected at electron temperature above 12 keV. Tungsten emission will also be measured by extreme ultraviolet (EUV) and optical spectrometers to determine its concentration in the plasma and to assess power loss and the tungsten sputtering rate. The Wolfram Project at Livermore produces data for tungsten in various spectral bands: L-shell X-ray emission for CIXS development, soft X-ray and EUV M-shell and N-
shell tungsten emission for understanding the edge radiation from ITER plasmas, and O-shell EUV emission for developing spectral diagnostics of the ITER divertor. For the design of diagnostics one requires data on the primary lines of interest but also data on any possible contaminant lines after shifting and Doppler broadening.

Port space is a scarce resource on ITER and the present choice is to measure only a single X-ray line in the core plasma; a line at 9.1 keV from W\(^{64+}\). Dr Beiersdorfer showed some considerations that went into that choice; the principal alternative would have been a line at 13.1 keV from heliumlike krypton, Kr\(^{34+}\), which would be introduced as a controlled impurity. The tungsten line is about 8 times brighter per atom at identical plasma conditions, but the plasma can tolerate a higher krypton concentration. In any case, the present choice is to devote the X-ray spectrometer to the line at 9.1 keV from neonlike tungsten.

Measurements were carried out on SuperEBIT and EBIT-I at Livermore of L-shell transitions of W\(^{62+}\) through W\(^{66+}\) [1] as well as of M-shell transition of W\(^{48+}\) through W\(^{61+}\) [2] and these measurements were described here in the context of the CIXS design. At 30 keV the width of the 9.1 keV reference line is about 9 eV and at a velocity of 500 km/s the shift is about 10 eV. The closest neighbouring line is 30 eV away from the reference line, which affirms the choice.

As part of the Wolfram project measurements were made of \(\Delta n=0\) M-shell lines in W\(^{64+}\) to W\(^{48+}\) using a high-resolution grating spectrometer attached to SuperEBIT and EBIT-I. The FAC code was used to calculate theoretical spectra. The measured lines are mostly E1-allowed. Recently further measurements were carried out using EBIT-I and concentrating on lines relevant in the divertor region, conditions \(1 \text{ eV} \leq T_e \leq 150 \text{ eV}\) and \(10^{14}/\text{cm}^3 \leq n_e \leq 10^{15}/\text{cm}^3\). These EBIT-I measurements complement measurements of emission from W\(^{2+}\) to W\(^{10+}\) in the SSPX spheromak at LLNL.

Work performed under the auspices of the DOE by LLNL under contract DE-AC52-07NA27344.


Hiroyuki A. Sakaue: EUV Spectroscopy of highly charged tungsten ions with electron beam ion traps.

Dr Sakaue described EBIT studies to obtain atomic data for tungsten. The “Tokyo-EBIT” was constructed in 1995 and it has an electron energy range from \(~1\) keV to \(~200\) keV. The “CoBIT” Compact Electron Beam Ion Trap [1] provides a complementary energy range of \(~100\) eV to \(~2.5\) keV for which the accessible charge states for tungsten are about \(10-40\). Tungsten is injected in the form of W(CO)\(_6\). The presentation is focussed on extreme ultraviolet (EUV) spectra, wavelengths 15 to 45 Angstrom, obtained on CoBIT in the electron energy range 0.49 keV to 1.5 keV [2], involving charge states W\(^{19+}\) - W\(^{34+}\). Comparison is made with calculations using the HULLAC code in so-called configuration mode (with \(n<9\)) in which only configuration averaged energy and total angular momentum \(J\) characterize the state. The energy range for these CoBIT spectra matches conditions in the Large Helical Device (LHD) at NIFS and emissions from LHD with tungsten impurity clearly show transitions in tungsten charge states W\(^{24+}\) to W\(^{33+}\): transitions 6g-4f and 5g-4f in charge states 24~28 and transitions 5f-4d and 5p-4d in charge states 28~32 or 28~33.

Recent and ongoing work is concentrated on fine structure calculations and fine structure identification in the plasma spectra and also on identification of high Rydberg states.


Yuri Ralchenko: Magnetic-dipole lines from 3d\(^n\) ions of tungsten and other high-Z elements.

Dr Ralchenko reported on progress in interpretation and analysis of extreme ultraviolet forbidden (mainly M1) lines from the high-Z ions with an open 3d shell, following ref. [1]. The NIST Atomic Spectra Database (ASD) version 5.0 (2012) provides information on 2229 energy levels and 14510
spectral lines of W. Using the NIST electron beam ion trap, more than 130 new lines were measured in 3d\textsuperscript{n} ions of Hf, Ta and Au. The lines were identified with a large-scale collisional-radiative modeling of the EBIT plasma using the FAC (Gu, 2003) and NOMAD (Ralchenko and Maron, 2001) codes. It is also found that the M1 line intensity ratios from neighboring ions (e.g., Ca-like and K-like) are a good indication of LMN dielectronic resonances.

A detailed discussion of the collisional radiative modelling was presented following [2]. The spectrum is sensitive to \( n_e \) when \( n_e \sim 1 \times 10^{14} \text{ cm}^{-3} \) or larger. Anisotropy of the electron distribution has an important effect via dielectronic recombination.


**Fumihiro Koike: MCDF calculation and analysis of E1 and M1 lines from tungsten ions in LHD and EBIT plasmas.**

Dr Koike described computations aimed at understanding observations of LHD plasmas at NIFS. Many E1 lines and unresolved transition arrays (UTA) of tungsten highly charged ions have been seen on LHD. Many visible M1 lines were also observed in EBIT ion sources.

The presentation concentrated on detailed analysis of visible lines in W\textsuperscript{26+}. A series of atomic structure calculation has been carried out on those lines by using GRASP and its family of codes and also RATIP. Tentative results for line identification and spectral analysis will be presented. In contrast to the E1 transitions, M1 or E2 transitions may take place between the fine structure multiplets in atomic ions. In the case of transitions in the ground state multiplets of tungsten highly charged ions, visible lines may be generated. The work presented here extends the MCDF calculations that were reported in the first meeting of this CRP in 2010.

The emphasis in the present work is on calculations of visible M1 lines using a large CI basis with analysis of basis set convergence. In addition, for specific transitions special optimization was carried out for the pair of levels in terms of the MCDF method.

**Chihiro Suzuki: Interpretation of EUV spectra from tungsten ions observed in the Large Helical Device.**

Dr Suzuki described measurements of EUV spectra from tungsten ions in plasmas produced in the Large Helical Device (LHD). Quasi-continuum spectral features arising from unresolved transition array (UTA) are often observed in a variety of conditions. Atomic structure calculations for ions with open 5p, 5s and 4f subshells suggest large contributions of stages lower than Ag-like ions in lower temperature conditions. The FAC code is used to support identification and also comparison was done with Cowan code calculations. Major discrete lines are reproduced successfully in the high-\( T_e \) case (\( T_e \sim 2 \text{ keV} \)), but the measured spectrum cannot be reproduced in the low-\( T_e \) case (\( T_e \) below \( \sim 1 \text{ keV} \)). Below \( T_e = 1.0 \text{ keV} \) there should be a large contributions of charge states lower than Ag-like W\textsuperscript{27+}.

