Journal of Optoelectronics and Advanced Materials Vol. 7, No. 5, October 2005, p. 2413 - 2420

COMPLEX ATOMS MODELLING FOR PLASMA DIAGNOSTICS

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In this work we report atomic data calculations in intermediate couplig scheme, for tungsten ions with two electrons outside closed shell of type Ca-like, Ba-like and Hf-like. We used the atomic structure code by Cowan to output values of energy levels, radiative transition probabilities, oscillator strengths and wavelengths for transitions in the EUV region. Our calculation refers to configuration interaction method using Hartree-Fock approximations. Results are compared with those obtained from Hartree Fock Slater and Hartree Statistical Exchange approximations.

(Received January 18, 2005; accepted September 22, 2005)

Keywords: Atomic data, Atomic spectra, Spectroscopy

1. Introduction

High particle and energy fluxes in future fusion experiments demand the investigation of materials for plasma facing components. A promising alternative to the present frequently used low-Z materials carbon and beryllium is tungsten. Partially ionized ions of elements such as tungsten and tantalum in the second long period, however, have two problems, an atomic structure which increasingly should be described in intermediate coupling and a consequent description of their emitted spectrum lines into very many separated levels from many transition arrays often associated with partially inner shells. The spectral emission may appear as a quasi-continuum.

The importance of tungsten to many modern high-temperature plasma devices has induced new activity to measure the radiation from such ions. This is in addition to the purely spectroscopic interest inherent in this kind of research. Fusion devices constitute a prime example, where the specific characteristics of tungsten make it an important material for various structural components. Recent work has suggested that tungsten may be the best solution for reducing the divertor tile erosion in a fusion reactor [1,2]. Moreover, tungsten has excellent redeposition properties with the result that production of higher ionization stages and associated problems of self-sputtering are in large part suppressed. On the other hand, if sputtered tungsten penetrates into the central plasma region it can exist there in various ionization stages, which depend on electron temperature, and it has the effect of raising the radiation losses. The radiation from tungsten represents a serious limitation to the energy confinement in a fusion reactor and could quench the fusion reaction if the relative concentration of W ions in the core plasma is higher than about 10^{-5}[3].

As tokamak systems become increasingly more sophisticated, the ability to predict and monitor plasma properties becomes imperative. It is more important, then, to have accurate data on which to base these predictions. The intermediate charge of tungsten is some of most prominent in plasmas with ion temperature of a few keV. These ions radiate a significant portion of their spectra in the extreme ultraviolet from 40 to 85 Å.

While many measurements of particular lines and theoretical predictions of transitions from intermediate charge-state ions have been reported in the last 20 years, the most complete

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compilations of the wavelengths and intensities of these lines in tungsten appear to be that by Fournier [4] where transition wavelengths were derived from ab initio atomic-structure calculations.

In this work are reported atomic data for tungsten ions belonging to Ba-like, Ca-like, Hf-like, Sr-like and Zn-like iso-electronic sequences. The calculations were performed on the basis of the Cowan's code in Hartree-Fock method including relativistic effects. The code computes spin-orbit parameter from the central-potential formula and also via the Blume-Watson method. The latter method gives more accurate values for atomic parameters.

2. Calculations

In this work the radial wavefunctions were generated using pseudo relativistic Hartree-Fock (HFR) method originally introduced by Cowan & Griffin [5] with the computer code written by Cowan [6]. The relativistic corrections included in the differential equations are derived from Pauli-type approximation to the Dirac-Hartree-Fock equations and retain both the mass-velocity and Darwin operators. The Cowan's code calculates configuration-interaction radial Coulomb integrals and electric dipole and quadrupole reduced matrix elements, scales all energy-level-structure parameters and writes a complete file of input data for making energy level and spectrum calculations.

There is a suite of four routines that calculate atomic structures and spectra via the superposition-of-configuration method: a) the calculation of one-electron radial wavefunctions (bound and free) for each of any number of the specified configurations, using Hartree-Fock or any of several more approximate methods (Hartree-Fock Slater, Hartree plus Statistical Exchange, Hartree-Slater); b) the calculation of the configuration-interaction Coulomb integrals between each pair of interacting configurations, and the electric-dipole and/or electric quadrupole radial integrals between each pair of configurations; c) sets up energy matrices for each possible value of the total angular momentum J, diagonalizes each matrix to get eigenvalues (energy levels) and eigenvectors (multi-configuration, intermediate-coupling wavefunctions in various possible angular-momentum-coupling representations), followed by the computation of the magnetic dipole, electric- dipole and – quadrupole spectra, with wavelengths, oscillator strengths, radiative transition probabilities, and radiative lifetimes; d) for higher accuracy results a least-square fit of experimental energy levels is possible using an iterative procedure.

