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Theoretical calculation of the transition spectra of highly charged tungsten ions in the EUV region

Yong-Joo Rhee *, Duck-Hee Kwon

Laboratory for Quantum Optics, Korea Atomic Energy Research Institute, Daejeon 305-600, Republic of Korea

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To the memory of Yong-Ki Kim

Abstract

A relativistic atomic code, MCDF (Multi-Configuration Dirac–Fock), was used to calculate the transition probabilities of highly charged tungsten ions ranging from $W^{33+}$to W^{37+}. Transition probabilities at the wavelength range of 40–75 Å were obtained for the transitions from $4p^5 4d^{n+1}$+$4p^6 4d^{n-1}$ 4f to $4p^6$ $4d^n$ by using the electronic configuration of Mo ions.

Keywords: Tungsten spectra; Highly charged ion; Transition probability; Relativistic atomic calculation

1. Introduction

In a high temperature plasma many electrons are removed from the atomic shells of an atom and thus this atom becomes a highly charged ion. The spectroscopic characteristics of such kind of highly charged ions are not well known partly because it requires elaborate relativistic theories of interacting electrons and nuclei from a theoretical point of view and partly because it is very difficult to analyze the level-by-level transitions experimentally. Furthermore, it is not easy to generate such a high temperature experimental environment as to get highly charged ions of a specific ionization stage in small laboratories. High temperature plasmas may only be generated at a large facility such as a nuclear fusion device, EBIT (Electron Beam Ion Trap) machine, and so on.

Tungsten (W) has recently been regarded as a good candidate for a plasma facing material in a magnetic fusion devices and more and more applications are planned in many facilities such as the ASDEX (Axially Symmetric Divertor Experiment) Upgrade [1], ITER (International Thermonuclear Experimental Reactor) and so on, in spite of its strong radiative loss. The ASDEX Upgrade tokamak in Germany is designed to use tungsten in the divertor region to take advantage of the very low sputtering rates of tungsten, which is the same case as in ITER. Therefore the electronic structure of highly charged W ions and their interactions with electrons are essential data for high temperature experiments in a nuclear fusion research.

However, in spite of the importance of the spectral data of tungsten for the diagnostics and control of fusion plasmas the spectroscopic properties of highly charged W ions of all ionization stages are not completely known yet and vividly investigated now, although much of the spectral lines are identified [2]. Some experiments and numerical calculations have been reported in the range of UV or EUV using EBIT [3–9] and in soft X-ray range for a tokamak plasma [10].

As to the theoretical studies of highly charged ions, the calculations of the transition lines of the ions do not agree well with the experimental data without any kinds of adjustable parameters [4] due to the complexity of the atomic structures which require relativistic treatments. Meanwhile the *ab initio* MCDF code which was developed by Desclaux et. al. [11], has been successfully applied to the calculation of electron impact ionization cross sections of neutral and singly charged Mo [12] and W [13], in which relativistic wave functions are calculated by using MCDF code so as to obtain the binding energies, kinetic energies, and occupation numbers of the orbitals. From these successful applications of MCDF code we may assume that the MCDF code can calculate the dipole transition matrix elements

* Corresponding author.
E-mail address: yjrhee@kaeri.re.kr (Y.-J. Rhee).

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correctly using those relativistic wave functions in the highly charged ions of heavy elements such as Mo and W, as well.

In this article we report the results of applying the MCDF code, which solves the relativistic Dirac–Fock equation, to the calculation of a dipole transition probability of the tungsten ions of charge states ranging from $W^{33+}$to W^{37+}. Transition lines from each of the eigenstates of a total angular momentum to a ground state have been calculated and the transition lines are convolved with a Gaussian function to obtain the line width of the emission spectral lines.

