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Article

Tungsten Data for Current and Future Uses in Fusion and Plasma Science

Peter Beiersdorfer [1,*], Joel Clementson [1] and Ulyana I. Safronova [2]

[1] Physics Department, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA;
E-Mail: joel.clementson@gmail.com
[2] Physics Department, University of Nevada, Reno, NV 89557, USA;
E-Mail: Ulyana.I.Safronova.2@nd.edu

* Author to whom correspondence should be addressed; E-Mail: beiersdorfer1@llnl.gov

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Abstract: We give a brief overview of our recent experimental and theoretical work involving highly charged tungsten ions in high-temperature magnetically confined plasmas. Our work includes X-ray and extreme ultraviolet spectroscopy, state-of-the-art structure calculations, the generation of dielectronic recombination rate coefficients, collisional-radiative spectral modeling and assessments of the atomic data need for X-ray diagnostics monitoring of the parameters of the core plasma of future tokamaks, such as ITER. We give examples of our recent results in these areas.

Keywords: tungsten; X-ray spectroscopy; EUV spectroscopy; spectral modeling; atomic structure; EBIT; tokamak; ITER

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1. Introduction

Atomic physics has played a very important role throughout the history of experimental plasma physics. It has been crucial for understanding the plasma energy balance and for diagnostic development [1]. With the shift in magnetic fusion research toward the very high-temperature burning plasmas expected to be found in the ITER tokamak (Latin for "the way"; but originally, an acronym for "International Tokamak Experimental Reactor"), the atomic physics of tungsten has become of high importance [2]. The reason is that tungsten will be a constituent of ITER plasmas, because of its use as a

plasma-facing component able to withstand high heat loads and with a lower tritium retention than other possible materials [3–5].

ITER diagnostics are already being developed based on using tungsten radiation. In particular, the ITER Core Imaging X-ray Spectrometer (CIXS), which is designed to measure the ion temperature and bulk plasma motion of ITER's plasma core, is being based on the X-ray emission of neon-like tungsten ions (W^{64+}) [6]. In addition, tungsten emission will 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 [7,8]. Moreover, tungsten is used on present-day tokamaks in preparation for ITER [9–12].

In anticipation of the importance of tungsten for fusion plasmas, our group has focused on studying the atomic properties of tungsten and its many ionization stages for over a decade. We have been doing so primarily using the Livermore electron beam ion trap facility [13], which is a device that was first designed at Livermore explicitly for studying the atomic physics of ions of heavy elements [14,15]. Our measurements have included spectral data in the X-ray region [16–23], the extreme ultraviolet regime [24–26] and the optical wavelength band [27,28].

Electron beam ion traps are now being used at a variety of international laboratories [29]. Several of these machines are being used for tungsten spectroscopy complementary to that performed on our facility. This includes measurements at the Berlin [30–32], Gaithersburg [33–35], Shanghai [36,37] and Tokyo facilities [38].

In addition to our measurements on the Livermore electron beam ion traps, we have utilized magnetic fusion plasmas to study the spectra of tungsten. These include the Sustained Spheromak Physics Experiment (SSPX), the National Spherical Torus Experiment (NSTX) and the Alcator C-mod tokamak [39–41]. We have also been involved in a significant theoretical effort utilizing some of the most advanced atomic physics computer codes [42,43].

In the past five years, our research on tungsten was shaped by our participation in the Coordinated Research Project "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV", which was led by the International Atomic Energy Agency. We dubbed our effort at Livermore the "Wolfram Project". This project has had the goal of producing experimental and theoretical data for tungsten in various spectral bands relevant to magnetic fusion research. In the following, we present an overview of the results from this effort.

2. Experimental Results

The generation of experimental spectroscopic data has been a key component in our effort. Measurements were carried out at the Livermore electron beam ion trap facility, which includes the first electron beam ion trap ever built, dubbed EBIT-I , and a high-energy version, dubbed SuperEBIT [13,44]. The spectral lines we measured during recent years were emitted by ionization stages from as low as thulium-like W^{5+} to as high as oxygen-like W^{66+} [45–47].