Table 1. Electric –dipole and –quadrupole transitions as labeled in Table 2. The corresponding angular momentum J is also given in Table 2.

index	electric-dipole transitions $[Xe]n_1l_1\ n_2l_2\ (J_0) - [Xe]\ n_1l_1\ n_2l_2(J_1)$	electric quadrupole transitions $[Xe]n_1l_1\ n_2l_2\ (J_0) - [Xe]\ n_1l_1\ n_2l_2(J_1)$
1	$6s^2(J_0) - 6s7p(J_1)$	$6s^2\ (J_0) - 6s^2(J_1)$
2	$6s7s(J_0) - 6s8p(J_1)$	$6s7s(J_0) - 6s7s(J_1)$
3	$6s8s(J_0) - 6s9p(J_1)$	$6s8s(J_0) - 6s8s(J_1)$
4	$6s9s(J_0) - 6s7f(J_1)$	$6s9s(J_0) - 6s9s(J_1)$
5	$6s7d(J_0) - 6s8f(J_1)$	$6s7d(J_0) - 6s7d(J_1)$
6	$6s8d(J_0) - 6s9f(J_1)$	$6s8d\ (J_0) - 6s8d(J_1)$
7	$6s9d\ (J_0) - 6s7h(J_1)$	$6s9d(J_0) - 6s9d(J_1)$
8	$6s7g\ (J_0) - 6s8h(J_1)$	$6s7g(J_0) - 6s7g(J_1)$
9	$6s8g(J_0) - 6s9h(J_1)$	$6s8g(J_0) - 6s8g(J_1)$
10	-	$6s9g(J_0) - 6s9g(J_1)$

Table 1 presents the studied transitions in Ba-like W ion, W^{18+}, configuration [Xe] $6s^2$. The corresponding atomic data, in jj coupling scheme, are shown in Table 2. The energies E_i, E_j, corresponding to the resolved transitions, oscillator strength, gf, radiative transition probability, gA, and wavelength, λ, are listed as output from the code. Comparisons with other method are also provided in this table: Hartree-Fock (HF), Hartree-Fock-Slater (HFS), Hartree plus Statistical exchange (HX).

Table 2. Atomic data calculations for W^{18+}. The lower and upper levels are denoted by 0 and 1, respectively. The transition energy, ΔE, and level energies E_0, E_1, are given in units of $1000cm^{-1}$, while the transition probability, ga, is in units of sec^{-1}. gf stands for the oscillator strengths.

		E_0 ($1000cm^{-1}$)	J_0	Config.	E_1	J_1	$Config_p$.	ΔE	$\lambda(A^0)$	gf	$ga(s^{-1})$
Ba-like	HF	electric-quadrupole transitions									
		-0.0446	0.0	1 (1S 0.0)	1380.7671	2.0	6 (2S 0.5)	1380.8117	72.4212	0.00001	7.709E+06
		-0.0446	0.0	1 (1S 0.0)	1386.3147	2.0	6 (2S 0.5)	1386.3593	72.1314	0.00002	2.535E+07
		-0.0446	0.0	1 (1S 0.0)	1590.0829	2.0	7 (2S 0.5)	1590.1276	62.8880	0.00001	8.997E+06
		-0.0446	0.0	1 (1S 0.0)	1593.6343	2.0	7 (2S 0.5)	1593.6789	62.7479	0.00002	2.617E+07
		electric-dipole transitions									
		-0.0446	0.0	1 (1S 0.0)	1275.6028	1.0	2 (2S 0.5)	1275.6474	78.3916	0.01464	1.589E+10
		-0.0446	0.0	1 (1S 0.0)	1299.9194	1.0	2 (2S 0.5)	1299.9640	76.9252	0.03761	4.239E+10
		-0.0446	0.0	1 (1S 0.0)	1521.5188	1.0	3 (2S 0.5)	1521.5634	65.7219	0.00800	1.235E+10
		-0.0446	0.0	1 (1S 0.0)	1537.0958	1.0	3 (2S 0.5)	1537.1405	65.0559	0.01958	3.086E+10
	HFSL	quadrupole-Slater's exchange term									
		-0.0431	0.0	1 (1S 0.0)	1381.0062	2.0	6 (2S 0.5)	1381.0494	72.4087	0.00001	1.238E+07
		-0.0431	0.0	1 (1S 0.0)	1386.9822	2.0	6 (2S 0.5)	1387.0254	72.0967	0.00003	3.763E+07
		-0.0431	0.0	1 (1S 0.0)	1590.5700	2.0	7 (2S 0.5)	1590.6131	62.8688	0.00001	1.265E+07
		-0.0431	0.0	1 (1S 0.0)	1594.4217	2.0	7 (2S 0.5)	1594.4649	62.7170	0.00002	3.427E+07
		dipole-Slater's exchange term									
		-0.0431	0.0	1 (1S 0.0)	1274.1988	1.0	2 (2S 0.5)	1274.2420	78.4780	0.02065	2.236E+10
		-0.0431	0.0	1 (1S 0.0)	1301.2161	1.0	2 (2S 0.5)	1301.2592	76.8486	0.05185	5.855E+10
		-0.0431	0.0	1 (1S 0.0)	1520.9398	1.0	3(2S 0.5)	1520.9830	65.7470	0.01046	1.614E+10
		-0.0431	0.0	1 (1S 0.0)	1538.2732	1.0	3(2S 0.5)	1538.3164	65.0061	0.02510	3.961E+10
		quadrupole-Kohn & Sham's									
		-0.0415	0.0	1 (1S 0.0)	1380.6209	2.0	6 (2S 0.5)	1380.6624	72.4290	0.00001	1.264E+07
		-0.0415	0.0	1 (1S 0.0)	1386.5049	2.0	6 (2S 0.5)	1386.5463	72.1216	0.00003	3.913E+07
		-0.0415	0.0	1 (1S 0.0)	1590.0325	2.0	7 (2S 0.5)	1590.0739	62.8902	0.00001	1.363E+07
		-0.0415	0.0	1 (1S 0.0)	1593.7915	2.0	7 (2S 0.5)	1593.8329	62.7418	0.00002	3.754E+07

