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

Summary Report of the First Research Coordination Meeting

IAEA Headquarters, Vienna, Austria
13-15 December 2010

Prepared by
B. J. Braams and H.-K. Chung
June 2012
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Abstract

Experts representing 14 research groups and the International Atomic Energy Agency met at IAEA Headquarters for the first research coordination meeting of a coordinated research project (CRP) on spectroscopic and collisional data for tungsten ions in fusion plasma. Participants presented their research following which a work plan was developed for the remainder of the CRP and outstanding data needs were identified. The proceedings and conclusions of the meeting are summarized here.

June 2012
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1. Introduction

Tungsten (symbol W, atomic number 74) is the leading candidate for use as wall material in the regions of high heat and particle flux in a fusion reactor and in ITER. The attractiveness of tungsten is due to its high thermal conductivity, its high melting point, its resistance to sputtering and erosion and its low propensity to trap tritium. However, as high-Z plasma impurity tungsten does not become fully stripped of electrons and radiates copiously, so that the tolerable fraction of tungsten impurity in the plasma is at most \(2 \times 10^{-5}\). Thus, the radiative properties of tungsten impurity are of great concern and are the subject of experiments and of numerical simulation. These considerations led the IAEA Nuclear Data Section (Atomic and Molecular Data Unit) to initiate a Coordinated Research Project (CRP) on “Spectroscopic and Collisional Data for Tungsten in Plasma from 1 eV to 20 keV”. The principal objectives of the CRP are to generate experimental and calculated data for radiative and collisional processes involving tungsten ions in a fusion plasma environment. Processes include 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 and spectroscopic signatures.

Thirteen research groups are represented in the CRP at the start. Representatives from these groups plus one invited expert met at IAEA in Vienna for a first Research Coordination Meeting (RCM) on 13-15 December 2010. The objectives of the meeting were to review the work of the participants in the CRP, to promote future collaboration and exchange of information and to prepare a work plan for the expected duration of the CRP through 2014. 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 the proceedings of the meeting. Section 3 presents the work plan that was developed during the meeting. Section 4 provides a review of the principal data needs. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2.

2. Proceedings

The meeting was opened by Dr D. Abriola, acting Section Head of the Nuclear Data Section. He noted the importance of tungsten in the fusion programme and the interest in atomic properties of tungsten impurity in plasma, both for plasma diagnostics and for plasma modelling. Dr B. Braams, scientific secretary of the meeting, extended his welcome and reminded participants of the objectives of this First Research Coordination Meeting (RCM): to review the status of experimental and theoretical work on spectroscopic and collisional properties of tungsten in fusion plasma, to identify data needs, to establish collaborations and to develop a work plan for the remainder of the CRP (2010-2015). Participants briefly introduced themselves after which the meeting turned to participant presentations.

N. Nakamura: Spectroscopy of multiply charged tungsten ions at the Tokyo electron beam ion trap

Dr Nakamura reported on the recent results on visible spectroscopy and EUV spectroscopy of tungsten using two electron beam ion traps, Tokyo-EBIT and CoBit. The Tokyo-EBIT built in 1995 can generate high energy and high current electron beams with maximum energy of 180 keV and maximum current of 330 mA. This is enough to ionize even high-Z atoms such as iodine completely. On the other hand, the CoBIT (Compact, Corona EBIT) that was built in 2007 may generate electron beams with energy in the range of 100 – 2500 eV and maximum current of 20 mA. With two EBIT machines the group can study tungsten plasmas in the wide range of temperatures, 100 – 18000 eV.

Many atomic lines of W ions are needed above 450 nm and from charge states below W XXVII (Ag-like) for spectral identification used in Tokamak research. Several W XXVII lines in the visible range were measured using CoBIT and compared with calculations by Ding and Koike. An EUV spectrometer is also available for CoBIT, which was used to study density diagnostics by Fe XIII
intensity ratios. A new EUV spectrometer was installed in the Tokyo EBIT for W XL-LX ions studies. An X-ray spectrometer has been used to measure dielectronic recombination and ion abundance of highly charged ions and the technique will be applied for Tungsten studies.

**P. Beiersdorfer: The WOLFRAM project at Livermore**

Dr. Beiersdorfer summarized the WOLFRAM project at Lawrence Livermore National Laboratory on tungsten atomic data relevant to fusion applications. He first reported that the atomic data community is very keen on tungsten data production as shown in the 2010 ASOS (Conference on Atomic Spectra and Oscillator Strengths) conference since a large number of tungsten data are needed for x-ray spectroscopy of the core ion temperature and bulk plasma velocities of magnetic fusion machines. He also described the design of the core imaging x-ray spectrometer (CIXS) for the ITER project, which is the responsibility of the US. The design is based on emission from Ne-like tungsten ions, which exists for temperatures above 12 keV. Calculations show that the 3d→2p emission is a strong function of electron temperature between 5 keV and 40 keV.

Tungsten spectra have been measured at several tokamak facilities. The Livermore SSPX (Sustained Spheromak Physics Experiment, 1999-2007) facility was used for studies of cooler plasmas relevant to the start-up phase of ITER or divertor plasmas. An X-ray and VUV grating spectrometer (XEUS) from Livermore and a bolometer were installed in the MIT Alcator CMod tokamak for tungsten research. In these measurements and those of other devices such as ASDEX-Upgrading, LHD and NSTX many lines were unidentified. Therefore the Livermore EBIT facility was used to make detailed observations.

The EBIT facility (EBIT-I and SuperEBIT) is used for a variety of applications in atomic physics, laboratory astrophysics, laser plasma physics and magnetic fusion research. The maximum electron beam energy is up to 200 keV and the beam current is up to 280 mA with the radius of 35 µm. The electron density is $10^{15}$ cm$^{-3}$ and ion density is $10^{9}$ cm$^{-3}$ with total number of ions $10^{7}$.

