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Electron-Impact Ionization of the W Atom

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ABSTRACT: Electron-impact ionization cross sections for the ground configuration of the W atom are calculated using a combination of non-perturbative close-coupling and perturbative distorted-wave methods. Direct ionization of the 6s and 5d subshells leading to single ionization are presented. The results show a decrease in the cross section over previous calculations when more coupled channels are included and a furthur decrease when a polarization potential is included.

1. INTRODUCTION

Non-perturbative close-coupling and perturbative distorted-wave methods have been used to calculate direct ionization cross sections for both the W[1] atom and the W^+[2] atomic ion. Tungsten is an important element for magnetically confined fusion experiments, being used as a wall material[3]. The ionization of neutral tungsten is a critical atomic process in diagnostics for gross erosion of tungsten plasma facing components[4].

In this paper we extend the non-perturbative close-coupling calculations for the W atom to include more coupled channels. We also examine the effects of the inclusion of a polarization potential in both the close-coupling and distorted-wave calculations, as was recently explored for the electron ionization of the Pb atom[5].

The rest of this paper is organized as follows. In Section 2 we give a brief review of the non-perturbative close-coupling and the perturbative distorted-wave methods used to calculate electron-impact ionization cross sections. In Section 3 we present our cross section results for the electron-impact ionization of the W atom. We conclude with a brief summary and future plans in Section 4. Unless otherwise stated, we will use atomic units.

2. THEORY

The non-perturbative close-coupling cross section is given by[6]:

$$\sigma_{ion}(n_0l_0) = \frac{\pi w_0}{8(2l_0+1)E} \times \sum_{LS}(2L+1)(2S+1)P(n_0l_0LS) , \tag{1}$$

where $P(n_0l_0LS)$ is the non-perturbative theory partial ionization probability.

The perturbative distorted-wave cross section is given by[7]:

$$\sigma_{ion}(n_0l_0) = \frac{32w_0}{k_i^3} \int_0^{E/2} \frac{d(k_e^2/2)}{k_e k_f} \times \sum_{l_i l_e l_f} (2l_i+1)(2l_e+1)(2l_f+1) S(n_0l_0k_il_i \to k_el_ek_fl_f) \ , \tag{2}$$

where $S(n_0l_0k_il_i \rightarrow k_el_ek_fl_f)$ is the first order perturbation theory partial scattering probability. The bound and continuum orbitals are calculated in the Hartree-Fock Relativistic (HFR) approximation[8].

For both the non-perturbative close-coupling and the perturbative distorted-wave calculations we use a polarization potential given by:

$$V_{pol}(r) = -\frac{\alpha r^2}{2(r^2+r_c^2)} \ , \tag{2}$$

where $\alpha = 68.0$ and $r_c = 3.79815$ for W [9]. The polarization potential corresponds to the incoming electron polarizing the electron charge cloud.

3. RESULTS

3.1. Direct Ionization of the 6s subshell with no polarization potential

Non-perturbative close-coupling calculations for direct ionization of the 6s subshell of W using Eq.(1) with no polarization potential were made on a 480 × 480 point lattice with a mesh spacing of $\delta r = 0.20$ ranging from r = 0.0 to r = 96.00 for both sets of points. The non-perturbative close-coupling cross sections for direct ionization of the 6s subshell with no polarization potential are presented in Table 1. Perturbative distorted-wave calculations were used to topup the non-perturbative close-coupling calculations for l = 8-50.

We note that for L = 0-5 that the new calculations use 132 coupled channels that is larger than the 90 coupled channels used before for W[1]. We find that the new cross section for an incident energy of 20 eV and L = 0-5 is 194.84 Mb and thus 30% lower than the 276.90 Mb found before for W[1]. We also find that the new cross section for an incident energy of 30 eV and L = 0 - 5 is 140.53 Mb and thus 32% lower than the 207.70 Mb found before for W[1].

Both the non-perturbative close-coupling and the perturbative distorted-wave ionization cross sections for the 6s subshell of W are presented in Figure 1. We use simple analytical formulae to smoothly join the the 3 calculated non-perturbative close-coupling cross sections and to extend the results to higher energies. Numerical values for the perturbative distorted-wave and non-perturbative close-coupling cross sections are available on a fine energy mesh[10].