Dr Suzuki raised some issues for consideration. At low \( T_e \) (below about 1 keV) it is difficult to find good lines for interpretation. A \( \Delta n=1 \) transition in the 3 nm region may be useful for the interpretation of the dominant charge states. Difficulties in code calculations (Hullac, FAC) for open 4f ions need to be resolved. The charge state distribution in the plasmas seems to be insensitive to transport coefficients, but one needs a reliable database of ionization and recombination rate coefficients for lower charge states. For quantitative evaluation of tungsten ion concentration we need to resolve the absolute sensitivity calibration in the VUV region. Finally in order to reconstruct the tungsten density and radiation profile it would be desirable to measure the spatial profile of EUV spectra.

**Thomas Pütterich: Tungsten spectroscopy in fusion plasmas.**

Dr Pütterich gave an overview about the investigations on the spectral features and spectral lines of W from the VUV to X-ray region that are measured on present experiments, especially AUG. Bolometry is more or less routine, but it does not identify individual lines as 2Dnd it deconvolution is difficult.
The interpretation of soft X-ray data is very challenging and places high demands on the quality of atomic data.

For $T_e$ below 1 keV the emissions come from ions below $W^{28+}$ and the open 4f-shell makes the calculations very demanding. Many more configurations are needed because of configuration mixing and configuration interaction, and millions of transitions are calculated.

In the range 0.8 keV – 1.8 keV the spectrum is largely quasicontinuum. In the range 2.0 keV – 4.5 keV there are spectral lines from $-W^{24+}$ - $W^{45+}$ that are partly accessible with soft X-ray spectroscopy. Some experiments were done on AUG at very high temperature for that experiment, up to 18 keV, where X-ray lines are seen from $W^{60+}$ - $W^{65+}$. It is noted that these spectrometer measurements are line-of-sight integrated and 2D deconvolution is only possible if one has multiple views. The most important demand on the atomic data are the rate coefficients for ionization and recombination, and beyond that the emissivity of the line. The identification of the element (W) is simple.

Dr Pütterich also considered charge exchange recombination spectroscopy (CXRS) for tungsten, but finds that it will be very difficult due to the low expected signal. It may be possible to combine many spectral lines from large spectral range using an Echelle spectrometer + UV spectrometer, but still the background emissions would be a problem for this sensitive measurement.

In conclusion Dr Pütterich presented a data wishlist: (1) High quality ionization and recombination rates from first principles (not matched to tokamak experiment). (2) High quality dielectronic recombination spectra and higher n contributions to improve SXR interpretation. (3) Someone to do the needed huge model calculations for the ions with an open f-shell, $W^{14+}$ - $W^{27+}$.

Sebastijan Brezinsek: Tungsten source spectroscopy for the ITER-Like Wall on JET.

Since September 2011 the JET experiment is operating with an “ITER-Like Wall”: beryllium for the main wall and tungsten in the divertor where the highest heat load occurs. Dr Brezinsek described spectroscopy of low charge states of W in the divertor and the opportunity to use this spectroscopy as a real-time measurement of the rate of erosion. The principle of tungsten source spectroscopy was explained and relevant lines in W I and W II were discussed. In W I ($W^{60+}$) the best lines are at 400.875 nm, 429.459 nm, 505.328 nm and 434.811 nm. Calculations for these lines were compared with measurements on TEXTOR. The line at 400.1 nm looks best for purpose. The S/XB for this line was assessed on several experiments using different methods: Weigh loss, spectroscopy, injection of $WF_6$ and injection of W(CO)$_6$ and the resulting S/XB more or less agrees as a function of $T_e$ among the various measurements. Note that there is not a first-principles calculation of S/XB.

The ratio of emissions between W II and W I can be used as measurement of prompt redeposition. Data from JET indicate >50% redeposition, in agreement with earlier data form TEXTOR.


Intense lines in the spectrum of W VIII in the VUV region belong to the $4f^{13}5s^25p^6$ - ($4f^{13}5s^25p^65d + 4f^{13}5s^25p^5(5d+6s)$) and $4f^{14}5s^25p^5$ - $4f^{14}5s^25p^5(5d+6s)$ transitions. Because the low-lying configurations $4f^{13}5s^25p$ and $4f^{14}5s^25p^5$ coincide in energy, all these transitions are resonance transitions. 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. 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 $4f^{13}5s^25p^6$ - $4f^{13}5s^25p^5j_{1/2}5s$ [1] and $4f^{14}5s^25p^5$ - $4f^{14}5s^25p^56s$ transitions. The lines of the group at 200 Å are mostly identified as $4f^{13}5s^25p^6$ - ($4f^{13}5s^25p^5j_{1/2}5d + 4f^{13}5s^25p^5j_{3/2}6s$) transitions, contrary to a former suggestion [2] that they could belong to transitions from the $4f^{14}5s^25p^45d$ configuration. Intense lines in the 250 Å region belong mostly to the $4f^{13}5s^25p^6$ - $4f^{13}5s^25p^5j_{3/2}5d$ transitions.
The identifications are verified by isoelectronic regularities based on simultaneous analyses of the same transitions in the isoelectronic spectra Hf VI [3], Ta VII and Re IX.


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 and on the isoelectronic ions Hf VI, Ta VII and Re IX will be presented by A. N. Ryabtsev from Troitsk. We will report some revisions in spectra of more moderately charged tungsten ions allowed by new experimental data.


We discuss three research areas relevant to the plasma modeling of tungsten that are ongoing at Los Alamos National Laboratory.

Firstly, we present improvements to previously published electron-impact excitation collision strength data for the Be- and B-like iso-electronic sequences [1]. The new data have been calculated in the relativistic distorted-wave approximation for ions with 26 ≤ Z ≤ 92, involve Δn=0 transitions with n=2, and use a fully relativistic plane-wave Born top-up approach to obtain more accurate collision strengths at high impact energies [2]. The data for Be-like ions will be published in ADNDT [3] and examples will be presented for tungsten ions at the meeting.

Secondly, we will summarize the tungsten test case considered at the recent NLTE-7 Workshop that was held recently in Vienna in December 2011. This workshop provides a forum for detailed comparison of plasma and spectral quantities from NLTE collisional-radiative modeling codes. We will provide a brief discussion on the role of metastable states and multipole transitions for spectral modeling of tungsten at plasma conditions considered at the workshop.

Finally, as time allows, we will discuss collisional-radiative modeling of tungsten at very low (few eV) temperatures, which may be important in the tokamak divertor region. We will present our findings from a recent preliminary study.


V. S. Lisitsa, V. A. Astapenko and V. A. Shurygin: Ionization balance and polarization radiation emission of tungsten ions in plasmas.

The analysis of ionization equilibrium of tungsten ions in tokamak plasmas is presented. It is shown that the ionization state distribution is close to a Gaussian one in the ionic charge space in the plasma periphery. The effect is due to sharp gradients of mean charge of ionization equilibrium resulting in
dominant contribution of ionization processes as compared with recombination ones. The radiation emission processes in collision of free electrons with tungsten ions is analyzed in detail. The contributions of two radiation channels in free-free and free-bound radiative transitions are presented: electron emission in static statistical ion potential versus radiation polarization emission of tungsten ion core. The detail comparison of radiation spectra are presented together with total radiative recombination rates.