The Livermore electron beam ion traps have been optimized for spectroscopic measurements since their inception almost thirty years ago [48]. The electron beam ion trap is a modified electron beam ion source and built with the intent to spectroscopically study the interaction of highly charged ions

with an electron beam by looking directly into the trap. It is described in detail by Levine *et al.* [15]. In this device, the electrons pass through the 2 cm-long trap region and are compressed to a beam with a diameter of approximately 50 μm by a three-Tesla magnetic field generated by a pair of superconducting Helmholtz coils. Neutral atoms or ions with low charge are injected into the trap where they are collisionally ionized by the electron beam. The electrons can be accelerated to any energy between 0.05 keV (and lower) [49] and 200 keV (and higher) [50]. This energy is sufficient to produce any charge state of tungsten, including completely ionized tungsten W^{74+} [1]. The ions are longitudinally confined in the trap by applying the appropriate voltages to a set of three copper drift tubes through which the beam passes. Radial confinement is provided by electrostatic attraction of the electron beam, as well as flux freezing of the ions within the magnetic field. All three drift tube voltages float on top of a potential (the common drift tube voltage) that is supplied by a low-noise high-voltage amplifier, and the electron beam energy is determined by the sum of these potentials, provided the electron gun is grounded. The electron beam density is about 5×10^{11} cm^{-3}, but can be varied [51].

Spectroscopic instrumentation includes a large variety of crystal spectrometers and grating spectrometers that cover line emission from the X-ray to the visible regime. In addition, many X-ray measurements have been made with microcalorimeters.

In Figure 1, we show the X-ray spectrum of the $3s \rightarrow 2p$ transitions of neon-like W^{64+} near 8500 eV. The figure illustrates the power of our measurement approach: new lines are observed when the energy of the electron beam is increased to allow the production of a higher ionization state. Lines from fluorine-like and oxygen-like tungsten appear as the beam energy is raised from 15 to 21 keV. The lines are absent at the lower beam energy, because the ionization potential of neon-like W^{64+} is calculated to be 15,603.6 eV, while the ionization potential of fluorine-like W^{66+} is calculated to be 15,965.5 eV [1]. L-shell X-ray transitions from tungsten ions are of special interest for the ITER tokamak, because they are under consideration as an ion temperature diagnostic of the core plasma [6].

Spectral lines from aluminum-like W^{61+} and from charge states as low as iron-like W^{48+} were observed in the ultra-soft X-ray range between 26 and 44 Å [46]. These measurements utilized a high-resolution grating spectrometer [52] that provided a resolving power ($\lambda/\Delta\lambda \approx 1500$ to 2000) similar to that afforded by the crystal spectrometer [53] employed to make the X-ray measurements shown in Figure 1. Such a high resolving power is needed because of the high density of the $3d \rightarrow 3p$ and $3p \rightarrow 3s$ lines in this wavelength band. In fact, the large number of lines has so far precluded the identification of more than about half of the observed lines [46], which is a strong indication that more research is highly desirable.

Lines from nickel-like W^{46+}, which terminate in the closed $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$ shell, fall into the X-ray range near 4 to 5 Å and are best observed with a crystal spectrometer [17,54] or an X-ray microcalorimeter [55,56]. Using the calorimeter, we were able to identify $n = 7, 6, 5, 4 \rightarrow n = 3$ transitions in nickel-like W^{46+} through selenium-like W^{40+} [23] and to assess the charge balance evolution as a function of electron energy [57].

Spectral lines from thulium-like W^{5+}, erbium-like W^{6+} and holmium-like W^{7+} were produced at very low electron beam energies (30 to 300 eV) [47]. An extended-range grazing incidence spectrometer with resolving power as high as 5000 [58] was employed to record these lines in the extreme ultraviolet wavelength range between 188 and 206 Å [46]. The measurements enabled us to newly identify five W^{5+}

lines near 200 Å, as illustrated in Figure 2. The corresponding transitions have not yet been determined. However, we note that some of the transitions from erbium-like W^{6+} and holmium-like W^{7+} falling into this wavelength region have been identified as $5d \rightarrow 5p$ transitions [59,60].