Spectroscopic diagnostics are carried out with multiple spectrometers: von Hámos-type curved crystal spectrometer (1-5 Å), vacuum flat-crystal spectrometer (4-25 Å), grazing incidence spectrometer (10-400 Å) and XRS microcalorimeter (0.2-80 keV). In particular, the microcalorimeter measures ALL x-ray lines in a wide band with high resolution (~ 4.5 eV). Emission spectra of $2s_{1/2} - 2p_{3/2}$ transitions, $\Delta n=0, 1$ and 2 of M-shell transitions of highly charged tungsten ions were measured in the EBIT facility and compared with theoretical predictions in collaboration with LLNL, UC Berkeley, UNR and Lund university.

**A. Ryabtsev: Spectra of moderately charged tungsten ions in the region below 350 Å**

Dr. Ryabtsev presented the experimental work on tungsten emission spectra at the Institute of Spectroscopy in Troitsk performed in the vacuum spark. About 3000 lines in the range 100-300 Å were measured in the vacuum spark spectrum with estimated error 0.005 Å. The spectrum is very complex. It consists of at least 5 overlapping W VIII transition arrays formed by excitation of different electrons from $4f^{14}5s^25p^5$ and $4f^{13}5s^25p^6$ configurations. W VI, W VII and W IX can also give a large contribution to the spectrum.

The vacuum spark spectrum convoluted with 5 Å resolution was compared with a Tokamak spectrum of W VIII; however, the tokamak spectrum seemed to be shifted by 20 Å. It appears that in the tokamak spectrum the calibration is off or the observed emission is not due to W VIII. For reliable identification of tungsten vacuum spark spectrum isoelectronic spectra of neighbouring chemical elements need to be studied as well, and vacuum spark spectra of Re, Ta and Hf excited in the same conditions were presented. Thereby the short wavelength part of the $4f^{13}5s^25p^6 - 4f^{13}5s^25p^76s$ transition array in Hf VI – Re IX spectra can be isoelectronically traced and identified.

Dr Wyart reported on their theoretical work on moderately charged tungsten ions. Calculations were carried out by means of the Cowan codes with the radial integrals being treated as adjustable parameters. The transition energies and $g_A$ values were presented for the isoelectronic ions of W III – W IX in the wavelength range > 350 Å between excited configurations.

Dr Tchang-Brillet presented the experimental work performed with the Meudon Observatory 10 m high resolution normal incidence VUV spectrograph. The resolution of the spectrograph is ~ 150000 (8mÅ) and the semi-automatic comparator and calibration with reference lines may yield $\Delta \lambda = \pm 0.001$–0.005 Å. The ion emission light sources are high voltage discharges under vacuum. The spark spectra of ionized heavy elements previously produced include emission from Iron group (3d), Platinum group 95d), Lanthanides (4f) and some Pd-like ions (5p,5d,5f). Detections can be made for photographic plates or image plates (photostimulable phosphor). The photographic plate has no resolution limit but the intensity response is linear only over limited intensity range. The image plate has a linear intensity response over 5 orders of magnitude and a good sensitivity even to the short wavelengths, however, the resolution and precision on wavelength depend on the characteristics of the specific scanner ($\Delta \lambda = \pm 0.005$–0.008 Å). The precise measurements of wavelengths and level energies will benefit the parametric studies of atomic configurations by improving the wave functions and hence level energies, dynamic properties such as transition probabilities, opacities and collision cross-sections.

A. Müller: Exploratory studies towards experimental data for electron-impact ionization, electron-ion recombination and photoionization of tungsten ions

Dr Müller reported on experimental cross-section data for electron impact ionization, photoionization and electron-ion recombination of W ions. First it was noted that theoretical predictions for ionization and recombination of complex many electron ions are very unreliable as seen in the examples of Xe$^{22+}$ and Fe$^{15+}$ ions and hence experiments are needed to test and guide theoretical approaches.

His group has been using several storage ring facilities: ESR at GSI, TSR at Heidelberg and CRYRING at Stockholm. For electron-ion recombination, merged beam experiments deliver high-accuracy data and the state of art theory was found to provide good predictions for light few-electron ions. However, for complex ions such as W$^{26+}$, the theory is not satisfying and needs new approaches. Only experiments will be able to guide such developments. Photoionization cross-sections by synchrotron radiation (ALS) were measured and the corresponding recombination cross-sections obtained by the principle of detailed balance are shown to be in good agreement with the direct recombination measurement at CRYRING. A high energy resolution is possible and the detailed spectroscopy of excited states of ions is accessible for this technique and hence it complements electron-ion recombination studies employing detailed balance.

Electron-impact ionization cross-sections for ions are measured using the crossed beams facility at the institute in Giessen. The comparison with theory shows that the present state of art theory predicts cross-sections for direct single ionization of few-electron ions with high accuracy; however, it has difficulties for complex many electron ions where excitation-autoionization processes prevail. There is no theory for multiple ionization cross-sections of complex ions. Dr Müller concluded by showing some preliminary measurements of recombination, ionization of tungsten ions. Future plans involve recombination experiments in the Heidelberg storage ring, electron-impact ionization measurements at the Giessen facilities and photoionization experiments at the ALS and PETRA synchrotron sources.
Dr Ralchenko reported on the activities of the NIST Atomic Spectroscopy Group on the production, analysis and utilization of spectroscopic data for highly ionized tungsten and other high Z elements.

The NIST EBIT facility produces plasmas with electron density of $10^{11}$-$10^{12}$ cm$^{-3}$ with mono-energetic electrons of the energy range 1-30 keV and the width of 60 eV. The produced spectra can be measured with X-ray micro-calorimeter in the spectral range of 1-10 keV with 5 eV resolution (at several keV) and EUV flat-field grazing incidence spectrometer at 2-30 nm.