3.2. Direct Ionization of the 6s subshell with a polarization potential

Non-perturbative close-coupling calculations for direct ionization of the 6s subshell using Eq.(1) with the polarization potential of Eq.(3) were made on a 480 × 480 point lattice with a mesh spacing of $\delta r = 0.20$ ranging from r = 0.0 to r = 96.0 for both sets of points. The non-perturbative close-coupling cross sections for direct ionization of the 6s subshell with a polarization potential are presented in Table 2. Perturbative distorted-wave calculations with a polarization potential were used to topup the non-perturbative close-coupling calculations for l = 8 - 50.

We find that the cross section with a polarization potential for an incident energy of 20 eV and L = 0-5 is 183.56 Mb and thus 5.8% lower than the 194.84 Mb found above without a polarization potential. We also find that the cross section with a polarization potential for an incident energy of 30 eV and L = 0 - 5 is 131.76 Mb and thus 6.2% lower than the 140.53 Mb found above without a polarization potential.

Both the non-perturbative close-coupling and the perturbative distorted-wave ionization cross sections for the 6s subshell of W are presented in Figure 2. We use simple analytical formulae to smoothly join the 3 calculated non-perturbative close-coupling cross sections and to extend the results to higher energies. Numerical values for the perturbative distorted-wave and non-perturbative close-coupling cross sections are available on a fine energy mesh[10].

3.3. Direct Ionization of the 5d subshell with no polarization potential

Non-perturbative close-coupling calculations for direct ionization of the 5d subshell of W using Eq.(1) with no polarization potential were made on a 480 × 480 point lattice with the same mesh as used before for the 6s subshell. The non-perturbative close-coupling cross sections for direct ionization of the 5d subshell with no polarization potential are presented in Table 3. Perturbative distorted-wave calculations were used to topup the non-perturbative close-coupling calculations for l = 8 - 50.

We note that for L = 0-5 that the new calculations use 527 coupled channels that is larger than the 341 coupled channels used before for W[1]. We find that the new cross section for an incident energy of 20 eV and L = 0-5 is 185.66 Mb and thus 26% lower than the 252.00 Mb found before for W[1]. We also find that the new cross section for an incident energy of 30 eV and L = 0 - 5 is 214.35 Mb and thus 24% lower than the 281.70 Mb found before for W[1].

Both the non-perturbative close-coupling and the perturbative distorted-wave cross sections for the 5d subshell of W are presented in Figure 3. We use simple analytical formulae to smoothly join the 3 calculated non-perturbative close-coupling cross sections and to extend the results to higher energies. Numerical values for the perturbative distorted-wave and non-perturbative close-coupling cross sections are available on a fine energy mesh[10].

3.4. Direct Ionization of the 5d subshell with a polarization potential

Non-perturbative close-coupling calculations for direct ionization of the 5d subshell of W using Eq.(1) with the polarization potential of Eq.(3) were made on a 480×480 point lattice with the mesh as used before for the 6s subshell.

We find that the cross section with a polarization potential for an incident energy of 20 eV and L = 0 - 5 is 181.66 Mb and thus 2.2% lower than the 185.66 Mb found above without a polarization potential. Since the change in the cross section is so small, we did not carry out any furthur non-perturbative close-coupling calculations for direct ionization of the 5d subshell of W with a polarization potential.

4. SUMMARY

Electron-impact ionization cross sections for the single ionization of the neutral W atom have been presented. The new L = 0-5 calculations for the 6s subshell used 47% more coupled channels than used before for the W[1] atom, lowering the cross section by around 30%. The addition of a polarization potential lowered the cross sections by an additional 6%. The overall perturbative distorted-wave and non-perturbative close-coupling calculations for the 6s subshell with and without a polarization potential were presented for energies ranging from threshold to 100 eV. The new L = 0-5 calculations for the 5d subshell used 55% more coupled channels than used before for the W[1] atom, lowering the cross section by around 25%. The addition of a polarization potential had only a small effect on the cross section. The overall perturbative distorted-wave and non-perturbative close-coupling calculations for the 5d subshell without a polarization potential were presented for energies ranging from threshold to 100 eV. In the future we plan to carry out perturbative distorted-wave and non-perturbative close-coupling calculations for the outer subshells of other heavy atoms.

