Electron-impact ionization of tungsten ions in the configuration-average distorted-wave approximation

M. S. Pindzola
Department of Physics, Auburn University, Auburn, Alabama 36849

D. C. Griffin
Department of Physics, Rollins College, Winter Park, Florida 32749

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Single-ionization cross sections for W^{4+}, W^{5+}, and W^{6+} are calculated in the configuration-average distorted-wave approximation. Contributions from excitation autoionization are found to be strong for each ion. When comparing theory with the recent crossed-beams measurements of Stenke *et al.* [J. Phys. B **28**, 2711 (1995)], ionization from the ground configuration dominates for W^{4+} and W^{5+}, while ionization from metastables of excited configurations dominates for W^{6+}. [S1050-2947(97)06208-2]

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Various highly refractory metals, including tungsten, are currently being tested for use as plasma facing divertor plates in controlled fusion experiments. An important process for divertor modeling is the electron-impact ionization of the metallic atom in low charge states. In this paper, we calculate single-ionization cross sections for W^{4+}, W^{5+}, and W^{6+} using a configuration-average distorted-wave (CADW) approximation [1]. For complex atomic ions with many subshells available for both direct ionization and excitation autoionization, the CADW method provides a convenient starting place for sorting out the relative strengths of the many ionization pathways. The CADW method can yield surprisingly accurate results for certain charge-state ranges, as was recently shown for the Mo isonuclear sequence [2,3], and is again shown in this report when theory is compared with the crossed-beams experiments of Stenke *et al.* [4] for the W ions.

The total single-ionization cross section for complex atomic ions is dominated by contributions from direct ionization

$$e^- + A^{q+} \rightarrow A^{(q+1)+} + e^- + e^-, \tag{1}$$

and excitation autoionization

$$e^- + A^{q+} \rightarrow (A^{q+})^* + e^- \rightarrow A^{(q+1)+} + e^- + e^-, \tag{2}$$

where A represents an arbitrary ion with charge q. Since for low-charged ions the branching ratio for autoionization is approximately one, the total single-ionization cross section is given by

$$\sigma_{\rm tot} = \sum_f \sigma_{\rm ion}(i \rightarrow f) + \sum_j \sigma_{\rm exc}(i \rightarrow j), \tag{3}$$

where $\sigma_{\rm ion}$ is the direct ionization cross section and $\sigma_{\rm exc}$ is the inner-shell excitation cross section. In a configuration-average distorted-wave calculation the indices i,j refer to configurations of the initial N-electron ion, while the index f refers to a configuration of the final $(N-1)$-electron ion. For more detailed distorted-wave treatments, the indicies may refer to LS terms or LSJ levels. In any case, one averages over initial states and sums over final states. The energies and wave functions for the various W configurations are calculated using the relativistically corrected Hartree-Fock atomic structure code of Cowan [5]. The bound and continuum radial orbitals are solutions to radial Schrödinger equations, which contain both mass-velocity and Darwin operators [6].

The single-ionization cross sections from the $5s^2 5p^6 4f^{14} 5d^4 6s^2$ ground configuration of neutral W and the $5s^2 5p^6 4f^{14} 5d^4 6s$ ground configuration of W^+ are dominated by direct ionization from the outer subshells. Previous CADW calculations [7] for W and W^+ reported large shape resonances in the direct ionization cross sections for the $6s$ and $5d$ subshells of W, but no shape resonances were found in the same subshell ionization cross sections for W^+. After recent comparisons of the distorted-wave method with a more accurate time-dependent close-coupling method for the