Collisional-radiative modelling was carried out with a universal non-Maxwellian CR code NOMAD utilizing the atomic data generated by the FAC (Flexible Atomic Code). The analysis shows that the E2/M3 ratio of the transition complex 3d$^{10}$-3d$^{9}$4s has a great sensitivity to electron density. EUV spectra of W$^{39+}$-W$^{47+}$, W$^{46+}$-W$^{57+}$ and W$^{58+}$-W$^{71+}$ were measured in the spectral range of 4-20 nm by the beam energies 2-4.1 keV, 4.5-7 keV, and 8.8-25 keV, respectively. It is quite a challenge to analyse the spectra due to a large number of excited states in 3dn ions. With the lower 3l states modelled as atomic levels and the higher states n≥4 levels grouped into super terms, the CR calculations agree well with the measured spectra. New diagnostics methods for fusion plasmas were proposed based on density-sensitive linearities.

Tungsten spectroscopic data has been compiled by A. E. Kramida and T. Shirai for energy levels and spectral lines of all ions and by A. E. Kramida and J. Reader for ionization potentials for all ions. All data are in the NIST Atomic Spectra Database. The Bibliographic databases currently include 528 references for energy levels and spectral lines and 332 references for transition probabilities.

Dr Trzhaskovskaya presented relativistic Dirac-Fock (DF) calculations of total and partial radiative recombination cross-sections (RRCs) and partial photoionization cross sections (PCS). The presentation also includes relativistic expressions for PCS and RRCs, a description of electron exchange effects and the relativistic and non-dipole effects for heavy and highly charged ions at high energies. A contribution of non-dipole effects in RRCs, PCS, and RR rates has been shown to be significant (10-50%) at electron energies of the order of 10 keV and higher. A new fully relativistic formula for RR rates has been derived using the relativistic Maxwell-Jüttner distribution.

The PCS calculations and the total RR rates were compared with previous results for highly ionized tungsten ions. To condense a great body of data, PCS for states with n≤12 and l≤6 were fitted by an analytical expression involving 5 fit parameters. The total RR cross-sections were computed as the sum of available all final states. The convergence with respect to the principal number n of the series is rather slow, however, a cut off of bound levels from density effects can limit the series. For the electron density range of $10^{13}$ cm$^{-3}$, the summation was carried out up to n=20. The relativistic DF partial and total RR rates were presented in the wide temperature range of $10^3$ K ≤ T ≤ $10^{10}$ K for nine tungsten ions.

Dr Lisitsa described the quasi-classical methods of representing radiative-collisional processes with tungsten ions in tokamak plasmas including ITER conditions. The methods consider the following processes: 1) Bremsstrahlung (Br) in a frozen atomic core, 2) Radiative recombination (RR) in the frozen core, 3) Core polarization effects for complex ions (polarization Br, RR) and 4) Dielectronic recombination (DR) for core excitation without change of its principle quantum number. In this approach, electron-atomic processes for complex ions are estimated with small numbers of input.
parameters and the universal scaling laws for atomic processes are obtained. The quasi classical results were compared with quantum calculations.

These codes need the support of more complex codes both atomic ones (energy levels, oscillator strengths) and plasma modelling codes (B2-EIRENE, transport code ASTRA, etc.) In particular, configuration averaged atomic data are needed. The codes will be accessible at Kurchatov Institute website and RAS Institute of Spectroscopy website.

M. Imai: Charge exchange cross sections for W⁺ and W²⁺ ions

Dr Imai presented the experimental studies of charge exchange cross-sections for W⁺ and W²⁺ ions and summarized the data compilation activities on charge exchange cross-sections. Atomic and molecular collision has been studied in Kyoto University (in gas phase) and JAEA (solid targets). The experimental apparatus and the derivation of absolute cross-sections were described.

Absolute cross-sections have been measured for charge exchange collisions: Cq⁺ (q = 1,2,3), Crq⁺ (q = 1,2), Niq⁺ (q = 1,2), Feq⁺ (q = 1,2), Beq⁺ (q = 1,2), Bq⁺ (q = 1,2), and Wq⁺ (q = 1,2) projectile ions colliding with He, Ne, Ar, Kr, H₂, CO, CO₂, N₂, CH₄, C₂H₆ and C₃H₈ targets at 5-32 keV. Previous studies on the tungsten cross-sections are very scarce, both experimentally and theoretically. His group proposed to measure the electron capture cross-sections of W⁺ and W²⁺ ions in the targets of He, Ne, Ar, Kr, H₂, N₂, CH₄ and C₂H₆. They will collaborate on theoretical studies as well.

Finally, the compilation on charge exchanging cross-sections from 390 papers and the electronic database were presented.

C.-Z. Dong: Theoretical study on electron impact excitation and dielectronic recombinant of highly charged tungsten ions

Dr Dong presented the computations of electron impact excitation (EIE) and dielectronic recombinant (DR), as well as the polarization of the emitted photons following EIE and DR processes. His group uses GRASP92/2K to calculate energies and wave functions in the multi-configuration Dirac-Fock (MCDF) method. The Breit interaction and dominant QED contributions are included as well.

The polarization of emission lines from EIE and DR of highly charged tungsten ions, which are an important diagnostic tool of plasma anisotropy, were studied based on the MCDF method. However, DR cross-sections and rate coefficients required for ionization balance and level population of tungsten ions require a systematic calculation, particularly, for outmost 4s and 4p sub-shells and hence the calculations will be carried out with the FAC (Flexible Atomic Code). Some available energy levels of highly charged tungsten ions were compared among MCDF, FAC and NIST results. The total DR rate coefficients were produced with FAC for Ni-like, Cu-like, Kr-like and Rb-like tungsten ions and fitted to the semi-empirical formula.

F. Koike: Analysis of visible light emissions of tungsten highly charged ions in plasmas

Dr Koike described an analysis using the collisional-radiative model of visible M1 Lines measured in the Tokyo EBIT and co-(E)BIT. Highly charged tungsten ions with open valence sub-shells emit visible light from the fine structure transitions and the magnetic dipole (M1) resonance transitions between the ground state fine structure levels can be observed in the visible range. The less radiation trapping probability and the ease of visible spectroscopic measurement make the M1 line emission attractive for diagnostics use.

