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Electron Impact Excitation of Fe-like Tungsten Ion

Research Article

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Abstract. Electron impact excitation of Fe-like tungsten ion has been studied using relativistic distorted wave theory. Cross-sections are obtained in the energy range upto 20 keV and their fitting is also provided for their potential application in plasma modeling. Polarization of the photon emission following the decay of the excited states is also analysed.

Keywords. Electron-impact excitation; Relativistic distorted wave; Polarization; tungsten ions

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1. Introduction

Atomic data of tungsten is in great demand due to its prospective application in plasma diagnostics in the *International Thermonuclear Experimental Reactor* (ITER). Tungsten ions in their various charge states are expected to be present in the ITER plasma where electron induced processes are likely to be the dominant ones. There exist several theoretical and experimental investigations of transition probabilities, excitation energies, wavelengths and oscillator strengths of the transitions as well as spectra of tungsten ions [1–7]. The atomic data compilations of Kramida and Shirai [2] and Kramida [3] may be looked up for more references. However, there are very limited theoretical or experimental investigations related to the electron induced processes of tungsten ions e.g., excitation, ionization, dielectronic recombination and radiative electron capture.

To meet the great demand of atomic data of tungsten and its multiply charged ions required for design and development of the ITER, the *International Atomic Energy Agency* (IAEA) has formed a committee of scientists from all over the world. One of the authors RS is member of this committee, therefore, as a part of our contribution to tungsten data we have taken initiative to study electron impact excitation of highly charged tungsten ions using fully *relativistic distorted wave* (RDW) theory. In this connection, we have reported detailed RDW excitation cross sections for M- and L-shell excitations of W^{q+} where $q = 44$ to 66 and also provided the fitting of these cross sections so that they can be directly applied in plasma models [8–10]. Apart from cross-sections, linear polarization of the photon emissions arising due to decay of the excited states of the above tungsten ions is also analysed. These detailed calculations have been performed in the light of spectroscopic measurements of M- and L-shell emissions in various charged states of tungsten ions recorded at *electron beam ion trap* (EBIT) at the Lawrence Livermore National Laboratory by Beiersdorfer and his co-workers [4–6]. We have calculated cross sections data for those transitions that correspond to the intense lines in the L- and M-shell spectra of tungsten ions in the EBIT measurements [4–6] as such data would be vital for diagnostics of nuclear fusion plasmas. Recently, Clementson *et al.* [7] have calculated the atomic structure and spectra of germanium-like W^{42+} through vanadium-like W^{51+} ions using the *Flexible Atomic Code* (FAC). They reported calculations for energy levels, radiative lifetimes, spectral line positions, transition probability rates, and oscillator strengths for these ions. They have also implemented collisional-radiative model for high-temperature, low-density plasma to produce line emissivities for X-ray transitions in the 1-4 keV (3-12)A^0 spectral interval. In the light of these new calculations, we have considered in the present work electron impact excitation of Fe-like W^{48+} ion. In this brief paper, we have performed RDW calculations to obtain cross sections for the transitions which give intense lines in the spectra calculated by Clementson *et al.* [7]. In particular, we have considered the excitation from the ground state i.e., $(3d^4_{3/2}3d^4_{5/2})_{J=4}$ to the final state leading to excitation of one electron either from $3d_{3/2}$ or $3d_{5/2}$ orbital to $4f_{5/2}$ and $4f_{7/2}$ orbitals. The fitting constants of these cross sections are also made available for their use in plasma modeling. We have also calculated polarization of the photons emitted due to decay of the anisotropically excited ionic state.

2. Theoretical Method

The evaluation of all scattering parameter can be performed using T-matrix $T^{RDW}_{i\to f}(J_i, M_i, \mu_i; J_f, M_f, \mu_f, \theta)$ for excitation of one electron from initial state $|\alpha_i J_i M_i\rangle$ to the final state $|\alpha_f J_f M_f\rangle$ of the ion [8]. Here θ is the scattering angle i.e., angle between the wave vectors k_i and k_f of the incident and scattered electrons. $J_{i(f)}$ and $M_{i(f)}$ denote the total angular momentum and its magnetic components in the initial(final) state of the ion and $\mu_{i(f)}$ is spin projection of the incident(scattered) electron. $\alpha_{i(f)}$ refer to the other quantum numbers required to specify the ionic states before and after the excitation.