**Duck-Hee Kwon, Young-Sik Cho, Yong-Joo Rhee, Young-Ouk Lee: Theoretical cross section for electron impact ionization of W⁺ forming W²⁺.**

We have investigated electron impact ionization cross section for singly charged tungsten ion W⁺ by theoretical calculation using the flexible atomic code (FAC) based on a distorted wave (DW) approximation. We have found that DI for the ground state is very sensitive to the choice of local central potential for atomic orbital description. When the local central potential is optimized to the ionized target configurations 5d⁴+5d⁷6s, the DI cross section peak is about 35% smaller than when the initial target ground state configuration 5d⁷6s is used for the local central potential. In addition indirect EA cross sections for the 5d₆s→nl (5≤n≤35) and 5s₅p→nl (5≤n≤10) transitions have been calculated with the detailed branching ratios. Our results have been compared with experimental measurements and other previous theoretical works.

**Xiaoyun Ma, Zhongwen Wu, Chengzhong Dong and Jun Jiang: Electron impact excitation and dielectronic recombination of highly charged tungsten ions.**

Electron impact excitation (EIE) and dielectronic recombination (DR) of tungsten are the most essential atomic processes in the plasma. A systematical study on the cross sections of these processes is necessary for present fusion experiments and the modeling of plasma properties. Furthermore, the degree of linear polarization of radiation emitted from the unequally populated magnetic sublevels can provide a detailed knowledge about their dynamics processes and has been recognized as an important diagnostic tool to characterize plasmas anisotropy.

In the present work presented by Dr Dong the target ion and the continuum electron wavefunctions are generated by the codes GRASP92 and RATIP based on the MCDF method. The EIE and Capture cross sections of the individual magnetic sub-levels are calculated by using the codes REIE06 [1] and REDR05 [2]. Furthermore, these cross sections are employed in calculating the linear polarization of the strongest nf →3d (n=4,5,6) lines from both the EIE and DR processes for highly-charged Ni-like to Ge-like tungsten ions. The linear polarization of 4f→3d and 5f→3d lines following EIE increases sharply with increasing of incident electron energy before starting to decrease at higher energy region. The polarization for the same lines but formed by DR is very different from that formed by EIE.

Rajeesh Srivastava: Electron excitation of highly charged tungsten ions.

The RDW method is employed to study the electron impact excitation of highly charged tungsten ions. Despite a great amount of work reported for various W ions, there is in general serious lack of excitation cross section data for various transitions for all the different ionic stages of tungsten ions. In this connection, we performed extensive calculations of cross sections in the wide range of incident electron energies up to 50 keV for dipole allowed transitions resulting due to the electron impact excitation from their M-shell of the ground states of Zn-like through Co-like tungsten ions. Their respective ground states are \([(\text{Ar})3d^{10}4s^2]J=0\) for Zn-like, \([(\text{Ar})3d^{10}4s^1]J=1/2\) for Cu-like, \([(\text{Ar})3d^{10}]J=0\) for Ni-like and \([(\text{Ar})3d^9]J=5/2\) for Co-like W ions. These transitions have been identified to be among the most intense lines in the M-shell X-ray spectra of Zn-line through Co-like W ions [1-3].

The recently developed RDW code as discussed earlier for electron impact excitation of ions using fully relativistic distorted wave (RDW) theory has been used to perform the calculations. Using RDW method we have calculated the cross sections for excitation of the electrons from 3\(d\) to 4\(p\) and \(n\)\(f\) sub-shells. Here we have considered \(n=4\) – 6 for Zn-like W\(^{44+}\) and Cu-like W\(^{45+}\), \(n=4\) – 8 for Ni-like W\(^{46+}\) and \(n=4\) and 5 for Co-like W\(^{47+}\) which belong to most intense lines observed in the M-shell X-ray spectra [3]. Since all the transitions considered in this work are dipole allowed we have also provided analytic fits of our calculated cross sections at high energies to the Bethe-Born formula which can be useful to plasma application purposes. Recently the linear polarization measurements were reported for the Ni-like W ion by Clementson et al [4]. In the light of the possibility of such measurements, in addition to the cross sections, we have also calculated and reported the results for the linear polarization of the photon emissions following the decay of electron impact excited anisotropic states to the ground states for all the four ions.


M. (Alex) Imai: Charge exchange cross sections for W\(^{\text{q+}}\) ions at high energy.

A new experiment for producing ionization, electron capture and loss cross sections for H + W\(^{\text{q+}}\) collisions at NBI energy (up to 1 MeV/u) is under the preparation now. We will make use of the tandem accelerator in JAEA to provide 184 MeV (1 MeV/u) W\(^{\text{q+}}\) ions as well as an atomic hydrogen source to produce crossed-beam H target. In the plan, ionizations of W\(^{\text{q+}}\) projectile ions will be measured with a charge analyzer downstream firstly and coincidence measurements of the recoil H\(^+\) ions will be performed next. We have already measured charge state distribution of 184 MeV W\(^{30+}\) incident ion after penetrating a C-foil, assuming we have only to replace the target with atomic hydrogen to complete the first plan.


New relativistic Dirac-Fock calculations for 30 tungsten ions in the range W\(^{24+}\) – W\(^{57+}\) were carried out. The partial photoionization cross sections as well as partial and total radiative recombination (RR) cross sections were obtained at electron energies from 1 eV to 60 keV. The RR rate coefficients and radiated power loss rate coefficients were calculated for temperatures from 10\(^4\) K to 10\(^9\) K. Besides, the effect of the target core electron polarization on the RR cross section was estimated for tungsten highly-charged ions as well as for the Fe XVII ion where a comparison with experimental data might be performed. The polarization effect was assessed for highly-charged tungsten ions in the nonresonance energy ranges. The enhancement factor of the RR cross section due to the effect varies from
approximately 17% to below 1%. The factor depends on the photon energy, the principal quantum number of polarized electrons, the ion charge and does not practically depend on the final electron state in the RR process.

3. Discussion and Work Plan

Review of data needs

From the perspective of modelling of tungsten impurity in the core region of fusion plasma the largest uncertainty in the atomic physics is in the process of dielectronic recombination; this is where both experimental and theoretical data is most needed. Ionization stages larger than \( \sim W^{30+} \) are interesting for today’s experiments, while for hot ITER discharges one requires recombination rates for the ions above \( \sim W^{35+} \).

Another area of need is that of cross sections for excitation and ionization of very low charge states in conditions far from equilibrium and of the associated radiative rates, as is relevant for source term spectroscopy. Tungsten atoms are sputtered into plasma that has electron temperature 100 eV or higher where they are rapidly ionized. The intensity of emissions from \( W^{1+} \) and \( W^{2+} \) may provide a measurement of the neutral tungsten source rate.

Review of experiments and data sources

**Spark plasma**: In this CRP spark plasma is represented by the work in Paris and Troitsk by W.-Ü L. Tchang-Brillet, J.-F. Wyart and A. Ryabtsev. Spark plasma sources can be used to study VUV emission spectra of low and moderately charged ions (e.g. \( W^{2+} \) to \( W^{8+} \)). The spark plasma is produced in a vacuum chamber by high voltage discharges through a low-inductance electric circuit. Depending on the discharge conditions (mainly the peak current) the temperature varies between a few eV and 20 eV and the electron density is up to \( 5 \times 10^{17} \) \( \text{cm}^{-3} \). The detection of the spectra is integrated over time. The complex emission spectrum of the source is recorded using high resolution spectrograph (\( \sim 100 000 \)) and analysed with the support of theoretical and parametric calculations (Cowan’s codes). The analysis provides fundamental data, such as precise wavelengths (\( \pm 0.005 \)Å). These plasmas produce intense spectral emission in very many lines, including lines from states that are only accessed by multi-stage excitation. Due to these features spark plasma are a beautiful source to determine many levels and transitions and match these lines to calculated transitions for assignment of energy levels and of semi-empirical wavefunctions and oscillator strengths. On the other hand, many ionization states are present at the same time in these plasmas and the measurements are integrated over a line of sight with variable conditions, so one doesn’t get clean experimental data on level populations or transition strength.