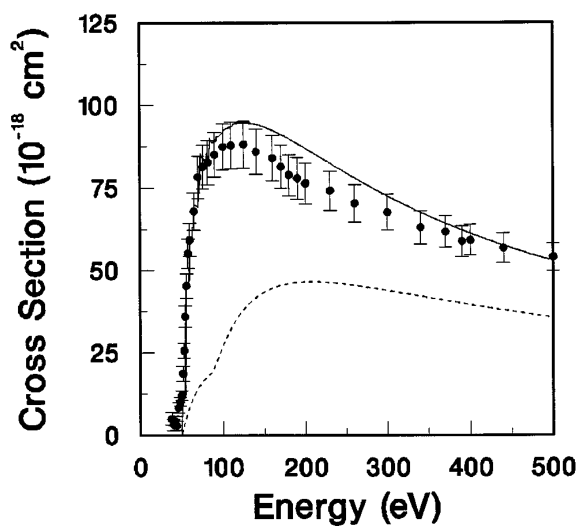

FIG. 1. Electron-impact single ionization of W^{4+}. Solid curve: total ionization from the $5s^2 5p^6 4f^{14} 5d^2$ ground configuration; dashed curve: direct ionization only; solid circles: crossed-beams measurements [4].

TABLE I. Direct ionization and inner-shell excitation cross sections for the $5s^25p^64f^{14}5d^2$ ground configuration of W^{4+}.

Transition	Threshold energy (eV)	Cross section (10^{-18} cm^2)
$5d\rightarrow kl$	50.03	20.56
$4f\rightarrow kl$	87.25	13.83
$5p\rightarrow kl$	94.82	12.81
$5s\rightarrow kl$	135.91	1.76
$4f\rightarrow 5d$	35.03	58.07
$4f\rightarrow 5f$	64.47	6.67
$4f\rightarrow 5g$	73.40	0.09
$4f\rightarrow 6s$	42.94	1.67
$4f\rightarrow 6p$	51.78	2.87
$4f\rightarrow 6d$	62.85	4.10
$4f\rightarrow 6f$	72.89	3.29
$4f\rightarrow 6g$	77.65	0.08
$5p\rightarrow 5d$	43.95	173.80
$5p\rightarrow 5f$	72.11	6.01
$5p\rightarrow 6s$	50.91	5.51
$5p\rightarrow 6p$	59.68	11.28
$5p\rightarrow 6d$	70.65	6.92
$5p\rightarrow 6f$	80.52	2.69
$5s\rightarrow 5d$	84.35	6.06
$5s\rightarrow 6s$	92.01	1.30
$5s\rightarrow 6p$	100.69	0.50
$5s\rightarrow 6d$	111.66	0.57

TABLE II. Direct ionization and inner-shell excitation cross sections for the $5s^25p^64f^{14}5d$ ground configuration of W^{5+}.

Transition	Threshold energy (eV)	Cross section (10^{-18} cm^2)
$5d\rightarrow kl$	63.98	6.24
$4f\rightarrow kl$	103.62	11.45
$5p\rightarrow kl$	109.58	9.75
$5s\rightarrow kl$	151.44	1.43
$4f\rightarrow 5d$	37.22	62.57
$4f\rightarrow 5f$	71.32	9.05
$4f\rightarrow 5g$	83.66	0.20
$4f\rightarrow 6s$	48.16	1.33
$4f\rightarrow 6p$	58.11	2.43
$4f\rightarrow 6d$	71.03	3.83
$4f\rightarrow 6f$	83.25	3.85
$4f\rightarrow 6g$	89.79	0.17
$5p\rightarrow 5d$	44.79	214.96
$5p\rightarrow 5f$	77.47	8.06
$5p\rightarrow 6s$	54.64	5.48
$5p\rightarrow 6p$	64.50	11.34
$5p\rightarrow 6d$	77.30	6.58
$5p\rightarrow 6f$	89.32	3.04
$5s\rightarrow 5d$	85.88	7.31
$5s\rightarrow 6s$	96.49	1.41
$5s\rightarrow 6p$	106.25	0.52
$5s\rightarrow 6d$	119.05	0.59

direct ionization of hydrogen [8], we now believe that the shape resonances in neutral W are due to a poor choice of potentials for the low angular momentum states of the scattered electron and do not exist.

The single-ionization cross section from the $5s^25p^64f^{14}5d^4$ ground configuration of W^{2+} has a strong $5p\rightarrow 5d$ excitation-autoionization contribution. CADW calculations yield a $5d$ ionization cross section of 144.83 Mb at twice the threshold energy of 24.87 eV and a $5p\rightarrow 5d$ cross section of 106.26 Mb at the threshold energy of 42.29 eV. Alone, these two contributions to the total ionization cross section are about 50% higher than the peak experimental cross section of 170 Mb [4]. For low charged ions, correlation effects beyond the single configuration approximation found in the CADW method can produce healthy reductions in both the direct ionization and inner-shell excitation cross sections.