Table 3 gives the electric-quadrupole transitions studied for Ca-like W ion, W^{54+}, configuration [Ar] $4s^2$. A selection of atomic data corresponding to a few of these transitions are shown in Table 4. Data are calculated using HF configuration-interaction method.

Table 3. Electric – quadrupole transitions as labeled in Table 4. The corresponding angular momentum J_0, J_1 is also given in Table 4.

index	electric quadrupole transitions $[Ar]n_1l_1\ n_2l_2\ (J_0)$ – $[Ar]\ n_1l_1\ n_2l_2(J_1)$	index	electric quadrupole transitions $[Ar]n_1l_1\ n_2l_2\ (J_0)$ – $[Ar]\ n_1l_1\ n_2l_2(J_1)$
1	$4s^2\ (J_0)$ - $4s^2(J_1)$	10	$4s6g(J_0)$ - $4s6g(J_1)$
2	$4s5s(J_0)$ - $4s5s(J_1)$	11	$4s7g(J_0)$ - $4s7g(J_1)$
3	$4s6s(J_0)$ - $4s6s(J_1)$	12	$4s4p(J_0)$ - $4s4p(J_1)$
4	$4s7s(J_0)$ - $4s7s(J_1)$	13	$4s5p(J_0)$ - $4s5p(J_1)$
5	$4s4d(J_0)$ - $4s4d(J_1)$	14	$4s6p(J_0)$ - $4s6p(J_1)$
6	$4s5d(J_0)$ - $4s5d(J_1)$	15	$4s7p(J_0)$ - $4s7p(J_1)$
7	$4s6d(J_0)$ - $4s6d(J_1)$	16	$4s4f(J_0)$ - $4s4f(J_1)$
8	$4s7d\ (J_0)$ - $4s7d(J_1)$	17	$4s5f(J_0)$ - $4s5f(J_1)$
9	$4s5g(J_0)$ - $4s5g(J_1)$	18	$4s6f(J_0)$ - $4s6f(J_1)$

Table 4. Atomic data calculations for W^{54+}. The lower and upper levels are denoted by 0 and 1, respectively. The transition energy, ΔE, and level energies E_0, E_1, are given in units of $1000cm^{-1}$, while the transition probability, ga, is in units of sec^{-1}. gf stands for the oscillator strengths.