**Laser produced plasma**: Not represented in this CRP. Laser produced plasma provides higher temperature and higher charge states than spark plasma, with emission spectra in the EUV and X-ray regions.

**EBIT experiment**: This CRP has contributions from EBITs at Livermore (P. Beiersdorfer), NIST (Yu. Ralchenko), Tokyo (N. Nakamura and H. Sakaue), and at the Second RCM also Heidelberg (J. R. Crespo López-Urrutia).

The strength of measurements with an electron beam ion trap is the possibility to observe the photon emission as a function of the energy of the electrons using ions that are thermally cold. This allows the use of very high-resolution spectrometers to get very good spectroscopic data (wavelengths). It also produces information on excitation processes, which includes dielectronic recombination, electron-impact excitation, charge exchange, and to a lesser extent excitation by radiative recombination. From this one can extract cross sections for dielectronic recombination, resonance excitation, and electron impact excitation. The electron energy can be more than 100 keV or as low as about 100 eV; the lower bound is associated with space charge effects and spreading of the beam. The data provide very accurate benchmarks for theory, especially for highly charged ions, but data can be collected for essentially all charge states of any element (even neutral). The magnetic trapping mode of operation of an electron beam ion trap allows the measurement of metastable lifetimes of highly charged ions. The ion
plasma in an electron beam ion trap represents an ideal testbed for benchmarking ionization balance calculations, because the ionization balance of the ion plasma is determined by a limited, selectable subset of ionization and recombination processes.

For interpretation of measurements it is very important to take account of polarization of the line, which depends on the magnetic sublevels involved. Crystal spectrometers are sensitive to polarization.

The EBIT has uses beyond spectroscopy. One can do rapid variation of the beam energy and thereby obtain data on recombination and ionization rate coefficients. On the other hand, known partial cross sections for radiative recombination (into Rydberg states?) are used for normalization and also for measurements of charge state balance. The variation of beam energy may also be done in order to mimic a Maxwellian distribution.

Background neutral gas is a problem as it affects the ionization balance and the emissions. One has to take it into account.

**Ion beam experiments:** These are represented in this CRP by the work of A. Müller and colleagues. The cleanest experiments involve ions in a storage ring where they are generally in the ground state. For merged beam electron-ion collisions at low collision energy one may resolve the final state as well; at higher collision energy there is a bigger spread and one cannot resolve the final state anymore. Merged beam experiments are also done using an ion source, but then there are always problems with metastable ions; one does not have the same clean resolution of the incoming state. The principal uses of merged beam experiments are measurements of radiative and dielectronic recombination and electron impact ionization; indirectly also electron impact excitation. Merged beam (and crossed beam) experiments do not provide a comprehensive dataset, but they provide precise tests. The Heidelberg storage ring is shutting down in late 2012 and this is a big loss for atomic data measurements. The Darmstadt storage ring is oversubscribed for other work.

Photoionization experiments are also done on ion beams, but at present there is no combination of storage ring and light source. The photoionization experiments are restricted to beams from an ion source, so there is the problem of metastable states. (Some special techniques exist to get rid of metastables, but nothing in general.) These experiments provide information about oscillator strengths, radiative recombination and electronic structure; they are valuable for fusion plasma atomic data even for photoionization processes that are not directly relevant to fusion plasma.

**Strengths and weaknesses of merged and crossed beams experiments:** Interacting beams experiments involving electrons and photons on one side and ions on the other have the advantage that mass and charge analysis can be done on the ion beams after the interaction. The parent ion beam typically consists of one defined isotope in one defined charge state. The ions usually have been accelerated to an energy sufficient to guarantee 100% detection efficiency of the product ions. In the collisions of electrons or photons with ions little momentum is transferred to the ions. So the ions undergoing a collision do not significantly change their direction. The recombined or ionized ions travel along with the parent ions, they are magnetically separated and the total angular distribution of the products is found within the acceptance of the detector. So, the measurements cover the whole angular range of the product, i.e. one has $4\pi$ collection of the products. The problem of characterizing beam overlap is technically demanding, but it can be solved and the result is that absolute cross sections can be determined in an almost straightforward manner.

Electron beams can be produced with a quite narrow energy spread. In crossed beams the Giessen group uses an electron beam with almost spectroscopic energy resolution of 2 to 3 eV at 1000 eV. With that resolution (and no contribution from the ion beam to the energy spread) details in the cross sections become accessible and resonances in electron impact ionization can be made clearly visible. Measuring recombination in cross beams is possible but would suffer from enormous levels of background primarily arising from electron capture by the parent ions in the residual gas. Therefore, the method of choice for recombination is to use merged beams with relatively fast ions (e.g. 10% of the speed of light) which have small cross sections for electron capture from the residual gas and thus produce little background. The merged beam arrangement has the advantage that the collision energy resolution in the center-of-mass frame strongly exceeds that of the laboratory frame. At low relative velocities between electrons and ions one can reach energy resolutions of a few meV with ions that
have an energy of hundreds of MeV. But also at 10 keV center-of-mass electron-ion collision energies, the kinematical advantage of the merged-beam technique still offers energy spreads as low as about 2 to 5 eV depending on the laboratory electron beam quality.

Photon beams from synchrotron radiation sources offer excellent energy resolution. Band widths as narrow as about 1 meV have been employed in photon-ion absorption experiments at resolving power 40000.

A problem in most of the interacting beams experiments is the low density in the beams which leads to relatively low signal rates. Therefore, the interacting beams techniques are mainly restricted to the measurement of total cross sections only differentiated by the number of electrons ejected in the interaction (i.e., one can distinguish between single and multiple ionization channels).

A problem in crossed beams experiments (single-pass experiments) is the possible presence of long lived excited ions in the parent ion beam. This disadvantage can also be used to get information on collisions involving excited states provided the mixture of ground-state and metastable ions is not too complex. Storage rings provide the possibility to start a collision experiment after a certain time span after production of the ions, so that excited states have time to decay. Therefore, storage rings offer the opportunity to measure with ions in a well defined electronic state: the ground state.

Fusion plasma experiments: Primarily we view the fusion plasma community as the user of atomic data, not as the producer. However, arguably fusion plasma diagnostics can produce accurate and robust information for the fractional abundances of important charge states. If this is to be used to test atomic data then one has to have accurate \( n_e \) and \( T_e \) profiles as well. Note that standard spectroscopic measurements are integrated over a line of sight, but charge exchange recombination spectroscopy is spatially resolved. Line ratios of groups of spectral lines may be used to determine the relative abundance of different charge states along the line of sight of the spectrometers.

For special discharges that feature the phenomenon of impurity accumulation, very accurate shapes of the fractional abundance curve vs. electron temperature can be obtained. In these discharges the transport levels are very low such that effects of transport which are anyhow small for W are further diminished and can be neglected. These measured fractional abundance curves do not rely on absolute numbers for the line intensities and on the other hand only give normalized shapes of the fractional abundances. However, they yield an ultimate benchmark for the ionization equilibrium in a Maxwellian plasma at fusion relevant electron densities. No information can be derived about the separate role of ionization and recombination.