The M1 transitions between the W²⁶⁺ ground state multiplets were calculated with GRASP2K MCDF wave functions and RATIP (Relativistic Atomic Transition and Ionization Properties, CPC library). The correlation between valence and core orbitals is very strong and is included for the ground state
energy levels. The calculated visible transitions between the W\textsuperscript{26+} ground state multiplets were compared with the EBIT measurements and HULLAC calculated values.

A collisional-radiative (CR) model in the steady state condition was developed for spectral analysis. The ratios of calculated line intensities of the W\textsuperscript{26+} ground state multiplets are sensitive to electron temperatures and densities and will be good candidates for plasma diagnostics. Dr Koike also presented another CR model for W\textsuperscript{35+}, W\textsuperscript{36+} and W\textsuperscript{37+} ions constructed with HULLAC generated atomic data and discussed the results at N\textsubscript{e} = 3\times1013/cm\textsuperscript{3} and T\textsubscript{e}=100-1000 eV. This model will be developed further by including more levels and the recombination rates.

**R. Srivastava: Relativistic distorted wave calculations for electron excitation of atoms and ions**

Dr Srivastava presented the fully relativistic distorted wave (RDW) theory applied to electron impact excitation of noble gases and atomic ions (including tungsten ions). The RDW method solves the Dirac equations to describe both the bound and continuum electrons. Thus the relativistic effects are incorporated to all orders in a natural way including spin-polarized electrons and the method is suitable for calculating atomic data for tungsten ions.

Electron impact excitation cross-sections from the ground states of Ar and Kr were compared with the available experimental and for some cases, theoretical results of R-matrix and non-relativistic Distorted Wave. The RDW method produces reliable results for the excitation of higher lying excited states of the odd parity levels, especially at higher impact energies. Analytic fits to integrated cross-sections of krypton were presented

Electron impact excitation cross-sections from 5p\textsuperscript{5}6s J=2 metastable state of Xe were presented and a collisional radiative model incorporating the results was developed for Xe near-infrared emission. For the CR model, both RDW method and semi-relativistic Breit-Pauli B-Spline R-matrix (BSR) method were used.

The RDW theory is also applied to the electron impact n\textsuperscript{2}S-n\textsuperscript{2}P resonant excitation of singly charged metal atoms with one valence electron (Mg\textsuperscript{+}, Ca\textsuperscript{+}, Zn\textsuperscript{+}, Cd\textsuperscript{+} and Ba\textsuperscript{+}) ions and to the electron impact cross-sections of W\textsuperscript{43+}-W\textsuperscript{45+} and W\textsuperscript{12+}.

**N. Badnell: Dielectronic recombination of heavy species: the tin 4p\textsuperscript{6}4d\textsuperscript{q} - 4p\textsuperscript{6}4d\textsuperscript{q+1}4f + 4p\textsuperscript{5}4d\textsuperscript{q+1} transition arrays for 1\leq q\leq 10**

Dr Badnell presented the theoretical study on the dielectronic recombination of the Tin open 4d subshell. Tin is of interest to EUV microlithography and is used on MAST (Mega Amp Spherical Tokamak) to study marker species diagnostics and impurity transport. Three programs were compared: 1) AUTOSTRUCTURE, 2) Burgess-Bethe General Program (BBGP) and 3) Configuration-Average (CA) method.

The results show that the dipole \(\Delta n=0\) promotion dominates in Sn\textsuperscript{11+}, which is in contrast to the case of W\textsuperscript{35+} where both non-dipole and \(\Delta n=1\) promotions contribute significantly. Configuration mixing between 4p\textsuperscript{5}4d\textsuperscript{q+1}4f and 4p\textsuperscript{5}4d\textsuperscript{q+1} states has a small effect on the total DR rate coefficients though individual radiative rates are significantly affected.

The BBGP results are systematically lower than those of AUTOSTRUCTURE while the CA results are systematically and significantly higher than the configuration mixed Breit-Pauli results obtained from AUTOSTRUCTURE. Similar calculations for Tungsten d-shell and the f-shell will be explored in the future.
J. Colgan: The LANL atomic kinetics modelling effort and its application to W plasmas

On behalf of Dr J. Colgan, Dr Chung presented the work of the LANL group on atomic kinetics modelling. There are various levels of detail in the LANL suite of atomic physics codes: 1) Non-relativistic configuration average kinetics (nln) + UTA spectra, 2) Relativistic configuration average kinetics (nlj) + UTA spectra, 3) Mixed UTA (MUTA) – configuration average kinetics and spectra composed of mixture of UTAs and fine-structure features and 4) Fine-structure levels. The LANL suite of atomic physics codes consists of 5 codes: 1) CATS/RATS atomic structure codes (semi-relativistic Cowan code or Dirac-Fock-Slater code), 2) ACE collisional excitation code (Plane-wave Born, Columb-Born and distorted-wave methods) and 3) GIPPER ionization code (scaled-hydrogenic and distorted-wave methods). An on-line version of the codes is available at http://aphysics2.lanl.gov/tempweb.

ATOMIC kinetics modelling code uses the atomic data for LTE or NLTE population kinetics models and spectral modelling of a broad range of plasma applications. The mixed UTA (MUTA) approach was developed for the spectra of complex ions and the results are in very good agreement with the Sandia-Z Iron opacity experiments. The LANL configuration-average/MUTA calculations were applied to tungsten problems of the non-LTE kinetics code comparison workshops. The LANL group plans to perform much larger calculations to assess the accuracy of the older results and to investigate low-temperature tungsten processes relevant to the divertor modelling.

L. Vainshtein: Ionization cross-sections for W I and W II and the ATOM and MZ codes

On behalf of L. Vainshtein, Dr Braams presented the ionization cross-sections of W I and W II produced by ATOM and MZ codes at Lebedev Physical Institute. The details of ATOM and MZ codes were described.

The atomic systems have 73-74 electrons with two or three open shells in the ground configuration, and there exist hundreds of SLJ levels in the ground configuration of 5d⁶6s². Both direct ionization and excitation autoionization processes contribute significantly as well as the double ionization. These processes can be calculated by code ATOM. Since there is no direct experimental data for W I but there is data for W II, the ionization cross-sections of W II were calculated first both for single and double ionization. The agreement is rather good for W II.