2. Transition probability and oscillator strength

The transition probability for going from an upper level n to a lower level n' by emitting a photon is called Einstein's A coefficient:

$$A_{nn'} = \frac{4e^2\omega^3}{3\hbar c^3}|\langle\Psi_n|\Sigma_j r_j|\Psi_{n'}\rangle|^2, \quad (1)$$

where the angular frequency $\omega = (E_n - E_{n'})/\hbar$ with the total energies E. This is called the dipole or $E1$ transition matrix element in the length form. Einstein's A coefficient (dimension = s^{-1}) is the total number of photons emitted per second. Alternatively, the dipole oscillator strength $f_{n'n}$ is used for a photo-absorption:

$$f_{n'n} = \frac{2m\omega g_n}{3\hbar g_{n'}}\langle\Psi_n|\Sigma_j r_j|\Psi_{n'}\rangle|^2 = \frac{mc^3 g_n}{2e^2\omega^2 g_{n'}}A_{nn'}, \quad (2)$$

where g is the multiplicity of the respective state. The above definition of the oscillator strength applies only to a dipole transition with the operator of e**r**. The dipole oscillator strength is often called the f-value, and it is dimensionless.

When the photon energy is high, non-dipole transitions become significant. Multipole transition probabilities are calculated by expanding the photon field into a multipole electromagnetic field. The magnetic dipole transition is called the $M1$ transition, the electric quadrupole transition the $E2$ transition, the magnetic quadrupole transition the $M2$ transition, and so on.

When wave functions from a local potential are used, the length and velocity forms of the f-value and hence its matching length and velocity forms of the transition probability agree exactly. Results from Hartree–Fock wave functions will not agree, because they are computed with non-local potentials. The difference between the length and velocity forms of the f-value *is not* an indication of the accuracy of the f-value. Numerical convergence of the f-value as the wave functions are improved is the only way to assure the accuracy.

When the MCDF code is used to calculate the electromagnetic transition probabilities, appropriate Slater coefficients aregenerated internally to calculate the Dirac–Fock wave functions specified in the input data and the requested types of transition probabilities. The accuracy of the *En* and *Mn* transition probabilities is determined by the accuracy of the Dirac–Fock wave functions used.

3. Calculation process

Since the electronic structures of Mo ions are relatively well known [14], we used the electronic configuration of Mo ions for highly charged tungsten ions, as shown in Table 1, instead of using those of neutral isoelectronic sequence atoms.

The spectra of tungsten ions with a charge state $q = 33+$ to $37+$ in the range of a wavelength from 40 to 75 Å are obtained by the transitions from the upper level configurations $4p^5 4d^{n+1}$ and $4p^6 4d^{n-1} 4f$ to the ground configuration $4p^6 4d^n$. The *ab initio* calculations of the atomic spectra were performed with the relativistic MCDF code [11]. The energies of the ground states and the ground multiplets of the configuration $4p^6 4d^n$were obtained by solving the Dirac–Fock equation with the self-consistent field (SCF) method. In the self-consistent field calculation, the relativistic correction to the Coulomb interaction between the bound electrons so called the Breit interaction was included as a perturbation by considering

Table 1
Configurations and energies of ground state of Mo ions [14]

Ionization stages	Ground configuration	Term symbol	Angular momentum J	Energy (eV)	Corresponding W ions
Mo^{1+}	[Kr] $4d^5$	^6S	5/2	0.0000000	W^{33+}
Mo^{2+}	[Kr] $4d^4$	^5D	0	0.0000000	W^{34+}
			1	0.030009	
			2	0.082851	
			3	0.151752	
			4	0.232137	
Mo^{3+}	[Kr] $4d^3$	^4F	3/2	0.0000000	W^{35+}
			5/2	0.096462	
			7/2	0.218183	
			9/2	0.355163	
Mo^{4+}	[Kr] $4d^2$	^3F	2	0.0000000	W^{36+}
			3	0.195631	
			4	0.416257	
Mo^{5+}	[Kr] 4d	^2D	3/2	0.0000000	W^{37+}
			5/2	0.320410	

only an average contribution for individual J values. The energies of the upper states of the transitions were calculated with the mixed configuration of $4p^5 4d^{n+1}$ and $4p^6 4d^{n-1} 4f$. For this mixed configuration, extended-average-level (EAL) wave functions were used as the starting orbitals. In the EAL calculation, radial wave functions are chosen such that the average energy of all the configurations weighted by their respective statistical weights becomes stationary with respect to the variations of the radial wave functions. The energies of the upper levels were then obtained by using the configuration interaction (CI) wave functions which come from applying the variational principle only to the configuration mixing coefficients while keeping the radial functions frozen. In the CI calculation, the radial functions are those produced by the EAL calculation. The oscillator strengths of the electric E1 transitions from $4p^5 4d^{n+1}$+$4p^6 4d^{n-1} 4f$ to $4p^6 4d^n$ were calculated with the wave functions of the lower levels and the upper levels which were obtained by the SCF and CI methods, respectively. The

transition wavelength were adjusted with a scaling factor which is a ratio of the published values of the ionization energy