Charge exchange cross section measurements: It may be possible for M. Imai (Kyoto) to carry out total cross section measurements working with a JAEA tandem beam line for ions in the range W\(^{25+}\) to W\(^{40+}\). It is probably too difficult to resolve partial cross sections using the available spectrometer.

Overlap and complementarity between experiments: EBIT and storage ring experiments are mainly complementary; EBIT can measure DR down to about 100 eV and this barely overlaps with storage ring data. On the EBIT one mainly looks at photons while on the storage ring one mainly looks at charged particles. Storage ring experiments sometimes gives energy resonances that can’t be obtained from EBIT, because no photons are emitted. Beam experiments involve a single charge state whereas on an EBIT there is a mix of charge states. If one wants to reproduce more nearly the beam conditions in an EBIT then ion cyclotron resonance provides a way to clean the charge states in the trap.

Photoionization and photoexcitation studies are done when the EBIT is attached to a synchrotron or free-electron laser light source; there is no similar facility on storage rings.
Plans for experimental work

J. R. Crespo López-Urrutia and Z. Harman: Multi-band spectroscopy on highly charged tungsten ions at the Heidelberg Electron Beam Ion Trap facility

Tungsten has ideal properties for a wall material for the chambers and divertors of the next generation of tokamaks. Its ions play major roles in plasma cooling and energy transfer to the walls. Thus, understanding its complex emission spectrum can benefit from multi-band spectroscopy using electron beam ion traps (EBITs). At the Max-Planck-Institute für Kernphysik in Heidelberg a starting research program on tungsten ions has started to generate abundant data on the resonant photorecombination processes (KLL, LMM, MNN).

In the next two years, we plan to expand this work with further measurements and corresponding state-of-the-art calculations. For the experimental work, three EBITs are available. The theory group of Z. Harman is specialized in high-level multiconfiguration Dirac-Fock calculations [1], but also operates configuration-interaction Dirac-Fock codes, and the standard Flexible Atomic Code.

Theoretical work will focus on the effect of resonant photorecombination with multiple excitations, such as dielectronic, trielectronic, and quadruelectronic recombination. In this field, seminal work has been carried out recently by Dr. Harman's group [2]. The various contributions from a multitude of resonant channel have a strong and sometimes dominant effect on the ionization balance of tungsten plasma ions, and in the X-ray emission from those ions.

Hyper-EBIT, one of the MPIK EBITs is equipped with two grating spectrometers, a silicon drift detector and a metallic magnetic microcalorimeter to simultaneously cover the photon energy range from 40 eV to 30 keV. The different spectral ranges are recorded as a function of the electron energy in the range 1 keV to 12 keV, which has an excitation energy resolution between 6 eV and 30 eV in this range. Hyper-EBIT can currently produce ions from W VI to W LXV, and is particularly well suited for the study of dielectronic resonances.

In the field of photoionization, where very scarce data are available, FLASH-EBIT [3,4] will be used to study the photoionization and photoexcitation of tungsten ions from W VI to W XXXVII, around the Ni-like shell closure, with photons in the range up to 1 keV. For this purpose, one experimental campaign at the synchrotron radiation facility BESSY II will be planned. These experiments can reach an enormous resolution in the photon channel and will therefore also help identify the different transitions in the soft X-ray unresolved transition arrays. Those experiments will also utilize the ion extraction capabilities for the investigation of the ratio of autoionization to photonic relaxation.

Additionally, both an optical spectrometer [5,6] and a laser spectroscopy laboratory [7] attached to the Heidelberg EBIT serve for high resolution investigation of forbidden optical transitions in tungsten ions with in charge states from 6+ to 56+. Data in this spectral range are useful to diagnose and gauge the wall erosion rate in the future divertor of ITER, and to clarify the level structure of such complex ions.

References


Simon, M.C., Schwarz, M., Epp, S.W., Beilmann, C., Schmitt, B.L., Harman, Z., Baumann, T.M., Mokler, P.H., Bernitt, S., Ginzel, R., Higgins, S.G., Keitel, C.H., Klawitter, R., Kubiček, K.,


VUV spectrometer will be installed in the Compact EBIT (CoBIT) making possible the observation in the range from 1 nm to 1000 nm continuously with EUV, VUV and Visible spectrometer. We will search for previously unreported lines. In collaboration with Dr. Suzuki and LHD group the EUV and visible spectra of CoBIT will be compared with LHD plasma spectra. In collaboration between H. A. Sakaue and Prof M. Imai we plan to measure the charge transfer (exchange) cross sections of tungsten HCl with H atom at low energy region by using EBIS.


2012-2013: Wavelengths of lines in the 30 - 60 Ångstrom soft X-ray band of tungsten ions around Pd-like W will be measured at the EBIT-1 electron beam ion trap. The data will be compared with spectra obtained at the NSTX and Alcator tokamaks. Measurements of near neodymiumlike tungsten (W$^{3+}$ to W$^{12+}$) in the 150-300 Å region will be attempted a resolving power of about 3000 to 4000, which will be 10x higher than before. L-shell lines of additional charge states of tungsten (W$^{62+}$ and lower) in the 8 - 12 keV spectral range will be measured to build up a complete L-shell tungsten spectrum, in order to be able to analyze spectra expected to be produced by ITER and other hot magnetic fusion plasmas. An attempt will be made to measure the tungsten ionization balance under specific, possibly Maxwellian, conditions. We will also continue calculations of tungsten energy levels, radiative rates, autoionizing rates, and dielectronic recombination rates using three set of codes (HULLAC, Cowan code, and many-body perturbation theory code). In 2012 this will mean a calculation of the Cu-like tungsten energy levels and rates.

A. Ryabtsev: Spectra of W VIII and W IX and Isoelectronic Ions of Hf, Ta and Re.

2012-2013: Continuation of production of high resolution VUV spectra of tungsten and of Hf, Ta and Re; measurement of wavelengths and intensities of the lines, differentiation of the charge state of the spectral lines using a variety of the spark source conditions. Theoretical calculations of the spectra using Cowan codes. Elimination of possible misidentifications in W VIII by continuation of isoelectronic analyses of Hf VI – Re IX and by search for transitions in W VII and isoelectronic spectra. Studies on W IX and isoelectronic spectra.

Plans for 2012-2013: Continued work on high-resolution VUV spectra of tungsten and of neighbouring ions (Hf, Ta, Re) in the normal incidence wavelength region. Spectra will be produced using spark sources operated in various conditions to differentiate the charge states of the emitting ions. Submit common publications with A.N.Ryabtsev’s group reporting results obtained on W VIII and Hf VI. Make data available on http://das101.isan.troitsk.ru and http://molat.obspm.fr.

Take advantage of the newly purchased high resolution scanner for image plate to get better resolution in the short wavelength region (lambda < 500Å) and better calibration of intensity measurements.

Analysis of the normal incidence region of tungsten spectra and of neighbouring ions (Hf VI and Ta VII). In W V: identification of 6p-6d and 6p-7s transitions and core-excited 5p65d2 - 5p5d3 and -4f135d1 transitions. In W VIII: 5p'6s and 5p'5d - 5p'6p, 4f135p'5s6s and 4f135p'5d - 4f135p'6p transitions.