In order to obtain T-matrix, one requires accurate wave functions for bound as well as continuum orbitals. GRASP2K code [11] is used to calculate the wavefunction of the bound orbitals within *multi-configuration Dirac-Fock* (MCDF) approach in which the initial and final states of the ion are expressed as linear combination of other configuration state functions with same J and parity. The wavefunction of projectile electrons are obtained by solving Dirac equation in the field of spherically averaged static potential of the final state of the ion. For the given normalization of the distorted waves, the cross section for the excitation of an ion to its magnetic sublevel M_f can be written as

$$\sigma(\alpha_f J_f M_f) = (2\pi)^4 \frac{k_f}{2(2J_i+1)k_i} \int \left| T^{RDW}_{i\to f}(J_i, M_i, \mu_i; J_f, M_f, \mu_f, \theta) \right|^2 d\Omega, \tag{2.1}$$

where integration has been carried over the solid angle of the scattered electron. The sum of all magnetic sublevel cross sections yields the total cross section corresponding to the fine-structure level J_f, i.e.,

$$\sigma(\alpha_f J_f) = \sum_{M_f} \sigma_{M_f}.$$

Further, using magnetic sublevel cross sections of the excited state σ_{M_f} linear polarization of the characteristic photon emission can be obtained with the help of density matrix theory [8, 12].

3. Results and Discussion

The ground state of Fe-like tungsten ion is $(3d^4_{3/2}3d^4_{5/2})_{J=4}$. We have considered transitions from the ground state to the excited state with a vacancy in $3d$ orbital and with one valence electron in $4f$ orbital. The list of transitions considered in the present work is given in Table 1. The ground state and excited state wavefunctions are obtained by using GRASP2K code [11]. To ascertain the accuracy of these bound state wave functions we have also calculated the excitation energies and oscillator strengths of these transitions and included them in Table 1. A comparison of our calculations with the FAC results reported by Clementson *et al.* [7] is also shown in Table 1. We find that our calculated excitation energies are within 0.03% while oscillator strengths are within 5% of the corresponding values calculated by Clementson *et al.* [7], except for Fe-1 transition, which shows a difference of 18%. Thus overall agreement between the two theoretical results is fairly good.

Further, using the bound orbital wavefunctions we have calculated the magnetic sublevel cross sections σ_{M_f}, equation (2.1) for excitation of Fe-like tungsten ion from ground state $(3d^4_{3/2}3d^4_{5/2})_{J=4}$ to the higher lying states as listed in Table 1. Excitation cross section $\sigma(\alpha_f J_f)$ is obtained by summing the cross sections of all the magnetic substates and shown in Figure 1 in the incident electron energy range from excitation threshold to 20 keV. It can be noticed from Figure 1 that with increasing electron energy magnitude of the cross section decreases while its order either remains same or fall off by one. Moreover, the magnitude of the cross sections is governed by the value of oscillator strength associated with the transition and hence the Fe-12 line shows maximum cross-sections of all the transitions considered. Therefore, it can be said that the cross-section curves show the typical behaviour of a dipole allowed transition.

Table 1. Comparison of our calculated excitation energies (in eV) and oscillator strengths of the transitions in Fe-like W^{48+} ions with the FAC calculations [7].

Transition	Upper Level	E_{present}	E [7]	f_{present}	f [7]
Fe-1	$[3d^4_{3/2}(3d^3_{5/2})_{9/2}4f_{7/2}]_{J=3}$	2184.33	2183.92	0.106	0.086
Fe-2	$[3d^4_{3/2}(3d^3_{5/2})_{9/2}4f_{7/2}]_{J=5}$	2185.70	2185.24	0.044	0.042
Fe-3	$[3d^4_{3/2}(3d^3_{5/2})_{9/2}4f_{7/2}]_{J=4}$	2192.84	2192.19	0.135	0.132
Fe-4	$[3d^4_{3/2}(3d^3_{5/2})_{5/2}4f_{5/2}]_{J=4}$	2198.19	2197.50	0.151	0.153
Fe-5	$[3d^4_{3/2}(3d^3_{5/2})_{3/2}4f_{7/2}]_{J=5}$	2299.95	2199.19	0.310	0.311
Fe-6	$[3d^4_{3/2}(3d^3_{5/2})_{5/2}4f_{7/2}]_{J=4}$	2201.50	2201.09	0.141	0.146
Fe-7	$[3d^4_{3/2}(3d^3_{5/2})_{5/2}4f_{7/2}]_{J=5}$	2206.50	2206.69	0.356	0.371
Fe-8	$[(3d^4_{3/2}(3d^3_{5/2})_2)_{5/2}4f_{5/2}]_{J=3}$	2266.33	2265.74	0.194	0.203
Fe-9	$[(3d^4_{3/2}(3d^3_{5/2})_2)_{5/2}4f_{5/2}]_{J=5}$	2268.91	2268.33	0.178	0.170
Fe-10	$[(3d^4_{3/2}(3d^3_{5/2})_4)_{11/2}4f_{5/2}]_{J=3}$	2269.54	2269.68	0.581	0.567
Fe-11	$[(3d^4_{3/2}(3d^3_{5/2})_2)_{5/2}4f_{7/2}]_{J=4}$	2271.42	2270.91	0.995	0.998
Fe-12	$[(3d^4_{3/2}(3d^3_{5/2})_4)_{5/2}4f_{5/2}]_{J=5}$	2274.60	2274.11	2.144	2.188
Fe-13	$[(3d^4_{3/2}(3d^3_{5/2})_2)_{5/2}4f_{7/2}]_{J=4}$	2274.89	2274.41	0.456	0.462

Table 2. Values of fitting coefficients Eq.(3.1) for electron impact excitation cross-sections for all the transitions in Fe-like W^{48+}ion. The number in the parenthesis refers to the power of 10 by which the quantity has been raised.