Yu. Ralchenko: Report from the non-LTE Code Comparison workshop NLTE-6

As a special report, Dr Ralchenko gave a brief overview of tungsten cases at the non-LTE (NLTE) code comparison workshops. The NLTE workshops are designed to verify and validate collisional radiative codes used in plasma diagnostics by understanding why code results differ through comparison of large sets of calculated population kinetics parameters. The elements so far compared are C, Ne, Al, Ar, Fe, Kr, Xe, W and Au. Tungsten has been studied in the 5th (2007) and 6th (2009) workshops and will be studied again in the 7th (2011) workshop in Vienna co-hosted by IAEA A+M data unit.

The workshop organization is as follows: 1) Cases are announced (~ 6 months before) for 3-5 elements and several plasma conditions per elements for steady-state or time-dependent cases, or for Maxwellian or non-Maxwellian cases. 2) Results are submitted (~ 2 months before). 3) Online data base of results is set up (~ 1 month before). 4) At the meeting, each case is compared for submitted code results and explored on the effects and sensitivities of assumptions and methods used by codes. 5) Calculations are resubmitted (~ 3 months after) for publication.

For the tungsten cases at the 6th workshop, four temperatures of 4 keV to 20 keV at electron density of 10¹⁴/cm³ were compared for various parameters such as the mean charge states, charge distributions, power loss rates, rate coefficients and spectra. The key issue of this particular workshop was to explore the effect of dielectronic recombination (DR) processes on result discrepancies. Each code
submitted cases with and without DR processes and, remarkably, all codes agree within a charge of 1 or 2 without DR processes. However, with DR process, the mean charge state could differ by more than 10. It was concluded that the DR processes are the most important source of uncertainty in tungsten modelling.

H.-K. Chung: Database and knowledge base developments at IAEA

Dr Chung gave a brief introduction on the IAEA A+M Data unit activities featured at the unit home page http://www-amdis.iaea.org. The CRP is the main mechanism by which the unit encourages new research and the results of CRP will be hosted at the databases or knowledge base maintained by the unit. In addition to databases, there exist several online capabilities maintained by the unit, one of which is the FLYCHK code. The FLYCHK code provides a rough estimate of mean charge, charge state distributions, or radiative power loss rates of elements up to gold over a wide range of plasma conditions. The code was originally developed to help experimentalists design experiments and hence it uses a simple model. Hence, a care is needed to apply the results for cases requiring a sophisticated result.

3. Work plan

During and following the presentations participants’ work plans were discussed.

N. Nakamura: Spectroscopic Studies of Highly Charged Tungsten Ions Using Electron Beam Ion Traps (EBITs)

Plans for 2011: Visible spectra of tungsten ions with charge state in the range 6-30 will be measured using a low energy EBIT. The observed lines will be identified through observation of their electron energy dependence and comparison with theoretical calculations. A high resolution EUV spectrometer (1-5 nm or 5-20 nm depending on grating) has been developed and will be used for measurements.

Later: EUV spectra of tungsten ions will be measured using a low energy EBIT for ions with charge state in the range 6-30 and a high energy EBIT for ions with charge state in the range 30-70. The dependence of the line ratios on electron energy and density will be measured and compared with a theoretical model. X-ray emission from dielectronic recombination (DR) will be measured. The corresponding DR cross-section will be deduced through change in ion abundance and through the renormalization to a reliable theoretical radiative recombination cross section. The experimental DR cross sections will be compared with theoretical ones.

P. Beiersdorfer: Atomic Physics of Tungsten Ions for Magnetic Fusion Diagnostics

Plans for 2011: The Livermore EBIT-I electron beam ion trap will be used to generate and measure the L-shell lines of neon-like tungsten ($W^{64+}$) in the 8 – 12 keV spectral range. The measurements will also determine the associated inner-shell and dielectronic satellite lines from sodium-like $W^{63+}$. In addition, measurements will be made of the wavelengths of W V through W XV in the extreme ultraviolet wavelength band (15 nm to 35 nm) as well as in the optical (3000 to 5500 Å) and will be compared to existing data from magnetic fusion devices, e.g., the Sustained Spheromak Physics Experiment.

Later: Measurements will be made of the electron-impact excitation cross sections of the L-shell x-ray lines of neon-like $W^{64+}$ in the 8 – 12 keV spectral range (normalization is a challenge for absolute cross sections). 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-I electron beam ion trap. The data will be compared with spectra obtained at the NSTX and Alcator tokamaks. 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 radiative lifetime of the...
fastest neon-like W$^{64+}$ transition by studying its Lorentzian line shape as well as to produce data on x-ray line polarization and data on line formation by charge exchange. An attempt will also be made to use the fast-switching electron beam to measure ionization balance under specific, possibly Maxwellian, conditions.

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

Plans for 2011: Continuation of production of high resolution VUV spectra of tungsten and of Hf, Ta and Re in the region below 35 nm where resonance transitions of W VIII and W IX and corresponding isoelectronic spectra of Hf, Ta and Re are expected. 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. Analysis of the $4f^{14}5s^25p^6 - 4f^{14}5s^25p^5(5d+6s)$ and $4f^{13}5s^25p^6 - 4f^{13}5s^25p^5(5d+6s)$ transitions in W VIII. Identification of the same transitions in the isoelectronic spectra of Hf VI, Ta VII and Re IX. Verification of the W VIII analysis using isoelectronic regularities in the studied spectra.

Later: W IX.


Plans for 2011: Complete recording of high-resolution VUV spectra of tungsten and of neighbouring ions (Hf, Ta, Re) in the normal incidence wavelength region (above 30 nm). Spectra will be produced using spark sources operated in various conditions to differentiate the charge states of the emitting ions. Photographic plates and image plates will be used for complementary detections. Measurements of wavelengths and reduction of data will be completed. With the support of theoretical calculations (parametric method by means of Cowan codes) it is hoped that ambiguous attributions may be removed from earlier line lists of W III to W VII. Analysis of W VIII and isoelectronic ions will be initiated.