Table 2
Number of eigenstates of the upper levels

Ionization stages	Upper state configuration	Lower state J	Upper state J	Number of eigenstates	Total number of transition lines
W^{33+}	$4p^5 4d^6$+ $4p^6 4d^4 4f$	5/2	3/2	83	282
			5/2	100	
			7/2	99	
W^{34+}	$4p^5 4d^5$+ $4p^6 4d^3 4f$	0	1	56	878
		1	0	19	
			1	56	
			2	80	
		2	1	56	
			2	80	
			3	84	
		3	2	80	
			3	84	
			4	73	
		4	3	84	
			4	73	
			5	53	
W^{35+}	$4p^5 4d^4$+ $4p^6 4d^2 4f$	3/2	1/2	28	547
			3/2	48	
			5/2	55	
		5/2	3/2	48	
			5/2	55	
			7/2	52	
		7/2	5/2	55	
			7/2	52	
			9/2	39	
		9/2	7/2	52	
			9/2	39	
			11/2	24	
W^{36+}	$4p^5 4d^3$+ $4p^6 4d^1 4f$	2	1	22	222
			2	29	
			3	28	
		3	2	29	
			3	28	
			4	22	
		4	3	28	
			4	22	
			5	14	
W^{37+}	$4p^5 4d^2$+ $4p^6 4f$	3/2	1/2	7	63
			3/2	11	
			5/2	12	
		5/2	3/2	11	
			5/2	12	
			7/2	10	

by Kramida and Reader [2] to the calculated ionization energy, which were obtained using the EAL wave function and the SCF wavefunction for the ionization state $W^{(q+1)+}$ and for the ground state of the W^{q+} ion, respectively. The line intensities of the transitions are considered proportional to the line strength or $g_j A_{ji}$ values assuming that the upper levels are statistically populated to a Boltzmann distribution.

4. Spectral lines of highly charged W ions

In order to calculate the transition probabilities, transitions from all the eigenstates of an upper level in the JJ coupling scheme, internally generated from the LS coupling scheme in the MCDF code, to the first eigenstate of a lower level, which is the lowest eigenstate, have been calculated. For the calculation of the electronic structure, instead of using the configuration of the isoelectronic sequence atoms, we used the Mo-ion-like configurations. The configurations of a lower level of Mo ions are shown in Table 1 together with the energy values. The same configurations are used for lower levels of the W ions as denoted in the table. The configurations and the number of eigenstates of each upper level are shown in Table 2. For each transition, the *gA* value is calculated in the length form. In Figs. 1 and 2, transition lines of W^{35+}, for instance, are shown corresponding to the different *J* values of the lower levels and upper levels.