Acknowledgments

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Table 1. Non-perturbative close-coupling calculations for the ionization of the 6s subshell of W

Initial Channel	L Values	Coupled Channels	20 eV	30 eV	40 eV
$6sks$	0	9	1.99 Mb	1.90 Mb	1.87 Mb
$6skp$	1	16	10.24 Mb	7.37 Mb	5.76 Mb
$6skd$	2	22	21.88 Mb	15.74 Mb	12.13 Mb
$6skf$	3	26	34.77 Mb	25.69 Mb	20.27 Mb
$6skg$	4	29	67.95 Mb	49.05 Mb	34.21 Mb
$6skh$	5	30	58.01 Mb	40.78 Mb	28.88 Mb
$6ski$	6	30	55.82 Mb	48.38 Mb	36.88 Mb
$6skj$	7	28	49.55 Mb	49.56 Mb	40.03 Mb
		partial total	300.21 Mb	238.47 Mb	180.03 Mb
		topup	81.29 Mb	130.89 Mb	151.63 Mb
		final total	381.50 Mb	369.36 Mb	331.66 Mb

Table 2. Non-perturbative close-coupling calculations with a polarization potential for the ionization of the 6s subshell of W

Initial Channel	L Values	Coupled Channels	20 eV	30 eV	40 eV
$6sks$	0	9	1.88 Mb	1.77 Mb	1.77 Mb
$6skp$	1	16	9.68 Mb	6.98 Mb	5.48 Mb
$6skd$	2	22	20.65 Mb	14.94 Mb	11.57 Mb
$6skf$	3	26	31.95 Mb	24.00 Mb	19.27 Mb
$6skg$	4	29	63.94 Mb	46.02 Mb	32.46 Mb
$6skh$	5	30	55.46 Mb	38.05 Mb	27.39 Mb
$6ski$	6	30	52.93 Mb	46.03 Mb	35.30 Mb
$6skj$	7	28	46.84 Mb	47.23 Mb	38.39 Mb
		partial total	283.33 Mb	225.02 Mb	171.63 Mb
		topup	79.63 Mb	123.36 Mb	140.43 Mb
		final total	362.96 Mb	348.38 Mb	312.06 Mb

Table 3. Non-perturbative close-coupling calculations for the ionization of the 5d subshell of W

Initial Channel	L Values	Coupled Channels	20 eV	30 eV	40 eV
$5dks$	2	22	5.59 Mb	5.40 Mb	4.90 Mb
$5dkp$	1	16	5.05 Mb	4.74 Mb	4.42 Mb
$5dkp$	2	14	8.27 Mb	6.73 Mb	5.42 Mb
$5dkp$	3	26	11.54 Mb	9.42 Mb	8.16 Mb
$5dkd$	0	9	1.73 Mb	1.77 Mb	1.77 Mb
$5dkd$	1	8	13.40 Mb	10.56 Mb	8.16 Mb
$5dkd$	2	22	8.68 Mb	7.30 Mb	6.17 Mb
$5dkd$	3	19	26.75 Mb	19.82 Mb	14.52 Mb
$5dkd$	4	29	18.86 Mb	14.64 Mb	12.00 Mb
$5dkf$	1	16	3.12 Mb	4.83 Mb	5.43 Mb
$5dkf$	2	14	4.50 Mb	8.48 Mb	9.73 Mb
$5dkf$	3	26	7.20 Mb	8.12 Mb	8.58 Mb
$5dkf$	4	22	7.37 Mb	14.70 Mb	17.81 Mb
$5dkf$	5	30	10.15 Mb	8.92 Mb	11.49 Mb
$5dkg$	2	22	2.09 Mb	2.52 Mb	3.03 Mb
$5dkg$	3	19	3.79 Mb	5.58 Mb	6.05 Mb
$5dkg$	4	29	5.11 Mb	7.69 Mb	8.16 Mb
$5dkg$	5	24	12.72 Mb	18.40 Mb	18.34 Mb
$5dkg$	6	30	13.02 Mb	22.15 Mb	23.84 Mb
$5dkh$	3	26	1.81 Mb	2.36 Mb	2.49 Mb
$5dkh$	4	22	1.78 Mb	2.90 Mb	3.47 Mb
$5dkh$	5	30	2.89 Mb	5.36 Mb	6.42 Mb
$5dkh$	6	24	3.66 Mb	7.74 Mb	9.75 Mb
$5dkh$	7	28	6.58 Mb	14.22 Mb	18.52 Mb
$5dki$	4	27	1.17 Mb	2.06 Mb	2.37 Mb
$5dki$	5	24	1.06 Mb	2.08 Mb	2.58 Mb
$5dki$	6	30	1.89 Mb	4.17 Mb	5.44 Mb
$5dki$	7	25	1.80 Mb	4.60 Mb	6.44 Mb
$5dki$	8	25	3.64 Mb	9.76 Mb	14.20 Mb
$5dkj$	5	28	0.78 Mb	1.69 Mb	2.21 Mb
$5dkj$	6	24	0.61 Mb	1.44 Mb	1.97 Mb
$5dkj$	7	28	1.16 Mb	3.02 Mb	4.35 Mb
$5dkj$	8	20	0.99 Mb	3.01 Mb	4.62 Mb
$5dkj$	9	20	1.97 Mb	6.54 Mb	10.64 Mb
		partial total	200.73 Mb	252.72 Mb	273.45 Mb
		topup	16.75 Mb	57.23 Mb	105.65 Mb
		final total	217.48 Mb	309.95 Mb	379.10 Mb