A. Müller: Crossed- and merged-beams experiments on tungsten ion interactions with photons and electrons.

New for 2012-2013: The group of A. Müller and their collaboration partners (Max-Planck-Institute for Nuclear Physics, Heidelberg, Columbia Astrophysics Laboratory, New York, University of Nevada, Reno, Advanced Light Source, Berkeley ) had agreed to contribute to the present CRP by providing experimental data for electron-ion recombination, electron-impact ionization and photoionization of selected tungsten ions. The emphasis of this work is on collisions, however, the spectroscopic techniques employed primarily by using monochromatized synchrotron radiation but also by performing high-resolution energy scans of cross sections reveal structural details in the ionization and recombination spectra associated with specific levels of the investigated parent and product ions.

Progress:

The group has measured storage-ring electron-ion recombination rate coefficients for W18+, W19+, W20+ and W21+ ions. For W20+ the data analysis was completed, absolute storage-ring and plasma rate coefficients were determined and the results have been published.

The Giessen group has measured absolute cross sections for electron-impact ionization of W6+, W8+, W11+, W13+ and W17+ ions at electron-ion collision energies up to 1 keV. The data for W6+ and W8+ are in excellent agreement with previous measurements of Stenke et al. Both the previous and the new experiments made use of the electron-ion crossed-beams technique employing different experimental arrangements. The analysis of the measurements on W17+ ions (single and double ionization) was finalized and configuration-average distorted wave calculations were carried out to determine the direct single-ionization contributions from different subshells of W17+ ions using the Los Alamos Atomic Physics Codes package. Comparison of the theoretical result with the experimental data indicates substantial additional contributions beyond direct ionization arising most likely from inner sub-shell excitations with subsequent autoionization. The results of this work (on W17+ ions) have been published.

The Giessen-Reno-Berkeley collaboration has measured photoionization spectra for W1+, W2+, W3+, W4+ and W5+ ions within a wide range of photon energies in the accessible range from about 20 eV to 300 eV. Monochromatized synchrotron radiation from the Advanced Light Source was employed in a photon-ion merged-beam arrangement. Beside single ionization also multiple ionization was addressed where experiments were feasible. First spectroscopic results have been published. For some of the measured (relative) spectra absolute cross section measurements have been performed so that the spectra can be put on an absolute cross section scale. Although photoionization is not of immediate interest in connection with the relatively thin fusion plasmas in tokamaks or similar machines, the joint experimental and theoretical effort is undertaken to better understand the structure of the complex many-electron tungsten ions and its influence on their collisional behavior.
Future plans:
The raw data obtained at the Heidelberg heavy-ion storage ring for W$^{18+}$, W$^{19+}$, and W$^{21+}$ ions are presently being analyzed. Finalized electron-ion recombination storage-ring rate coefficients will be determined for these ions and absolute plasma rate coefficients will be derived as a function of temperature. For easy use in plasma modeling, the rate coefficients will be fitted by suitable functions and the fitting parameters will be provided. In close interaction with the theory group around Nigel Badnell, University of Strathclyde, the Giessen group will contribute to the detailed understanding of the physics behind the observations and will help in the process of optimizing the theoretical treatment of electron-ion recombination of complex many-electron ions. Since the Heidelberg TSR storage ring will be shut down by the end of 2012, no more recombination measurements on tungsten ions will be possible in the near future.

The Giessen group will fill in the gaps between the existing experimental ionization data up to charge state W$^{17+}$. Absolute electron-impact ionization cross sections will be determined. Detailed energy-scan measurements will be carried out to reveal fine details of the cross section function from which one can draw conclusions about ionization mechanisms and processes contributing to the observed net single- (or multiple) ionization cross sections. The group will also perform calculations on direct ionization and excitation-autoionization contributions to the observed cross sections. The possible influence of long-lived excited states in the parent ion beam on the measurements will be investigated. An attempt will be made to extend the electron energy range beyond the present limit (1000 eV) to much higher energies (e.g. 5 keV).

The Giessen-Reno-Berkeley collaboration will complete the raw-data measurements carried out at the Advanced Light Source. For example, the present state of the measurements indicates, that a detailed scan measurement of the photoionization cross section for W$^{4+}$ ions at high energy resolution would be desirable. Moreover, the absolute measurements that have been started for the lower charge states up to W$^{3+}$ will be completed so that all photoionization spectra taken to date can be normalized and thus be put on an absolute scale. For understanding the details of photo single ionization of low-charge tungsten ions, the close collaboration with B. M. McLaughlin, The Queen’s University, Belfast, and C.P. Ballance, Auburn University, will be continued. Extensive R-matrix calculations will be performed and compared to the experimental results aiming at the development of suitable close-coupling basis sets that can deliver converged cross sections and accurate level energies.

**Plans for theoretical work**

**Yu. Ralchenko:** Experimental and Theoretical Analysis of EUV and X-ray Spectra from Highly-Charged Ions of Tungsten and isoelectronic ions of other high-Z elements.

Plans for 2012+: Analysis of LMn inner-shell dielectronic resonances in 3dn ions of W and other high-Z elements using ratios of magnetic-dipole lines. A new X-ray spectrometer will be installed on the NIST EBIT and test measurements will be performed. Prepare an extensive publication of the W results from the NLTE-7 Code Comparison Workshop. In collaboration with D. R. Schultz (UNT) initiate calculation of charge-exchange cross sections (W$^{q+}$ + H) with the Classical Trajectory Monte-Carlo method. Prepare a set of test cases for W at NLTE-8. New W spectroscopic data from all available sources will be critically compiled and added to the NIST Atomic Spectra Database.

**M. Trzhaskovskaya and V. Nikulin:** Unified Database of Radiative Recombination and Photoionization Cross Sections as well as Radiative Recombination and Radiated Power Loss Rate Coefficients for Tungsten Ions in Plasmas.

Plan for 2013: 1. Development of the code for determination of quantum mechanical spectrum, wave functions and level populations of ions embedded in the high-temperature uniform electron gas (fusion plasma). We will modify the self-consistent “average atom” model employed in the Los-Alamos IN-FERNO code for study of the high-temperature and high-density metallic plasma. Implementation of our new code will be based on our computer code package RAIN (Relativistic Atom. Interaction of electromagnetic radiation and Nucleus with atomic Electrons).
2. To perform relativistic calculations of photoionization and radiative recombination cross sections (PCS and RRCS) for ground and excited states for a number of tungsten ions \( \text{W}^{q+} \) with charges in the range \( 58 \leq q \leq 71 \) in the kinetic electron energy range from 1 eV to 50 keV. The relativistic Dirac-Fock method is used. All multipoles of the radiative field are taken into account. To carry out calculations of partial and total radiative recombination rate coefficients (RR rates) and radiated power loss rate coefficients for these ions in the temperature range from \( 10^4 \) K to \( 10^9 \) K. To determine fit parameters for approximation of partial PCS which allow one to obtain PCS, and consequently RRCS, at any photon energy. To fit total RR rates by the analytical expression involving four fit parameters. New calculations will be supplemented the unified electronic database for tungsten ions.

Later: Study of effect of the plasma electron density on energies and probabilities of the strong X-ray E1, M1, E2 transitions in tungsten ions important for the ITER plasma diagnostics. The code package RAINE and the new developed code mentioned above will be used.