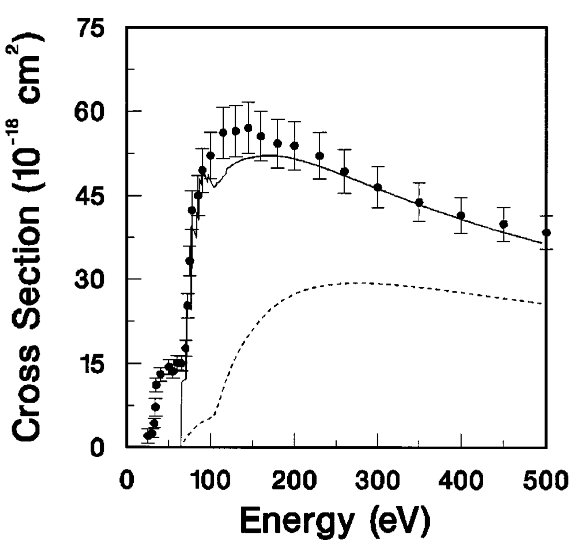

FIG. 2. Electron-impact single ionization of W^{5+}. Solid curved: total ionization from the $5s^25p^64f^{14}5d$ ground configuration; dashed curve: direct ionization only; solid circles: crossed-beams measurements [4].

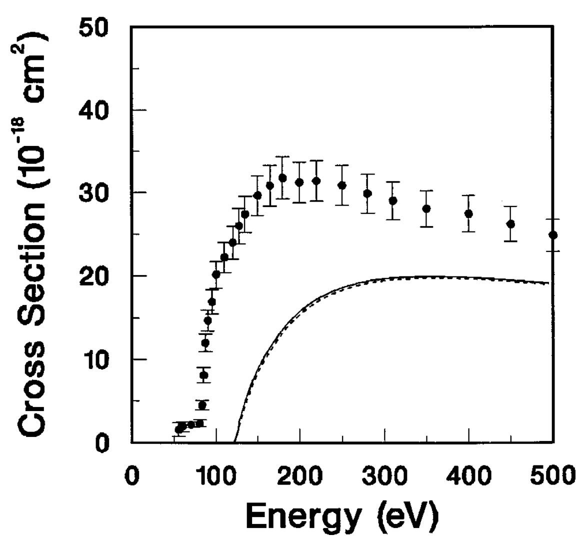

FIG. 3. Electron-impact single ionization of W^{6+}. Solid curve: total ionization from the $5s^25p^64f^{14}$ ground configuration; dashed curve: direct ionization only; solid circles: crossed-beams measurements [4].

TABLE III. Direct ionization and inner-shell excitation cross sections for the $5s^2 5p^6 4f^{14}$ ground configuration of W^{6+}.

Transition	Threshold energy (eV)	Cross section (10^{-18} cm^2)
$4f \to kl$	120.98	9.76
$5p \to kl$	125.07	7.40
$5s \to kl$	167.76	1.15
$5p \to 5d$	45.60	258.21
$5p \to 5f$	82.43	9.69
$5p \to 6s$	58.52	5.38
$5p \to 6p$	69.44	11.25
$5p \to 6d$	84.00	6.16
$5p \to 6f$	98.08	3.14
$5s \to 5d$	87.46	8.61
$5s \to 6s$	101.17	1.48
$5s \to 6p$	111.98	0.53
$5s \to 6d$	126.55	0.60