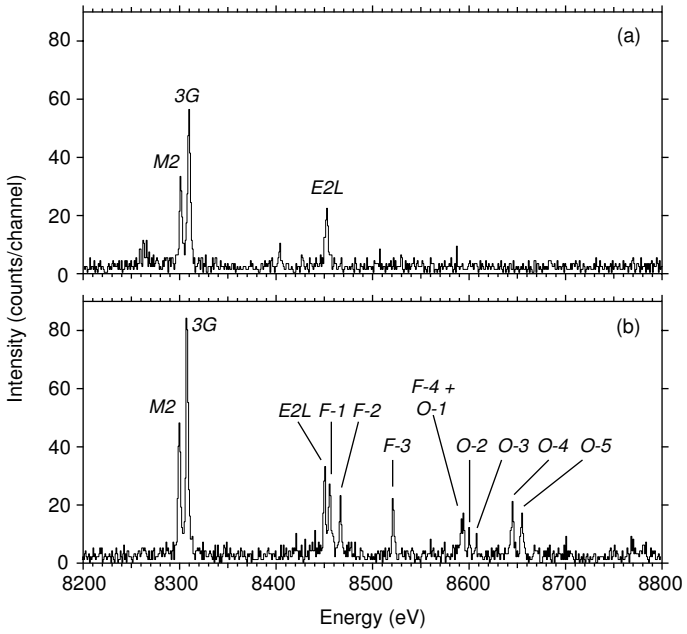

Figure 1. X-ray emission of highly charged tungsten ions at an electron beam energy of (**a**) 15 keV and (**b**) 21 keV. The strongest lines are from neon-like W^{64+} and are labeled $M2$, $3G$ and $E2L$. Lines from fluorine-like W^{65+} and oxygen-like W^{66+} are labeled by F and O, respectively.

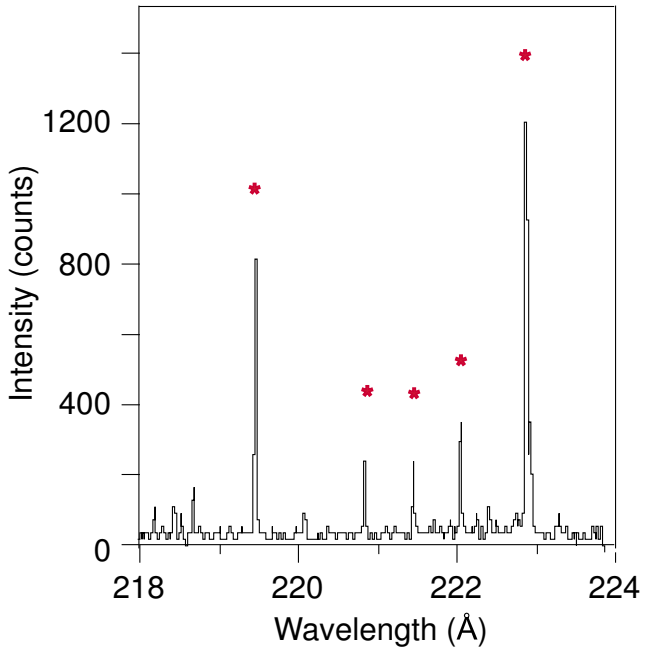

Figure 2. Emission of thulium-like W^{5+} in the extreme ultraviolet spectral band. The five lines marked with an asterisk have been newly identified.

Because several of our spectrometers have been installed on magnetic fusion devices in the United States [61–66], we can obtain tungsten spectra also from these sources, provided that tungsten is introduced into these machines. One such spectrum is shown in Figure 3. It was obtained on the Alcator C-mod tokamak at the Massachusetts Institute of Technology [67] and shows bright tungsten emission near 50 Å. Comparison with spectral data from other fusion machines, notably from the Large Helical Device in Japan [68], points to charge states silver-like W^{27+}, palladium-like W^{28+} and ruthenium-like W^{29+} as the strongest emitters, as described by Podpaly *et al*. [67].