1. Investigation of collective effects in spectra of complex atomic systems which includes:
   1.a. development of plasma atomic models for tungsten ions;
   1.b. Calculations of quasicontinuum spectra of tungsten ions for different temperatures;
   1.c. Estimations of radiative-collision processes rates on the basis of statistical models of complex ions.

The advantage of statistical models is their universal nature which is of both fundamental interest (as collective effects in atomic physics) and applied interest (as fast codes for tungsten spectra calculations to be combined with more complicated transport codes- ASTRA, DINA, etc.).

2. Development of quasiclassical method for calculations of dielectronic recombination rates, which includes:
   a) calculations of dielectronic recombination rates differential in principal and orbital momentum quantum numbers in spherical basis;
   b) calculations of DR rates in parabolic basis in order to account for the presence of external electric field in plasmas;
   c) calculations of total DR rates in both bases and comparison between the approximations.

The selective (in principle quantum numbers ) DR rates are necessary for population kinetics of highly excited atomic states responsible for background radiation in visible and infrared spectral range essential for plasma diagnostics. The quasiclassical approach to DR rates with core excitation without change of principal quantum numbers is based on following estimations: the captured electron energy \( E \) has to smaller as the core excitation energy which is of the order of \( Z \) (a.u.) and it is small as compare with the ionization energy being of order of \( Z^2 \); the last inequality just corresponds to the condition \( Z^2/E \gg 1 \) of classical electron motion in the field of highly charged ions (see Landau – Quantum mechanics). The classical consideration makes it possible to obtain universal results for DR rates selective in quantum numbers.

The effect of external electric field on DR rates was tested theoretically and confirmed experimentally (A. Muller et al., 1995). It results in the increase of DR rates several times (3 times in experiment). So the calculation of DR rates in the presence of plasma microfield (related to the transition from spherical to parabolic basis) is of interest for applications.

Chenzhong Dong: Dielectronic Recombination Cross Sections and Rate Coefficients of Highly Ionized Tungsten Ions.

The DR cross sections and rate coefficients, maybe electron impact excitation and excitation-autoionization and resonance photoionization will be calculated for As-like to Zn-like W ions (\( \text{W}^{41+} \) to \( \text{W}^{44+} \)). Possibly resonance photoionization for some lower charge states. Analytical expressions as function of electron temperature will be produced. The DR cross sections and rate coefficients will be
calculated for Br-like and Se-like W ($W^{39+}$ and $W^{40+}$). The research report and comprehensive data tables for DR cross sections and rate-coefficients will be produced.

1. The polarization of the strongest L lines from both the EIE and DR processes tungsten ions will be studied by our own codes REIE and REDR, which are based on MCDF and RATIP packages.

2. The DR rate coefficients of tungsten ions from $W^{26+}$ to $W^{37+}$ with outmost 4d sub-shells will be calculated by FAC code, and all results will be fitted as an analysis formula.

3. Laser produced plasmas source will be used to measure the EUV spectra from some low ionization states less than $W^{15+}$.

**Fumihiro Koike**: Atomic Physics in Weakly, Moderately or Highly Charged Ions of Tungsten Atoms.

1. Extend and improve the method of GRASP92 and GRASP2K calculations to cover all the lines that have been or that are to be observed by Tokyo-EBIT and CoBIT.

2. Further investigate the level structures and the characteristics of the dynamical processes in $4f^n$ open sub-shells for $n = 1 \sim 13$ with closed and single vacancy 4d sub-shells.

3. Also investigate the $4d^n$ open 4d sub-shells for $n = 1 \sim 9$.

4. Search the lines that can be good candidates for the diagnostic purpose, i.e., for the electron density measurement.

5. For the spectroscopic analysis of E1 X-ray/EUV lines, Dr. Suzuki has presented the case of LHD plasmas and Dr. Sakaue has presented the EBIT plasmas. Suzuki has compared the experimental spectra with FAC code calculation, and Sakaue compared the experimental spectra with HULLAC calculation. The use of FAC and/or HULLAC code for W X-ray/EUV spectra looks basically OK. However, some GRASP calculations might be necessary for several selected spectra to justify or verify the FAC/HULLAC calculation. In collaboration with Prof. I. Murakami and her group, the spectral analysis for LHD plasmas will be carried out.

6. As far as we look into the spectra, their detailed structures are not resolved and in this sense any too sophisticated calculations for entire range of the experimental results will not be necessary as long as the purpose is to analyze the current experimental spectra

**James Colgan et al.:** Collisional Data Calculations and Collisional-Radiative Modeling for Tungsten.

Construct atomic structure and collision models for lower charged states of W, centered around $W^{20+}$ (as many as $W^{14+}$ to $W^{27+}$, if possible), i.e. open f-shell ground state ions. Assess convergence of these atomic data calculations with respect to the number of configurations (levels) included. Perform collisional-radiative modeling, and compare resulting CSD, ionization balance, radiative losses, with other NLTE modeling efforts. This will mainly be done through NLTE8 workshop test cases. Also perform other NLTE8 workshop cases.

Examine feasibility of lower-temperature W CR modeling in the 10-80 eV temperature range. Perform test atomic-structure and collision calculations of relevant ions. Perform CR modeling if feasible and explore possibility of TD modeling of relevance to the neutral W atoms in a 40 eV plasma.

Perform detailed state-to-state comparisons of atomic collisional data with other calculations and/or measurements, depending on what else is available with which to compare, and depending on time & manpower constraints.

**R. Srivastava**: Plasma Based Fully Relativistic Distorted Wave Calculations of Electron Impact Excitation and Ionization Cross Sections and Associated Photon Emissions of Atoms and Ions.

1. Explore electron impact excitation of tungsten ions for which P. Beiersdorfer measured X-ray spectra and more to come from his group.

2. We will try to fill up gaps of cross section data which are not reported in the literature whose literature survey we have already done.
3. Report ionization cross section results in the light of A. Müller’s ionization results.

4. We will apply or recently developed CR model for argon to low temperature tungsten ion plasma.

**D.-H. Kwon:** Electron impact ionization (EII) and recombination for lowly charged, near neutral W ions.

We calculated electron impact ionization cross section for W⁺ forming W^{2+} by FAC code based on distorted wave (DW) approximation and IP-IR (independent process and isolated resonance) approximation. Direct ionization (DI) cross section of 5d and 6s valence shell electrons is sensitive to the choice of atomic local central. When the local central potential is optimized on the ionized target configurations 5d^4 + 5d^3 6s, the DI cross section is largely reduced than when pre ionized target configuration 5d^4 6s is chosen for the local central potential. Excitation-autoionization (EA) cross sections for 5d,6s -> nl (n=5-35) and 5s,5p->nl (n=5-10) considering detailed branching ratios contributes largely to the total EII cross section. As a result, our newly calculated total EII cross section for W⁺ agree with available experiments better than previous theoretical works but still about 20% larger than experiment at the peak.

In the future, we will carry out R-Matrix calculations in an attempt to resolve the present discrepancy of our calculated EA cross section with experiments. Then we will extend our calculation method to EII of W^{2+} and W. The reliability of atomic potential and wave functions generated with FAC for near neutral ions will be verified by comparing energies and oscillator strengths obtained by FAC with NIST and other available data. As well, dielectronic recombination rate coefficient for W⁺ and W^{2+} will be calculated.
Appendix I: List of Participants

Mr Chenzhong Dong, Department of Physics, Northwest Normal University, 967 East Anning Road, 730070 Lanzhou, CHINA.