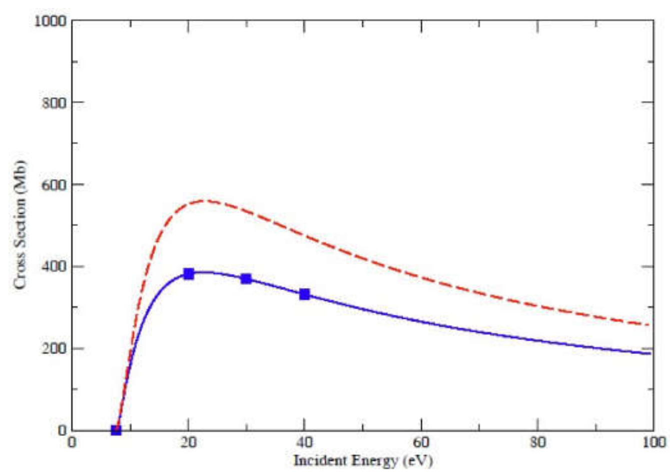

Figure 1. Electron-impact direct ionization of the 6s subshell of W. Dashed line (red): distorted-wave method, Solid squares (blue): non-perturbative close-coupling method (1.0 Mb = 1.0 × 10^{-18} cm^2).

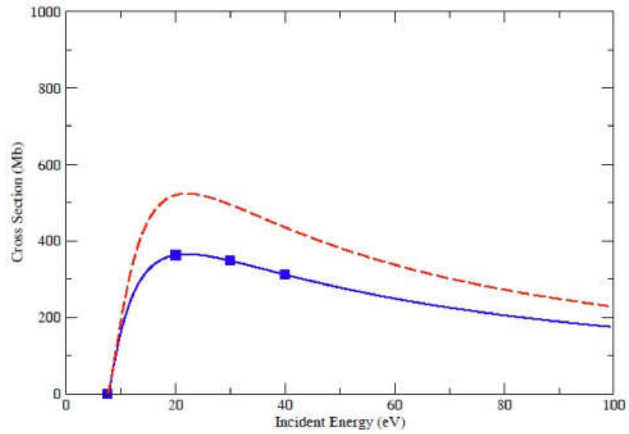

Figure 2. Electron-impact direct ionization of the 6s subshell of W. Dashed line (red): distorted-wave method with a polarization potential, Solid squares (blue): non-perturbative close-coupling method with a polarization potential (1.0 Mb = 1.0 × 10^{-18} cm^2).

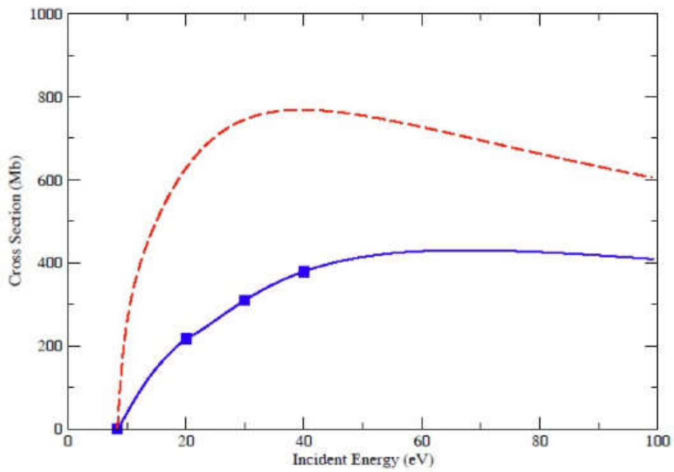

Figure 3. Electron-impact direct ionization of the 5d subshell of W. Dashed line (red): distorted-wave method, Solid squares (blue): non-perturbative close-coupling method (1.0 Mb = 1.0 × 10^{-18} cm^2).