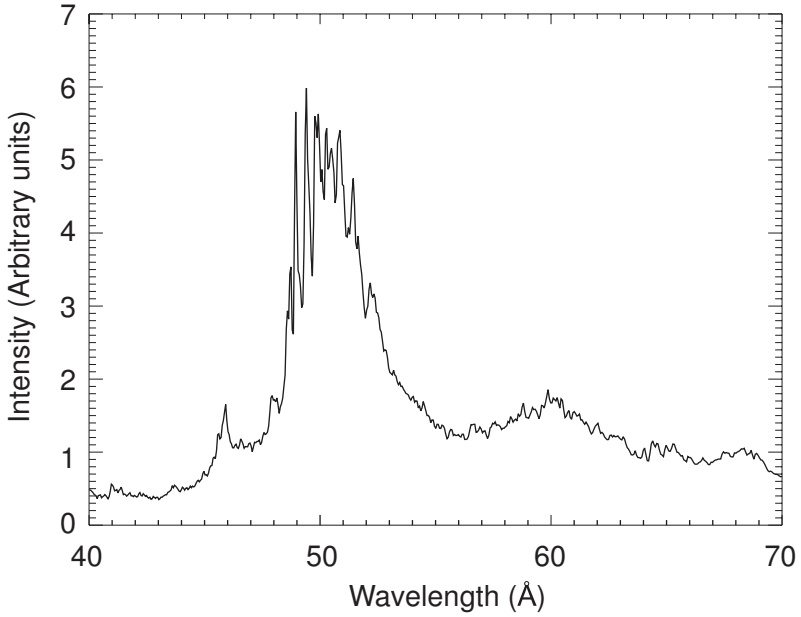

Figure 3. Emission from tungsten ions observed on the Alcator C-mod tokamak.

3. Theoretical Atomic Data and Spectral Modeling

Our Wolfram project includes a significant collisional-radiative modeling effort using atomic data that we have generated with the Flexible Atomic Code (FAC) developed by Gu [69]. For example, we have generated modeled spectra of the $n = 3 \rightarrow n = 2$ X-ray transitions of near neon-like tungsten ions (W^{56+} to W^{71+}) [2]. In addition, we have performed such modeling for essentially all of the ionization stages we investigated experimentally, and the results can be found in our papers mentioned above.

In Figure 4, we show a spectrum predicted by our modeling calculations for vanadium-like W^{51+} in the 1000 to 4000 eV X-ray range. This was part of a large effort that produced theoretical spectral data from germanium-like W^{42+} through vanadium-like W^{51+} [70].

Our collisional-radiative modeling effort has been augmented with calculations of the ionization potentials of all tungsten ions [1], as well as specific atomic parameters needed for spectral measurements and diagnostics. The latter calculations include energy levels, radiative rates, oscillator strengths and autoionization rates. We employed three very different atomic physics computer codes, *i.e.*, the Hartree–Fock-relativistic method (COWAN code), the multi-configuration relativistic Hebrew University-Lawrence Livermore Atomic Code (HULLAC code) and the relativistic many-body perturbation theory method (RMBPT code) [71–77], in order to estimate the reliability of the calculations from the spread of the obtained results.

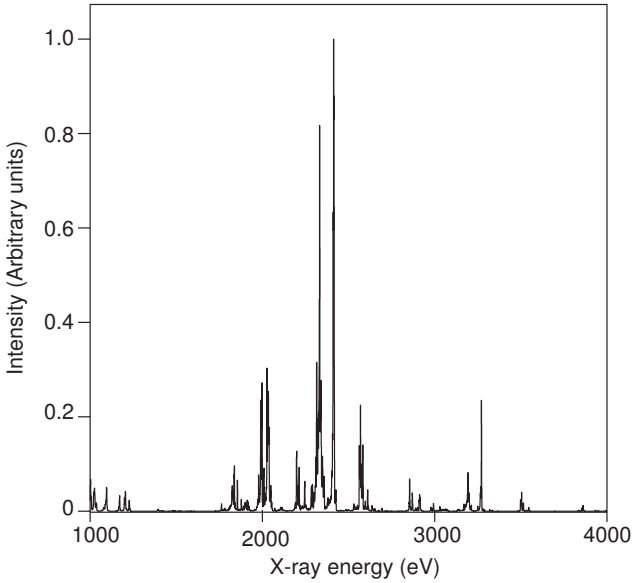

Figure 4. Spectral emission of vanadium-like W^{51+} in the 1000 to 4000 eV X-ray range predicted by calculations performed with the Flexible Atomic Code.