Transition	b_0	b_1	b_2	c_1	c_2	c_3
Fe-1	1.48058(−2)	3.34751(−4)	8.65562(−8)	1.49601(+2)	9.43692(+0)	2.29575(−2)
Fe-2	7.16988(−3)	5.65681(−5)	1.72660(−9)	1.49497(+2)	6.71077(+0)	6.45266(−3)
Fe-3	1.35213(−2)	3.67740(−4)	1.01659(−7)	1.48460(+2)	9.88939(+0)	2.66412(−2)
Fe-4	1.37178(−2)	4.48858(−4)	1.35358(−7)	1.48322(+2)	1.06317(+1)	3.04766(−2)
Fe-5	3.36154(−2)	1.18130(−3)	3.78171(−7)	1.47961(+2)	1.35110(+1)	4.05364(−2)
Fe-6	1.47188(−2)	3.68324(−4)	1.00140(−7)	1.48065(+2)	9.95143(+0)	2.57655(−2)
Fe-7	3.91507(−2)	1.23336(−3)	3.82740(−7)	1.47674(+2)	1.27392(+1)	3.6574(−2)
Fe-8	2.78572(−2)	9.74727(−4)	3.20606(−7)	1.47108(+2)	1.81534(+1)	5.56208(−2)
Fe-9	2.44115(−2)	9.18200(−4)	3.05294(−7)	1.47051(+2)	1.86108(+1)	5.74287(−2)
Fe-10	9.93902(−2)	3.47952(−3)	1.15840(−6)	1.46618(+2)	2.17741(+1)	6.71147(−2)
Fe-11	1.77555(−1)	6.41744(−3)	2.15419(−6)	1.46352(+2)	2.35057(+1)	7.28505(−2)
Fe-12	3.68332(−1)	1.38898(−2)	4.70626(−6)	1.46343(+2)	2.35577(+1)	7.35884(−2)
Fe-13	7.83587(−2)	2.81631(−3)	9.36372(−7)	1.46487(+2)	2.26508(+1)	6.95775(−2)

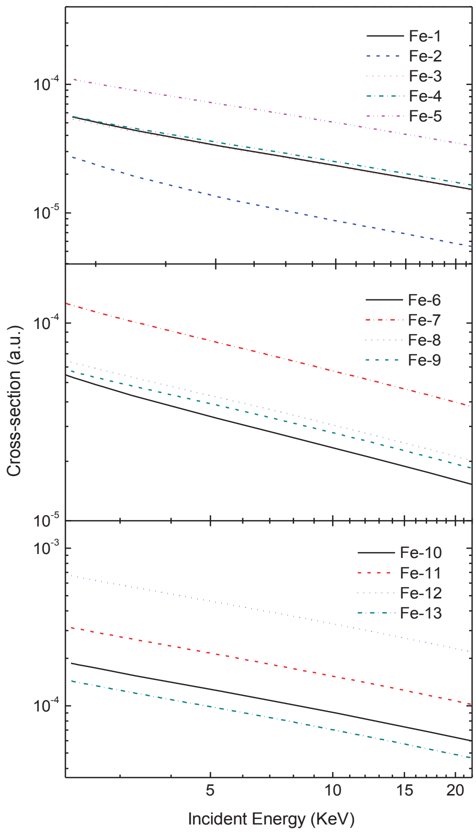

Figure 1. Electron-impact excitation cross-sections (in atomic units) for different transitions as given in Table 1 for Fe-like tungsten ions as a function of incident electron energy.