		E_0 ($1000cm^{-1}$)	J_0	Conf.	E_1	J_1	Config.	ΔE ($1000\ cm^{-1}$)	$\lambda(A^0)$	gf	$ga(s^{-1})$
Ca-like	HF	quadrupole									
		9837.0567	0.0	2 (2S 0.5)	11104.8523	2.0	6 (2S 0.5)	1267.7956	78.8771	0.00002	1.920E+07
		9778.0302	1.0	2 (2S 0.5)	11100.1869	1.0	6 (2S 0.5)	1322.1567	75.6340	0.00003	3.994E+07
		9778.0302	1.0	2 (2S 0.5)	11104.8523	2.0	6 (2S 0.5)	1326.8221	75.3681	0.00004	4.384E+07
		9837.0567	0.0	2 (2S 0.5)	11229.7400	2.0	6 (2S 0.5)	1392.6833	71.8038	0.00004	5.633E+07
		9778.0302	1.0	2 (2S 0.5)	11222.0011	3.0	6 (2S 0.5)	1443.9709	69.2535	0.00010	1.448E+08
		9778.0302	1.0	2 (2S 0.5)	11229.7400	2.0	6 (2S 0.5)	1451.7098	68.8843	0.00003	3.747E+07
		16030.1786	3.0	10 (2S 0.5)	17773.3164	1.0	4 (2S 0.5)	1743.1378	57.3678	0.00000	0.000E+00
		15645.7873	2.0	7 (2S 0.5)	17773.3164	1.0	4 (2S 0.5)	2127.5292	47.0029	0.00014	4.305E+08
		15642.4864	3.0	7 (2S 0.5)	17773.3164	1.0	4 (2S 0.5)	2130.8301	46.9301	0.00055	1.669E+09
		15645.7873	2.0	7 (2S 0.5)	17784.1987	0.0	4 (2S 0.5)	2138.4115	46.7637	0.00025	7.675E+08
		9778.0302	1.0	2 (2S 0.5)	11926.6028	3.0	9 (2S 0.5)	2148.5727	46.5425	0.00000	0.000E+00
		16049.5877	4.0	10 (2S 0.5)	18227.9861	2.0	8 (2S 0.5)	2178.3984	45.9053	0.00001	3.189E+07
		16032.8036	4.0	10 (2S 0.5)	18227.9861	2.0	8 (2S 0.5)	2195.1826	45.5543	0.00018	5.890E+08
		16030.1786	3.0	10 (2S 0.5)	18226.8567	1.0	8 (2S 0.5)	2196.6781	45.5233	0.00013	4.149E+08
		16030.1786	3.0	10 (2S 0.5)	18227.9861	2.0	8 (2S 0.5)	2197.8076	45.4999	0.00002	7.303E+07
		15575.2380	2.0	7 (2S 0.5)	17773.3164	1.0	4 (2S 0.5)	2198.0785	45.4943	0.00027	8.858E+08
		15573.1991	1.0	7 (2S 0.5)	17773.3164	1.0	4 (2S 0.5)	2200.1173	45.4521	0.00026	8.394E+08
		15575.2380	2.0	7 (2S 0.5)	17784.1987	0.0	4 (2S 0.5)	2208.9608	45.2702	0.00016	5.164E+08
		16049.5877	4.0	10 (2S 0.5)	18269.9749	3.0	8 (2S 0.5)	2220.3872	45.0372	0.00001	2.481E+07
		16049.5877	4.0	10 (2S 0.5)	18271.7877	2.0	8 (2S 0.5)	2222.2000	45.0004	0.00021	6.854E+08
		16043.7924	5.0	10 (2S 0.5)	18269.9749	3.0	8 (2S 0.5)	2226.1825	44.9199	0.00027	9.034E+08
		16032.8036	4.0	10 (2S 0.5)	18269.9749	3.0	8 (2S 0.5)	2237.1714	44.6993	0.00003	1.005E+08

Table 5 is concerned with the electric-quadrupole transitions in Sr –like W, W^{36+}, configuration $[Kr]5s^2$. They are labeled according to their appearance in the Table 6.

Table 5. Electric–quadrupole transitions as labeled in Table 6. The corresponding angular momentum J_0, J_1 is also given in Table 6.

index	electric quadrupole transitions $[Kr]n_1l_1\ n_2l_2\ (J_0)$ – $[Kr]\ n_1l_1\ n_2l_2(J_1)$	index	electric quadrupole transitions $[Kr]n_1l_1\ n_2l_2\ (J_0)$ – $[Kr]\ n_1l_1\ n_2l_2(J_1)$
1	$5s^2\ (J_0)$ - $5s^2(J_1)$	6	$5s6d(J_0)$ - $5s6d(J_1)$
2	$5s6s(J_0)$ - $5s6s(J_1)$	7	$5s7d(J_0)$ - $5s7d(J_1)$
3	$5s7s(J_0)$ - $5s7s(J_1)$	8	$5s8d\ (J_0)$ - $5s8d(J_1)$
4	$5s8s(J_0)$ - $5s8s(J_1)$	9	$5s5g(J_0)$ - $5s5g(J_1)$
5	$5s5d(J_0)$ - $5s5d(J_1)$	10	$5s6g(J_0)$ - $5s6g(J_1)$

Table 6. Atomic data calculations for W^{36+}. The lower and upper levels are denoted by 0 and 1, respectively. The transition energy, ΔE, and level energies E_0, E_1, are given in units of $1000cm^{-1}$, while the transition probability , ga, is in units of sec^{-1}. gf stands for the oscillator strengths.