The single-ionization cross section from the $5s^2 5p^6 4f^{14} 5d^3$ ground configuration of W^{3+} also has a strong $5p \to 5d$ excitation-autoionization contribution. CADW calculations yield a $5d$ ionization cross section of 55.29 Mb at twice the threshold energy of 36.95 eV and a $5p \to 5d$ cross section of 134.88 Mb at the threshold energy of 43.11 eV. The $5p \to 5d$ excitation cross section is calculated by averaging over the states in 8 LS terms or 19 LSJ levels of the initial $5s^2 5p^6 4f^{14} 5d^3$ configuration and summing over the 68 LS terms or 180 LSJ levels of the final $5s^2 5p^5 4f^{14} 5d^4$ configuration. The levels of the initial configuration are spread over a 6.7-eV energy range, while the levels of the final configuration are spread over a 25.4-eV energy range. With respect to the lowest level of the ground configuration, 175 of the 180 LSJ levels are autoionizing. Alone, the $5d$ ionization cross section and 97% of the $5p \to 5d$ excitation cross section are about 35% higher than the peak experimental cross section of 135 Mb [4]. Although

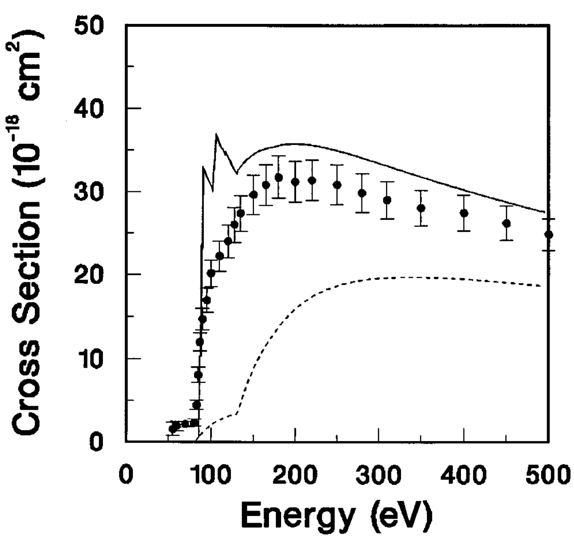

FIG. 4. Electron-impact single ionization of W^{6+}. Solid curve: total ionization from the $5s^2 5p^6 4f^{13} 5d$ excited configuration; dashed curve: direct ionization only; solid circles: crossed-beams measurements [4].

TABLE IV. Direct ionization and inner-shell excitation cross sections for the $5s^2 5p^6 4f^{13} 5d$ excited configuration of W^{6+}.

Transition	Threshold energy (eV)	Cross section (10^{-18} cm^2)
$5d \to kl$	81.34	3.77
$4f \to kl$	132.12	7.81
$5p \to kl$	129.92	6.92
$5s \to kl$	173.92	1.09
$4f \to 5d$	48.14	35.70
$4f \to 5f$	88.24	7.81
$4f \to 5g$	104.87	0.24
$4f \to 6s$	63.74	0.68
$4f \to 6p$	75.00	1.38
$4f \to 6d$	89.91	2.28
$4f \to 6f$	104.50	2.93
$4f \to 6g$	113.22	0.20
$5p \to 5d$	47.85	215.66
$5p \to 5f$	86.39	9.51
$5p \to 6s$	62.17	4.49
$5p \to 6p$	73.34	10.11
$5p \to 6d$	88.10	5.26
$5p \to 6f$	102.48	2.96
$5s \to 5d$	90.61	7.44
$5s \to 6s$	105.73	1.35
$5s \to 6p$	116.77	0.50
$5s \to 6d$	131.55	0.52

correlation effects in general decrease with higher charge state, they are still fairly sizable for W^{3+}.

The single-ionization cross section from the $5s^2 5p^6 4f^{14} 5d^2$ ground configuration of W^{4+} is compared with experiment [4] in Fig. 1. Various direct ionization and inner-shell excitation cross sections between configurations are presented in Table I. The ionization cross sections are reported at twice the threshold energy, while the excitation cross sections are reported at the threshold energy. The $5s \to kl$ ionization cross section is not included in Fig. 1 since its threshold energy of 135.91 eV is above the double-ionization threshold of 114.01 eV. The $5p \to 5d$ excitation cross section is calculated by averaging over the states in 6 LS terms or 9 LSJ levels of the initial $5s^2 5p^6 4f^{14} 5d^2$ configuration and summing over the states in 48 LS terms or 110 LSJ levels of the final $5s^2 5p^5 4f^{14} 5d^3$ configuration. The levels of the initial configuration are spread over a 6.4-eV energy range, while the levels of the final configuration are spread over a 22.0-eV energy range. With respect to the lowest level of the ground configuration, 26 of the 110 LSJ levels are autoionizing. We included 21% (148 autoionizing states out of 720 total states) of the $5p \to 5d$ excitation cross section at the average threshold energy for the autoionizing states of 54.46 eV to take into account its unique character of having the largest relative strength of all the inner-shell excitations and yet having its levels straddle the ionization threshold. Besides the $5p \to 5d$, the dominant excitations that contribute to ionization are $5p \to 6p$, $5p \to 6d$, and $4f \to 5f$. As seen in Fig. 1, the agreement between theory and experiment for this ion is reasonably good.