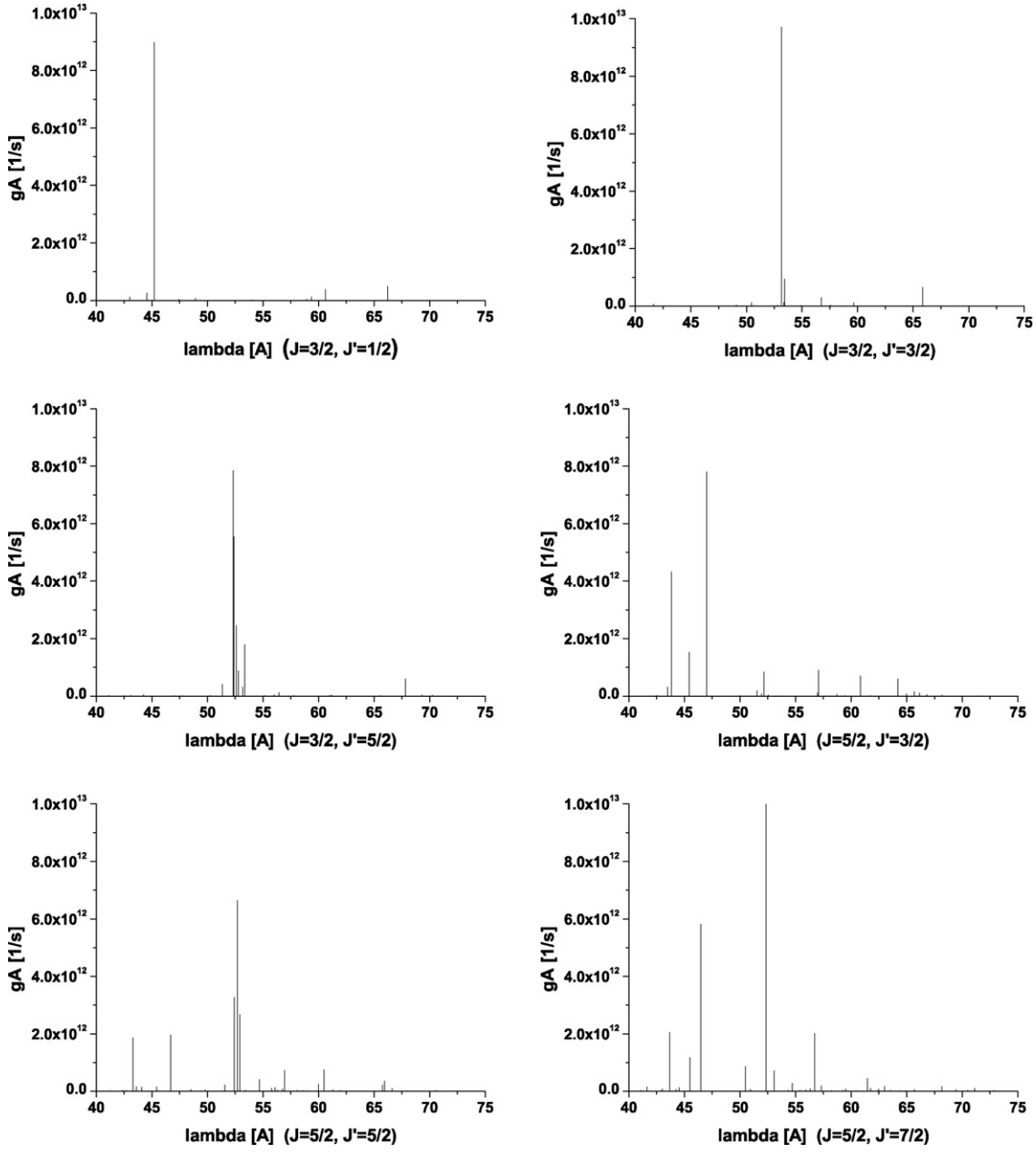

Fig. 1. *gA* values of the transitions to $J = 3/2$ and 5/2 of W^{35+}, where *J* is the angular momentum of the lower level and J' is that of upper level. The value of *gA* is clipped when it is larger than 1×10^{13}.