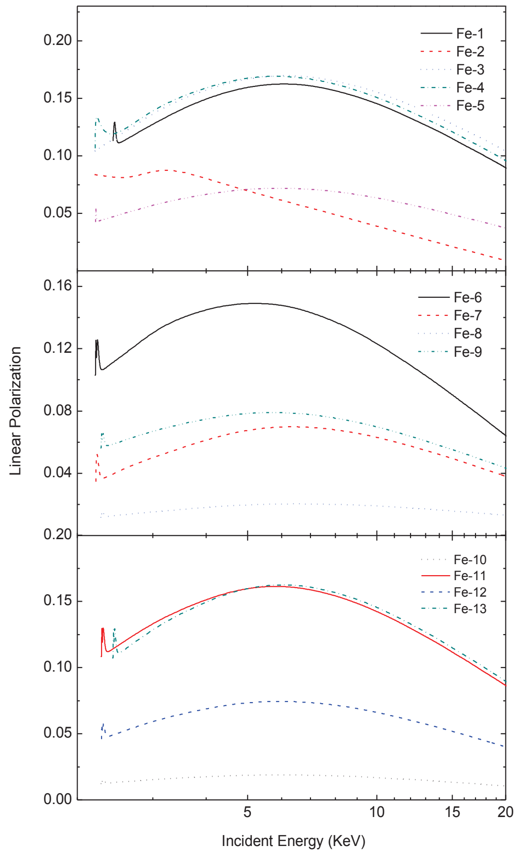

Figure 2. Polarization for the photon emission from anisotropic excited states through different transitions (as given in Table 1) for Fe-like, tungsten ions as a function of incident electron energy.

In order to provide the cross-section data at any energy, we have fitted our cross sections to the analytical expression which can be written as,

$$\sigma = \frac{\Sigma_{i=0}^{n}\, b_i E^i}{\Sigma_{i=1}^{n}\, c_i E^{i-1}}\, a_0^2 \,. \tag{3.1}$$

Here $b_i^{\prime s}$ and $c_i^{\prime s}$ are fitting coefficients; E is the energy of incident electron in atomic units and is the Bohr radius. We have found that only three terms are sufficient in expansion of summations appearing in the numerator and denominator. The values of these coefficients are given in Table 2 for all the 13 transitions considered in the present work. These fitting coefficients are valid from excitation threshold and provide cross-sections with a maximum of 5% deviation from the calculated RDW cross-sections.

In addition to the cross sections, we have also calculated the linear polarization of photon emission due to decay of the excited states of the ion. For this purpose, we have used our calculated magnetic sublevel cross sections in the following expressions simplified for the transitions considered in the present work and the resulting formulae are written as

$$P = \frac{-3(5\sigma_3 - 3\sigma_1 - 2\sigma_0)}{43\sigma_3 + 48\sigma_2 + 51\sigma_1 + 26\sigma_0}, \quad \text{for } J_f \rightarrow J_i (3 \rightarrow 4) \tag{3.2a}$$

$$P = \frac{28\sigma_4 + 7\sigma_3 - 8\sigma_2 - 17\sigma_1 - 10\sigma_0}{36\sigma_4 + 29\sigma_3 + 24\sigma_2 + 21\sigma_1 + 10\sigma_0}, \quad \text{for } J_f \rightarrow J_i \ (4 \rightarrow 4) \tag{3.2b}$$

$$P = \frac{-3(15\sigma_5 + 6\sigma_4 - \sigma_3 - 6\sigma_2 - 9\sigma_1 - 5\sigma_0)}{45\sigma_5 + 54\sigma_4 + 61\sigma_3 + 66\sigma_2 + 69\sigma_1 + 35\sigma_0}, \quad \text{for } J_f \rightarrow J_i \ (5 \rightarrow 4) \tag{3.2c}$$

We have considered only three types of transitions in which one electron de-excites to ground state with $J_i = 4$ from any of excited $J_f = 3,4$ and 5 states, thus leading to and +1, respectively.

The polarization curves with respect to the energy of the incident electron are shown in Figure 2. From the figure it can be seen that all the curves show a broad peak near 5 keV and then fall off with increasing electron energy. The only exception to this behaviour can be noticed for Fe-2 line which shows a narrower peak below 5 keV. Further, we observe that the transitions corresponding to i.e., $\Delta J = 0$ Fe-3, Fe-4, Fe-6, Fe-11 and Fe-13 show maximal polarization value about 17%, followed by lines Fe-2, Fe-5, Fe-7, Fe-9 and Fe-12, due to $\Delta J = 1$ transition, giving nearly 9% value of polarization. Two transitions causing $\Delta J = -1$ viz. Fe-8 and Fe-10 lead to emission to feebly polarized photons with a maximum of 2% polarization near 5 keV. Though Fe-1 line also arises due to $\Delta J = -1$ transition, it gives maximum of 16% polarized radiation at 6.4 keV.

4. Conclusions

We have studied electron impact excitation of Fe-like tungsten ion using RDW theory. Good agreement of our calculated excitation energies as well as oscillator strengths of all the transitions considered with FAC results of Clementson *et al.* [7] indicate the accuracy of the wavefunctions employed in our calculations. We have performed calculations to obtain magnetic sublevel cross sections which yield total cross section and polarization of the subsequently emitted photon. We hope that this work would extend the database on highly charged tungsten ions relevant to fusion plasma diagnostics.

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Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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