Published data will be available on http://molat.obspm.fr/

Later: Extension of the previous analysis to the transition arrays $5d^{10}(5f,7p) - 5d^8$ and $5d^{10}(6d,7s) - 5d^{9}16p$ in the W III and W IV spectra, determination of the ground energy level configuration ($5p^54f^{13}2f_{7/2}$ or $5p^34f^{14}2p_{3/2}$) in W VIII, and analyses of the strong transitions $6s-6p$ and $5d-6p$ between excited configurations in W VIII and W IX. Possibly analysis of Hf, Ta and Re spectra in order to get the support of isoelectronic regularities such as Hf VI - Ta VII - W VIII - Re IX, or Hf VII - Ta VIII - W IX - Re X.

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

Plans for 2011: Exploratory measurements of cross-sections will be conducted on electron-impact ionization and photoionization of W$q^+$ ions in charge states up to q=25 at the crossed beams apparatus of the Group in Giessen and at the Advanced Light Source in Berkeley (there up to at most q=10); test measurements on electron-ion recombination of W$q^+$ ions in intermediate charge states q (between 10 and 25) will be carried out at the Heidelberg heavy-ion storage ring; the Group will explore and start to develop techniques to cover the widest possible range of charge states and collision energies accessible to crossed and merged beams experiments with tungsten ions.

Later: A new electron gun will be implemented in crossed beams electron-impact ionization measurements aiming at intense electron beams up to 5 keV electron energy thus extending the present electron-ion collision energy range by a factor of 5; a facility for studying photon-ion interactions presently being set up at the PETRA III synchrotron in Hamburg will be commissioned for photoionization experiments with W$q^+$ ions covering photon energies up to 3 keV; a comprehensive
program on the measurement of single and multiple ionization of W$q^+$ ions by electron impact will be conducted at the institute of the Principal Investigator, absolute cross sections and detailed precision scans of the cross sections will be performed such as to extract information about excited states involved in the ionization processes.

The cross section measurements for ionization of tungsten ions will be finalized; recombination of selected highly charged tungsten ions will be measured at the Heidelberg storage ring and plasma rate coefficients will be determined; photoionization cross sections of W$q^+$ ions will be measured for selected charge states; experimental results of all measurements will be analyzed and compared to theory.

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 2011: Perform a detailed analysis of the recently measured magnetic dipole lines from tungsten ions (W XLI to W LVII) to assess their applicability to fusion plasma diagnostics. Prepare a new set of measurements on the NIST EBIT device; install and test a new CCD camera (EUV region) on the EBIT. Collect atomic data for tungsten from other groups and from publications and add it to the NIST Atomic Spectra Database (ASD). Develop plasma population kinetics cases for W to be compared at the NLTE-7 Code Comparison Workshop.

Later: Extend the measurements of tungsten spectra to cover yet unexplored spectral ranges and ions. Perform collisional-radiative (CR) modelling of the measured spectra in order to identify new spectral lines. Incorporate the new data in the NIST ASD. Perform a detailed analysis of the various atomic processes that affect the population balance of tungsten ions in fusion plasma and explore new methods of spectroscopic diagnostics. Critically assess the data and add the evaluated data to the NIST ASD.

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.

2011: Perform relativistic calculations by the Dirac-Fock method of partial photoionization cross-sections (PCS) and radiative recombination cross-sections (RRCS) for ground and excited states to states with principal quantum number \( n=20 \) for selected charges in the range approximately 24-46 (range is of interest for AUG, for example) and electron kinetic energy range 1 eV to 50 keV. Calculate associated rate coefficients by averaging over the Maxwell-Jüttner distribution. The DF method with proper consideration of the exchange interaction between atomic electrons and between bound and continuum electrons will be used as implemented in the computer code package RAINE. All significant multipoles of the field will be taken into account. Also calculate total RRCS for selected tungsten ions in the range W$^{24+}$ to W$^{46+}$ in the kinetic electron energy range from 1 eV to 50 keV. Obtain fitted analytical expressions for the partial cross-sections; tabulate the total RRCS and the fit parameters and partial and total radiative recombination and associated radiative power loss rates in the temperature range $10^4$K - $3\times10^8$K.

Later: Extend the charge range to 47-65 (range of interest for ITER and EBIT; possibly of interest for normalization of EBIT electron impact excitation cross-sections). Attempt will be made to estimate the effect of electron density of the plasma on the radiative recombination cross-sections.

V. Lisitsa and A. Kukushkin: Radiative-Collisional Processes in Electron-Tungsten Ion Collisions

Plans for 2011: Quasi-classical calculations (Thomas-Fermi potential) of Bremsstrahlung cross sections in collisions of plasma electrons with tungsten ions. Tests of calculated atomic data for tokamak core and SOL plasma conditions via comparison with quantum calculations. Estimation of
Bremsstrahlung radiation background in the visible spectral range for passive spectroscopic diagnostics and active diagnostics (CXRS and Thomson scattering diagnostics). Charge exchange cross section calculations from n=2 hydrogen level on highly charged ions with Z>>1 selective in n at E=100 keV/aum for CXRS in ITER.


C.-Z. Dong: Dielectronic Recombination Cross Sections and Rate Coefficients of Highly Ionized Tungsten Ions

Plans for 2011: The Dielectronic Recombination (DR) cross-sections and rate coefficients will be calculated for Kr-, Cu-, and Ni-like W ions (38+, 45+, 46+). The calculations will pay special attention to configuration interaction and relativistic effects as well as the contribution of different inner-shell excitations to the DR data at high collision energy.

Later: 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 (41+ to 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 (39+ and 40+). The research report and comprehensive data tables for DR cross-sections and rate-coefficients will be produced.