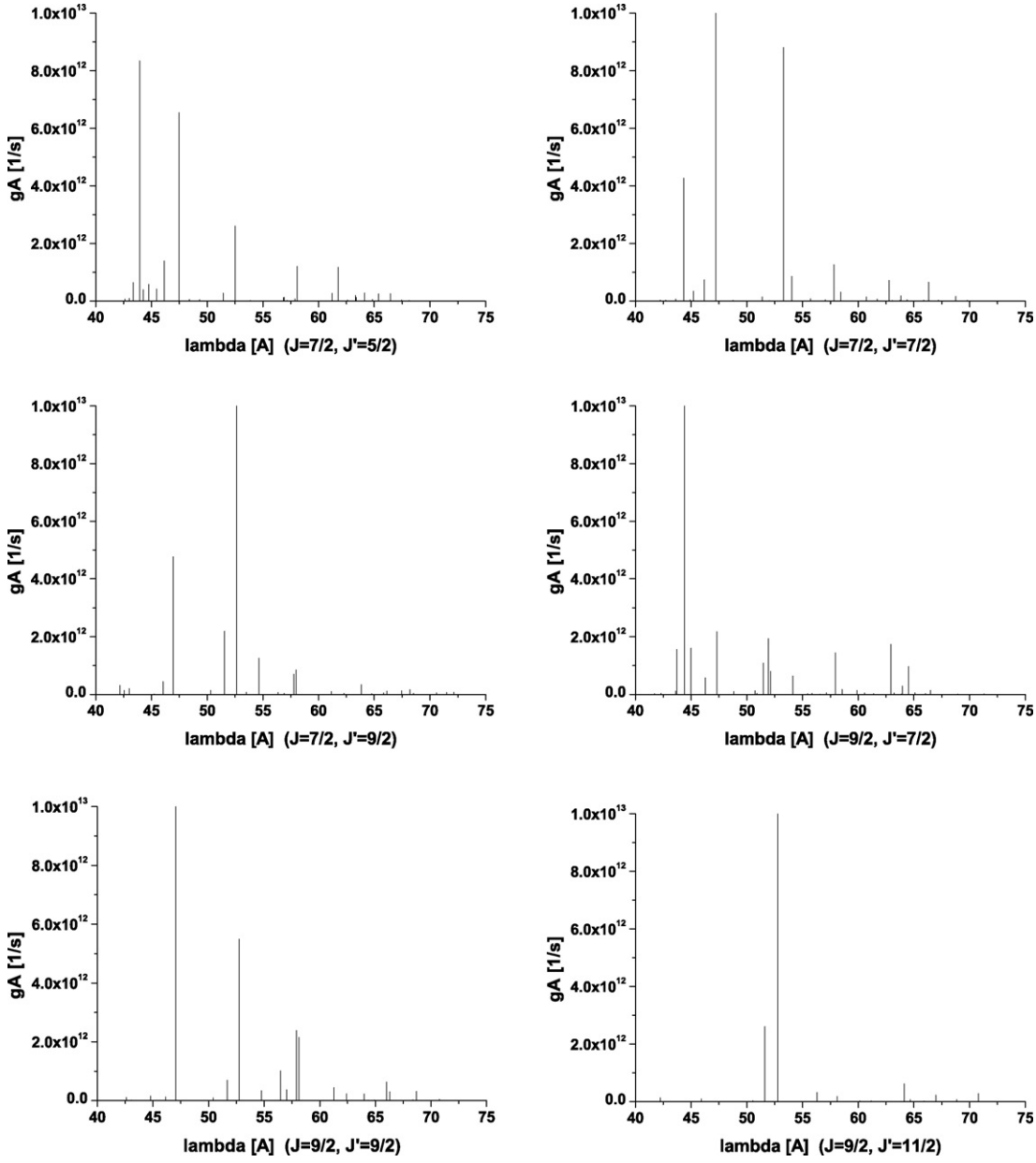

Fig. 2. *gA* values of the transitions to $J = 7/2$ and 9/2 of W^{35+}, where J is the angular momentum of the lower level and J' is that of upper level. The value of *gA* is clipped when it is larger than 1×10^{13}.

When these lines are gathered together and convolved with a Gaussian function with a variance of 0.138 Å we obtained the spectra as shown in Fig. 3 which shows the spectra of W^{33+} through W^{37+}. Here the value of the variance in the Gaussian function for a convolution is the same as that used in the analysis of the data from LHD (Large Helical Device). Theoretical data should be convolved with an impulse response function of an apparatus to be compared with the experimental data of the apparatus. This value should be chosen appropriately according to the experimental devices and we used an ad hoc value of 0.138. In total about 2000 transition lines were calculated to obtain the *gA* values.