Ms Wan-Ü Lydia Tchang-Brillet, LERMA, Observatoire de Paris, 61 Avenue de l’Observatoire, 75014 Paris, FRANCE.

Mr Jean-Francois Wyart, Laboratoire Aimé Cotton UPR 3321 du CNRS, Centre Université Paris Sud 11, 91405 Orsay Cedex, FRANCE.

Mr Sebastijan Brezinsek, Institut für Plasmaphysik IEK-4, Forschungszentrum Jülich GmbH, Leobrandt-Strasse, 52428 Jülich, GERMANY.

Mr Dmitry Kondratyev, Institut für Plasmaphysik IEK-4, Forschungszentrum Jülich GmbH, Leobrandt-Strasse, 52428 Jülich, GERMANY.

Mr Jose Ramon Lopez-Urrutia, Max-Planck-Institute of Nuclear Physics, Postfach 103980, 69029 Heidelberg, GERMANY.

Mr Alfred Müller, Institut für Atom- und Molekülphysik, Justus-Liebig-Universität Giessen, 39392 Giessen, GERMANY.

Mr Thomas Pütterich, Max-Planck Institute for Plasma Physics, EURATOM Association, Boltzmannstrasse 2, 85748 Garching, GERMANY.

Mr Rajesh Srivastava, Department of Physics, Indian Institute of Technology (IIT), Roorkee, 247667 Uttarakhand, INDIA.

Mr Makoto Imai, Department of Nuclear Engineering, Kyoto University, Yoshida, Sakyo-ku, 606-8501 Kyoto, JAPAN.

Mr Fumihiro Koike, Physics Laboratory, School of Medicine, Kitasato University, Kitasato 1-15-1, Sagamihara, 228 Kanagawa, JAPAN.

Mr Hiroyuki A. Sakaue, Fusion Systems Research Division, National Institute for Fusion Science, 322-6 Oroschi-cho, 509-5292 Toki, Gifu-ken, JAPAN.

Mr Chihiro Suzuki, National Institute for Fusion Science, 322-6 Oroschi-cho, 509-5292 Toki, Gifu-ken, JAPAN.

Ms Duck-Hee Kwon, Nuclear Data Center, Korea Atomic Energy Research Institute, Yuseong-Gu, 989-111 Daein-dong, KOREA.

Mr Valeryi Lisitsa, Nuclear Fusion Institute, Russian Research Centre “Kurchatov Institute,” Kurchatov Sqr. 1, 123182 Moscow, RUSSIAN FEDERATION.

Mr Alexander Ryabtsev, Institute of Spectroscopy of the Russian Academy of Sciences, Fizicheskaya Str. 5, 142190 Troitsk, Moskovskaya Oblast, RUSSIAN FEDERATION.

Ms Malvina Trzhaskovskaya, Petersburg Nuclear Physics Institute, Theoretical Department, Leningrad District, 188300 Gatchina, RUSSIAN FEDERATION.

Mr Vladimir Nikulin, Theoretical Astrophysics Department, Ioffe Physical Technical Institute, 26 Polytechnicheskaya, 194021 St. Petersburg, RUSSIAN FEDERATION.

Mr Peter Beiersdorfer, Lawrence Livermore National Laboratory, 7000 East Avenue, Mailstop L-611, Livermore, CA 94550, UNITED STATES OF AMERICA.

Mr James Colgan, Theoretical Division T-4 B-283, Los Alamos National Laboratory, Los Alamos, NM 87545, UNITED STATES OF AMERICA.

Mr Yuri Ralchenko, Atomic Spectroscopy Group, National Institute for Standards and Technology, 100 Bureau Dr., Stop 8422, Gaithersburg, MD 20899, UNITED STATES OF AMERICA.

Mr Bastiaan J. Braams, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.
Ms Hyun-Kyung Chung, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.
Appendix II: Meeting Agenda

Second Research Coordination Meeting of the Coordinated Research Project on “Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV”, Heidelberg, Germany, 29-31 August 2012.

Wednesday 29 August – Central Seminar Room

09:30-09:55: Welcome, adoption of the agenda. K. Blaum, A. Müller, B. Braams

Session 1: Chair: A. N. Ryabtsev

09:55-10:20: A. Müller: Experimental Data for Electron-Impact Ionization, Electron-Ion Recombination and Photoionization of Tungsten Ions

10:20-10:45: P. Beiersdorfer: Tungsten data for current and future uses in fusion and plasma science produced at Livermore

10:45-11:15: Break

11:15-11:40: H. A. Sakaue: EUV Spectroscopy of highly charged tungsten ions with electron beam ion traps

11:40-12:05: Yu. Ralchenko: Magnetic-dipole lines from 3dn ions of tungsten and other high-Z elements

12:05-12:30: F. Koike: MCDF calculation and analysis of E1 and M1 lines from tungsten ions in LHD and EBIT plasmas

12:30-13:00: All: Discussion, primarily on EBIT data and their interpretation

13:00-14:00: Lunch

Session 2: Chair: P. Beiersdorfer

14:00-14:25: C. Suzuki: Interpretation of EUV spectra from tungsten ions observed in the Large Helical Device

14:25-14:50: Th. Pütterich: Tungsten spectroscopy in fusion plasmas

14:50-15:15: S. Brezinsek: Tungsten source spectroscopy for the ITER-Like Wall on JET

15:15-15:45: All: Discussion, primarily on fusion plasma spectroscopy and its issues for W

15:45-17:30: Visit to storage ring and EBIT

19:30---: Social dinner

Thursday 30 August – Central Seminar Room

Session 3: Chair: Yu. Ralchenko

09:00-09:25: A. N. Ryabtsev: Resonance transitions of W VIII and isoelectronic Hf VI, Ta VII and Re IX spectra.

09:25-10:00: W.-Ü. L. Tchang-Brillet and J.-F. Wyart: Present status of experimental data on VUV spectra of moderately charged tungsten ions from Meudon and Troitsk

10:00-10:25: J. Colgan: Atomic Data Calculations and Collisional-Radiative Modeling of Tungsten

10:25-10:50: V. S. Lisitsa: Ionization balance and polarization radiation emission of tungsten ions in plasmas

10:50-11:20: Break


11:45-12:10: C.-Z. Dong: Electron impact excitation and dielectronic recombination of highly charged tungsten ions
12:10-12:35: R. Srivastava: Electron excitation of highly charged tungsten ions
12:35-13:00: M. Imai: Charge exchange cross sections for W$q^+$ ions at high energy
13:00-14:00: Lunch

**Session 4: Chair: A. Müller**

14:00-14:30: M. Trzhaskovskaya and V. K. Nikulin: Unified database of radiative recombination and photoionization data for highly-charged tungsten ions in plasma
14:30-15:00: J. Colgan and Yu. Ralchenko: Review of NLTE7 code comparisons for tungsten
15:30-16:00: All: Discussion, mainly on the state of collisional radiative modelling
15:30-16:00: Break
16:00-17:30: All: Questions, clarifications, discussion

**Friday 31 August – Central Seminar Room**

09:00-13:00: Break up for
(a) Status, needs and plans for spectroscopic data
(b) Status, needs and plans for collisional data
13:00-14:00: Lunch
14:00-16:30: Review and work plan