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

Plans for 2011 and later: Survey the theoretical and relevant experimental works on atomic properties of tungsten ions. Calculate transitions in the visible light emission region for moderately charged tungsten ions. Calculate the 3d-4f, 4d-4f, 4p-4d, 3p-3s transitions of moderately charged tungsten ions.

Carry out accurate calculations for magnetic dipole transitions that enter visible light or its neighbouring wave length region in moderately ionized tungsten atomic ions by means of multiconfiguration Dirac-Fock method using GRASP2K (and/or GRASP92) and RATIP (Relativistic Atomic Transitions and Ionization Property) codes. Investigate the tungsten ions which have a 4f open sub-shell as valence sub-shell, which are mostly in lack of the theoretical calculation due to the complexity of the electronic structure of the ions. Extend the GRASP2K + RATIP calculations to all the 18 lines that have been newly observed by Tokyo-EBIT and CoBIT. Complete the calculation for W$^{26+}$ [Kr]4d$^{10}$4f$^{2}$, and next proceed to the calculations of the ions that have more or fewer 4f electrons in the system. They are W$^{16+}$ [Kr]4d$^{12}$4f$^{2}$, W$^{25+}$ [Kr]4d$^{10}$4f$^{3}$ and W$^{17+}$ [Kr]4d$^{10}$4f$^{11}$, and so on to the half-filled 4f shells. Calculations of W$^{27+}$ [Kr]4d$^{10}$4f$^{3}$ and W$^{15+}$ [Kr]4d$^{10}$4f$^{13}$ are also planned.

Later: Create new tabulation of the basic atomic properties such as energy levels, transition probabilities and lifetimes of tungsten ions. Calculate the spectator satellite transitions and shake-up satellite transitions of tungsten ions. Calculate the radiative transitions between excited states of tungsten ions. Calculate the radiative recombination processes of tungsten ions.
Search the line pairs that can be good candidates for the diagnostic purpose. And, try to enhance our CR model to include a huge number of the levels that are relevant to the analysis of tungsten lines. And further, try to establish the method of spectral analysis for the EUV range emissions from LHD plasmas, of which measurement are now on going in NIFS.

J. Colgan et al.: Collisional Data Calculations and Collisional-Radiative Modelling for Tungsten

Plans for 2011: Construct atomic datasets for relevant ion stages of tungsten, including structure data, collision strength data and electron-impact, photoionization, and autoionization data. The semi-relativistic structure code CATS will be used to generate these data. It will be investigated whether fully relativistic structure (and collisional) data are required for this project.

Later: Perform collisional-radiative modelling on tungsten for temperatures and densities of relevance to fusion plasma and to the CRP using the datasets generated previously. The modelling will produce, in particular, radiative power loss data, which is of key interest in fusion modelling. Provide emission spectra for selected temperature and density ranges in which tokamak experiments are performed. Provide critical analysis of the comparison between the modelling and experiment.

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

Plans for 2011: Systematic theoretical study of atomic and ionic excitation in inelastic collision processes will be carried out within the framework of the Dirac relativistic theory, the density matrix approach and relativistic distorted wave theory. Apart from total cross-sections special emphasis will be placed on the alignment of excited atomic states and the resulting photoemission. Detailed analysis of total and differential cross-sections will be carried out during the first year for the electron-impact excitation of neutral inert-gas atoms. In simultaneous work the implementation of the relativistic distorted wave theory will be extended to calculate the electron-impact excitation of an ion in a general manner; due to the residual ionic charge this involves different conditions on the projectile electron waves and greater complexity as compared to excitation of neutral atoms.

Detailed analysis of total and differential cross-sections will be carried out In simultaneous extended work the relativistic distorted wave theory will be extended to calculate the photon and electron-impact ionization of tungsten ions. These calculations are planned to supplement the experimental measurements of Alfred’s cross section and Peter’s line emissions in different spectral ranges.

N. Badnell: Dielectronic Recombination of Tungsten Ions

We have complete ADAS collisional-radiative density-dependent ionization balance for W based on Burgess-Bethe method for DR. The overall goal is to validate/replace this data by/with more advanced from AUTOSTRUCTURE.

Plans for 2011: Identify key ionization stages of tungsten in different plasma regimes, viz. core, edge and divertor. Produce a standalone version of the Burgess-Bethe General Program (BBGP) currently used by ADAS. Check the L-shell agreement between BBGP and AUTOSTRUCTURE. Also, explore validity of configuration average (CA) method in collaboration with Don Griffin (the DRACULA code).

Compare 4p-subshell results with FAC(?) work of Dr. Dong (timescale?).

Compare with experiments of Profs Müller and Nakamura?

Later: Carry out AUTOSTRUCTURE dielectronic recombination calculations for M-shell to Ar-like and then for open 3d-subshell tungsten ions. Make comparisons and first adjustments to BBGP. Start on open 4d-subshell and contrast with 3d-subshell results and comparisons. Move on to open 4f-
subshell BBGP and AUTOSTRUCTURE calculations. Finalize changes to BBGP in light of detailed comparisons with AUTOSTRUCTURE. Re-integrate BBGP within ADAS and compare new tungsten derived data, e.g. for ionization balance, density dependent DR rate coefficients for transport etc., with original predictions.

M. Imai:

Plans for 2011: Assemble data for tungsten charge exchange cross-sections. Will try to develop new experiment for H+W<sub>q</sub> crossed beams at high energy.

4. Data Needs

Overview

The work of the Atomic and Molecular Data Unit and of the present CRP is dedicated to the development of fusion energy and therefore the objective of the CRP is to provide data that are useful for fusion plasma modelling and for interpretation of experiments. The most important data for core plasma modelling are rate coefficients for ionization and recombination by electron impact and for electron energy loss, all as function of electron density and temperature. For diagnostics one needs in addition finely resolved information about spectral emissions, and the interaction of highly charged ions with a diagnostic or heating neutral beam is of special interest. In order to diagnose erosion of tungsten wall material via spectral emissions from the near wall plasma one requires spectroscopic data for near-neutral charge states of tungsten. These near-neutral tungsten ions may be in a highly ionizing regime far removed from any kind of ionization equilibrium.