In Fig. 3, it is clearly seen that the spectrum band near 45 Å is appearing at the same spectral position regardless of the ionization stages but the emission lines at 50 Å are shifting to a longer wavelength range as the ionization stage becomes closer to a higher ionization as in reference[4] where the HULLAC atomic code with a collisional-radiative (CR) model was used to analyze the EBIT data. For W^{37+} the emission band at 50 Å is no longer dominant. To compare with the experimental spectra, it is necessary to multiply the transition probabilities with the level population at a specific temperature. However, here, it is assumed that only the low lying excited states are contributing to the radiative transitions.

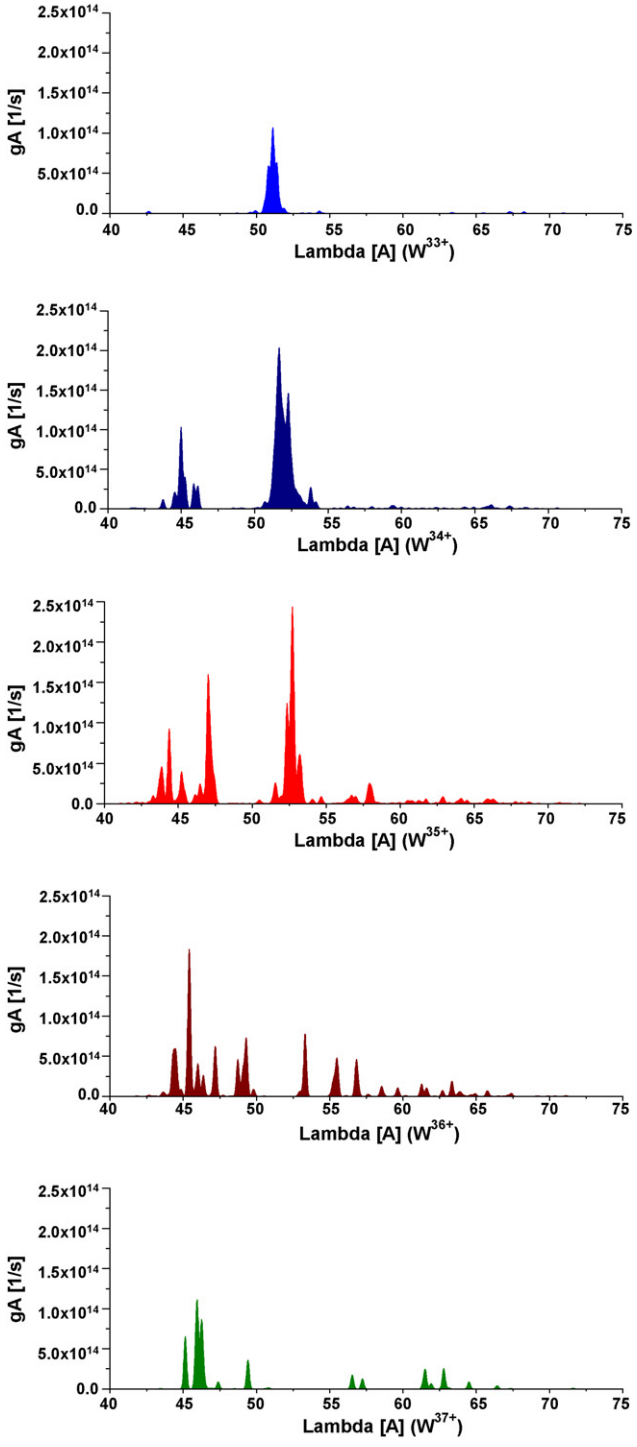

Fig. 3. Emission spectra constructed from the *gA* values convolved with a Gaussian function as a line spread function. The spectrum band at 45 Å and the shift of the emission lines at 50 Å is clearly notable.

5. Conclusions

To obtain the emission spectral lines of highly charged tungsten ions, the *ab initio* relativistic MCDF code is applied to the Mo-ion-like configurations. The preliminary result of this calculation of the transition probabilities shows a pretty good agreement, even though an accurate prediction of the spectra of highly charged tungsten ions is very difficult due to the complicated interactions of the electrons. The spectra obtained in this report agreed well with the available experimental results [4]. This method can be applied to higher ionization stages or lower ionization stages as well, and it is expected to be a good tool for a calculation of the atomic structure and transitions of high Z elements.

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