In Figure 5, we show the total dielectronic recombination rate coefficients we have calculated as a function of electron temperature for the recombination of neon-like W^{64+}, sodium-like W^{63+} and copper-like W^{45+} into their respective next lower ionization states. In all cases, it is assumed that the recombining ion is in its ground state. Because the ground state of neon-like W^{64+} is a completely closed shell, there are no low-energy dielectronic resonances. As a consequence, the dielectronic recombination rate vanishes as the electron temperature drops below 100 eV. By contrast, the ground state of both sodium-like and copper-like tungsten has a single valence electron outside an otherwise closed shell. This allows for low-energy resonances that contribute to the total recombination rate coefficient, even at very low plasma temperatures, as shown by the figure.

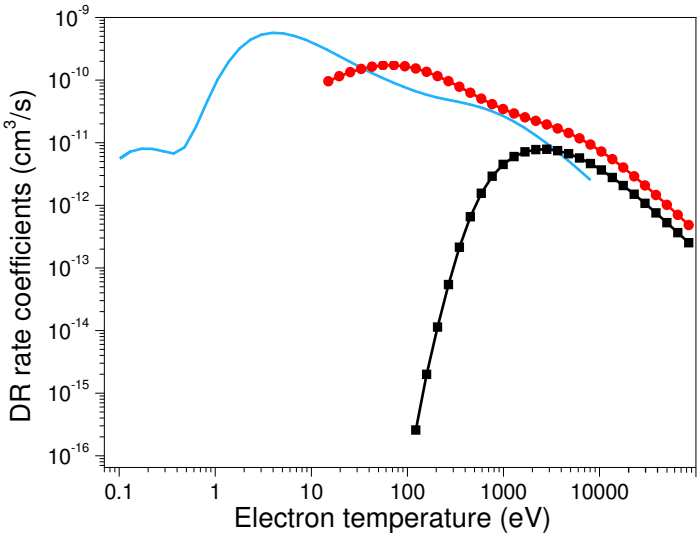

Figure 5. Total dielectronic recombination rate coefficients for neon-like W^{64+} (black trace with solid squares), sodium-like W^{63+} (red trace with solid circles) and copper-like W^{45+} (light blue trace) recombining into their respective next lower ionization state.

4. Assessment of Atomic Data Needs for ITER Core Diagnostics

Tungsten radiation will be observed on ITER with a variety of instrumentation. For example, various survey-type instruments will monitor plasma performance near the plasma edge [7,78], where lower ionization stages of tungsten will radiate. The core plasma will be monitored with the aforementioned CIXS instrument [6] and possibly an X-ray microcalorimeter [79]. Both of these instruments are designed to determine the ion temperature from the L-shell emission of tungsten ions.

Recently, we have compiled specific atomic data needs to increase the reliability of the core ITER X-ray diagnostics [80,81]. These include: (1) absolute wavelength measurements with accuracy lines on the order of about 0.02 eV of the L-shell lines of neon-like W^{64+} and of the neighboring sodium-like and fluorine-like tungsten lines; (2) measurements and calculations of the position and intensity of the dielectronic satellite lines associated with the neon-like W^{64+} lines, including those with a spectator electron in a high principal quantum number; and (3) calculation and measurement of the excitation rates at a level of accuracy of about 5%, including excitation by indirect processes [82], such as resonance excitation and cascade contributions.

There is also a growing need for reliable ionization balance calculations, which for tungsten is a nontrivial undertaking [83]. The reason for this need is that the CIXS will provide radial profiles of the ion abundance in ITER. When compared to accurate ionization balance calculations, such radial profile measurements can be used to extract the ion transport parameters, *i.e.*, the radial ion diffusion coefficient and the inward pinch velocities, as detailed recently by Beiersdorfer [81]. Diagnosing transport and ultimately controlling it is a prime objective in fusion research, and reliable atomic physics is a prerequisite for using the CIXS in this endeavor.

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Author Contributions

All three authors have substantially contributed to the physics presented in this article. All authors have read and approved the final manuscript.

Conflicts of Interest

The authors declare no conflict of interest.

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