Although fusion experiments are the focus of the CRP, in order to develop confidence in the data one wants to model any well-diagnosed experiment too. In many cases (EBITs and crossed beam experiments) this requires cross-section data rather than Maxwellian averaged rate coefficients.

Fusion plasma data needs

For fusion plasma modelling

Primarily rate coefficients (less important, cross-sections) for ionization, recombination and electron energy loss due to collisions e+W<sup>q+</sup>. All processes; most important are dielectronic recombination (DR), excitation, excitation-autoionization, direct ionization and also multiple ionization.

Data are needed also for conditions far away from equilibrium; e.g., rate coefficients for ionization of low-charged tungsten in plasma of several 100 eV electron temperature.

Generally electron impact is the dominant process, but also cross-sections for charge exchange are required; most important the process H+W<sup>q+</sup> → H<sup>+</sup>+W<sup>(q-1)+</sup> for energy of H (D, T) up to 1 MeV and for any charge state q. (There are no measurements of this process in the CRP; who can do this?) Maybe merged beam experiments at CFADC at Oak Ridge or maybe Kyoto?

For fusion plasma diagnostics

In the end one desires data to model all spectral emission from W in the plasma and assign the emissions to any of the possible reactions.

Spectrum of emission from DR, emission from excitation, etc. Spectrometer is planned for ITER with tungsten as the main source of impurity radiation. DR is primarily responsible for line shape and formation of satellite lines (exceeds Doppler broadening).
Charge exchange with H must be taken into account in order to calculate the charge state distribution. State-selective CXRS (charge exchange recombination spectroscopy) cross-sections are required for diagnostic purposes. Spectrum from CX with neutral beam is potentially a diagnostic for the charge distribution.

There is a special need to identify all lines in W$^{1+}$ and W$^{2+}$ that may be used to recognize and perhaps quantify tungsten erosion.

EUV, VUV spectrometers; many lines are still unidentified.

**Data needs for other experiments**

In the end we want to be able to model any well-diagnosed experiment and explain the measurements.

**Spark plasma**

What is the experimental setup (explain to the modeller). Non-stationary; measurements are integrated over time. Not a clean system for spectral synthesis.

**EBIT experiment**

It is possible to do rapid variation of beam energy and thereby create conditions away from ionization equilibrium. To model it one needs cross-sections for recombination and ionization. With rapid variation of beam energy a Maxwellian can be simulated, but in general cross-section data are needed rather than rate coefficients.

For interpretation of measurements it is very important to take account of polarization, because the beam is directional. Crystal spectrometers are sensitive to polarization.

Partial radiative recombination cross-sections are important for EBIT modelling; they are used for normalization and also for measurements of charge state balance.

For the NIST EBIT the most important data needs are those for EUV spectroscopy and related collisional radiative modelling.

Background neutral gas is always a problem. One tries to measure its effects by modulating the beam. Any special data needs for the background neutral gas?

**Merged beam experiments**

Merged beam experiments in a storage ring are very clean; ions generally in the ground state. For merged beam or crossed beam experiments using an ion source there are always problems with metastable ions and one needs cross-section data for metastables.
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Agenda

Monday, 13 December

Opening, Adoption of Agenda, D. Abriola and B.J. Braams

Session 1: Reports I

Chairperson: A. Müller

09:40 – 10:15  N. Nakamura: Spectroscopy of multiply charged tungsten ions at the Tokyo electron beam ion trap

10:15 – 10:50  P. Beiersdorfer: The WOLFRAM project at Livermore

10:50 – 11:10  Coffee Break

11:10 – 11:45  A. Ryabtsev: Spectra of moderately charged tungsten ions in the region below 350 Å

11:45 – 12:20  L. Tchang-Brillet and J.-F. Wyart: Experimental and theoretical study of vacuum ultraviolet spectra of weakly charged ions of heavy elements, including tungsten

12:20 – 14:00  Lunch

Session 2: Reports II

Chairperson: A. Ryabtsev

14:00 – 14:35  A. Müller: Exploratory studies towards experimental data for electron-impact ionization, electron-ion recombination and photoionization of tungsten ions

14:35 – 15:10  Yu. Ralchenko: NIST research on spectroscopy and collisional-radiative modeling of highly-charged ions of tungsten

15:10 – 15:30  Coffee Break

15:30 – 16:05  M.B. Trzhaskovskaya and V.K. 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

16:05 – 16:40  V. Lisitsa: Radiative-collisional processes in electron-tungsten ions collisions:

16:40 – 17:15  M. Imai: Charge exchange cross sections for W+ and W2+ ions

Tuesday, 14 December

Session 3: Reports III

Chairperson: V. Lisitsa

09:00 – 09:35  C.-Z. Dong: Electron impact excitation and dielectronic recombination of highly charged tungsten ions
F. Koike: Calculation of M1 visible transitions between the ground state multiplets of tungsten ions

Coffee Break

R. Srivastava: Relativistic distorted wave calculations for electron excitation of atoms and ions

N. Badnell: Dielectronic recombination of heavy species: the tin 4p64dq - 4p64dq-14f + 4p54dq+1 transition arrays for 1≤q≤10

H.-K. Chung on behalf of J. Colgan: The LANL atomic kinetics modeling effort and its application to W plasmas

B.J. Braams on behalf of L. Vainshtein: Ionization cross-sections for W I and W II and the ATOM and MZ codes

Lunch

Session 4: Data evaluation and data needs

Chairperson: F. Koike

Yu. Ralchenko: Report from the non-LTE Code Comparison workshop NLTE-6

H.-K. Chung: Database and knowledge base developments at IAEA

All: Prospects and plans for data evaluation

Coffee Break

All: Prospects and plans for data evaluation

Wednesday, 15 December

Session 5: Data needs

Chairperson: L. Tchang-Brillet

All: Comprehensive review and summary of status

Lunch

Session 6: Work plan

Chairperson: N. Nakamura

All: Development of work plan and meeting report

Adjourn