		E ($1000cm^{-1}$)	J	Conf.	E_p	J_p	$Conf_p$.	ΔE	$\lambda(A^0)$	gf	$ga(s^{-1})$
Sr-like	HF	quadrupole									
		1337.2889	3.0	5 (2S 0.5)	2511.7522	4.0	9 (2S 0.5)	1174.4633	85.1453	0.00000	7.872E+05
		1283.8980	2.0	5 (2S 0.5)	2490.3656	3.0	9 (2S 0.5)	1206.4677	82.8866	0.00003	2.890E+07
		1283.8980	2.0	5 (2S 0.5)	2492.6088	4.0	9 (2S 0.5)	1208.7108	82.7328	0.00017	1.643E+08
		1270.9786	1.0	5 (2S 0.5)	2490.3656	3.0	9 (2S 0.5)	1219.3870	82.0084	0.00013	1.290E+08
		1283.8980	2.0	5 (2S 0.5)	2511.7522	4.0	9 (2S 0.5)	1227.8542	81.4429	0.00001	1.334E+07
		2511.7522	4.0	9 (2S 0.5)	3780.4078	2.0	6 (2S 0.5)	1268.6557	78.8236	0.00001	1.082E+07
		-0.0497	0.0	1 (1S 0.0)	1283.8980	2.0	5 (2S 0.5)	1283.9476	77.8848	0.00004	4.026E+07
		4788.0969	0.0	3 (2S 0.5)	6075.3516	2.0	8 (2S 0.5)	1287.2547	77.6847	0.00005	5.570E+07
		2490.3656	3.0	9 (2S 0.5)	3777.6283	1.0	6 (2S 0.5)	1287.2626	77.6842	0.00004	4.117E+07
		2492.6088	4.0	9 (2S 0.5)	3780.4078	2.0	6 (2S 0.5)	1287.7991	77.6519	0.00004	4.864E+07
		2490.3656	3.0	9 (2S 0.5)	3780.4078	2.0	6 (2S 0.5)	1290.0422	77.5168	0.00001	8.072E+06
		4777.0804	1.0	3 (2S 0.5)	6074.7025	1.0	8 (2S 0.5)	1297.6221	77.0640	0.00008	9.135E+07
		4777.0804	1.0	3 (2S 0.5)	6075.3516	2.0	8 (2S 0.5)	1298.2712	77.0255	0.00009	1.004E+08
		2511.7522	4.0	9 (2S 0.5)	3813.3033	3.0	6 (2S 0.5)	1301.5511	76.8314	0.00000	3.204E+05
		4788.0969	0.0	3 (2S 0.5)	6089.8072	2.0	8 (2S 0.5)	1301.7103	76.8220	0.00010	1.131E+08
		2511.7522	4.0	9 (2S 0.5)	3818.4802	2.0	6 (2S 0.5)	1306.7280	76.5270	0.00005	5.954E+07
		4777.0804	1.0	3 (2S 0.5)	6088.7061	3.0	8 (2S 0.5)	1311.6257	76.2413	0.00020	2.249E+08
		4777.0804	1.0	3 (2S 0.5)	6089.8072	2.0	8 (2S 0.5)	1312.7268	76.1773	0.00005	5.525E+07
		2496.5545	5.0	9 (2S 0.5)	3813.3033	3.0	6 (2S 0.5)	1316.7488	75.9446	0.00008	9.392E+07
		2492.6088	4.0	9 (2S 0.5)	3813.3033	3.0	6 (2S 0.5)	1320.6945	75.7177	0.00001	1.266E+07
		2490.3656	3.0	9 (2S 0.5)	3813.3033	3.0	6 (2S 0.5)	1322.9376	75.5894	0.00000	8.740E+05
		2492.6088	4.0	9 (2S 0.5)	3818.4802	2.0	6 (2S 0.5)	1325.8714	75.4221	0.00001	1.032E+07
		2490.3656	3.0	9 (2S 0.5)	3818.4802	2.0	6 (2S 0.5)	1328.1146	75.2947	0.00000	4.034E+06

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Journal of Optoelectronics and Advanced Materials Vol. 7, No. 5, October 2005, p. 2413 - 2420

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