The single-ionization cross section from the $5s^2 5p^6 4f^{14} 5d$ ground configuration of W^{5+} is compared with experiment [4] in Fig. 2. Various direct ionization and inner-shell excitation cross sections between configurations are presented in Table II. The dominant excitations that contribute to ionization are $5p \rightarrow 6p$, $4f \rightarrow 5f$, and $5p \rightarrow 5f$. As seen in Fig. 2, the agreement between theory and experiment for this ion is quite good. The 19 LS terms associated with the $5s^2 5p^5 4f^{14} 5d^2$ final configuration of the $5p \rightarrow 5d$ excitation are now bound and thus do not contribute to ionization. Among the 19 LS terms are 6 quartet terms with relatively long lifetimes. The early onset of ionization seen in the experimental measurements of Fig. 2 may be due to a small amount of ionization from these metastable terms.

The single-ionization cross section from the $5s^2 5p^6 4f^{14}$ ground configuration of W^{6+} is compared with experiment [4] in Fig. 3. Various direct-ionization and inner-shell excitation cross sections between configurations are presented in Table III. The complete disagreement between theory and experiment in Fig. 3 is strong evidence that ionization in the experiment is taking place predominately through metastable states in excited configurations. Unfortunately, information on the fraction of metastable states in the W^{6+} ion beam is difficult to obtain experimentally. Only one excitation in Table III, the $5s \rightarrow 6d$, has a threshold energy above the $4f$ ionization potential. The single-ionization cross section from the $5s^2 5p^6 4f^{13} 5d$ excited configuration of W^{6+} is compared with the same experiment [4] in Fig. 4, while direct ionization and inner-shell excitation cross sections are presented in Table IV. Experiment is in much better agreement with calculations of ionization from the excited configuration, as seen in Fig. 4. The excited configuration contains many triplet terms with relatively long lifetimes. The dominant excitations in the excited configuration are $4f \rightarrow 5f$, $5p \rightarrow 5f$, and $5s \rightarrow 5d$. We also carried out calculations for the single-ionization cross section from the $5s^2 5p^5 4f^{14} 5d$ excited configuration of W^{6+}. The $5s^2 5p^5 4f^{14} 5d$ cross section is qualitatively quite similar to the $5s^2 5p^6 4f^{13} 5d$ cross section, thus making the identification of the precise metastable states in the experiment even more difficult.

There are as many as 5 configurations contributing to the ionization of W^{7+} as measured by the crossed-beams experiment of Stenke *et al.* [4]; the $5s^2 5p^6 4f^{13}$ ground configuration and the $5s^2 5p^6 4f^{12} 5d$, $5s^2 5p^5 4f^{14}$, $5s^2 5p^5 4f^{13} 5d$, and $5s^2 5p^4 4f^{14} 5d$ excited configurations. We did not carry out CADW calculations for W^{7+}, and higher charge states, due to the uncertainty as to what initial configurations are present in the experiment, and due to the increasing importance of radiation damping in the excitation-autoionization contributions.

In conclusion, configuration-average distorted-wave calculations for the single-ionization cross sections of W^{4+}, W^{5+}, and W^{6+} were found to be in reasonable agreement with recent crossed-beams measurements [4]. Strong excitation-autoionization contributions were found to be present in each cross section. Ionization from metastable states of excited configuration was found to dominate the experimental results for W^{6+}.

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