X-ray spectra of high temperature tungsten plasma calculated with collisional radiative model*

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Tungsten is regarded as an important candidate of plasma facing material in international thermonuclear experimental reactor (ITER), so the determination and modeling of spectra of tungsten plasma, especially the spectra at high temperature were intensely focused on recently. In this work, using the atomic structure code of Cowan, a collisional radiative model (CRM) based on the spin–orbit-split-arrays is developed. Based on this model, the charge state distribution of tungsten ions is determined and the soft X-ray spectra from high charged ions of tungsten at different temperatures are calculated. The results show that both the average ionization charge and line positions are well agreed with others calculations and measurements with discrepancies of less than 0.63% and 1.26%, respectively. The spectra at higher temperatures are also reported and the relationship between ion abundance and temperature is predicted in this work.

Keywords: tungsten plasma, high temperature X-ray spectra, collisional radiative model

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1. Introduction

As one of the best materials subjected to high temperature, tungsten can be used as plasma facing material in international thermonuclear experimental reactor (ITER). Therefore, the research of spectra from tungsten plasma plays a more and more important role in modern nuclear physics.[1–5] The electron temperature in ITER, which is associated with the position of the plasma, will range from below 0.1 keV at the edge to about 25 keV in the core of the plasma. The plasmas under different temperatures have different ionization degrees. A measured plasma spectrum is contributed by the different ionization ions with different abundances according to the ionization degree, which means that the measured spectrum often contains many spectral lines from several ionization ions. For understanding the measured spectrum, model calculation based on atomic data is very important. The calculation should consider all different ionization ions and their fractional abundances. However, spectrum data for high-Z atoms are scarce because of the complicated transitions and the pronounced relativistic effects for these ions. The spectrum data are also useful to diagnose laser-produced plasmas. So it is necessary to model the emission spectrum for high ionization tungsten.

Up to now, the researchers have done a lot of work on it and obtained many useful results.[6–12] Yuri Ralchenko *et al.*[9] presented a detailed collisional-radiative model for a benchmark X-ray spectrum of highly charged tungsten ions in a range between 3 Å and 10 Å (1 Å = 0.1 nm), produced in an electron beam ion trap (EBIT) with a beam energy of 4.08 keV. Putterich *et al.*[10] modeled the tungsten emission X-ray spectrum at 3.9 keV and reported on the spectral lines for tungsten at 4 Å–8 Å. Neu *et al.*[11] observed X-ray spectrum in a range of 7 Å–10 Å from highly charged W ions in the tokamak plasmas and lines emitted from W^{37+} to W^{47+} were calculated and identified. But at high temperature, the systematic data for the average ionization degrees and the spectral lines are rarely reported.

Up to now, several methods to calculate the spectrum of high-Z atomic plasma at high temperature have been developed.[13–15] Ma *et al.*[16] used the average atom (AA) model to obtain the spectral lines of high Z elements. Jin *et al.*[17] used the detailed term accounting (DTA) model to deal with hot ion plasma. Han *et al.*[18] treated emission spectrum under collisional radiative model (CRM). Zhang *et al.*[19,20] and Cheng *et al.*[21] used the CRM associated with SOSA model to study the charge state distribution. However, each method has its own restrictions. Owing to the fact that the tungsten ions not only have high Z but also are highly ionized at high temperature, an efficient and economic method is needed. In this work, relativistic Hartree–Fock (RHF) method associated with CRM model based on SOSA model is used to obtain the emission X-ray spectrum of highly ionized tungsten. The emitted X-ray spectra at different electronic temperatures are calculated. The fractional abundance of ionization degrees and the X-ray spectrum at 4 keV are obtained and compared with measured and calculated results. The results indicate that using this method to calculate the emission X-ray

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spectrum from highly charged tungsten is reliable. The spectra in the range of 1 keV to 10 keV are also provided for diagnosing the temperature of laser-produced plasma.

2. Method

Theoretical data for the ionization equilibrium and the excitation rate coefficient along with the atomic level structure and transition probability are the basic input quantities to model the emissions of tungsten. In this work, we use Cowan code to calculate atomic structure.[22] Cowan code uses a quasi-relativistic Hartree–Fock method with superposition of configurations. For high-Z atomic plasma like tungsten, the average transition energy of configuration cannot properly describe the real energy levels. Therefore, the average transition energy of subconfiguration is adopted instead.[23] The overlapping and broadening of spectra lines are due to the existence of many transition arrays in various ionization stages, so the observed spectra are often unresolved. In that case, unresolved transition array model (UTA) is an efficient way to describe such a spectral structure. In the UTA model,[24] the average transition energy is calculated from

$$T_{\rm av}(B-A) = [E_{\rm av}(B) - E_{\rm av}(A)] + \delta E, \tag{1}$$

where A and B are the upper and lower subconfigurations respectively, $T_{\rm av}(B-A) \equiv \mu_1$, $E_{\rm av}$ is the average wave number of a subconfiguration.

$$\begin{aligned}\delta E = N\Bigg[& -\sum_{\substack{k\neq 0\\ \text{even}}} \frac{(2j+1)(2j'+1)}{2j} \begin{Bmatrix} k & j & j \\ 1 & j' & j' \end{Bmatrix} \\ & \times \begin{bmatrix} j & k & j \\ 1/2 & 0 & -1/2 \end{bmatrix} \begin{bmatrix} j' & k & j' \\ 1/2 & 0 & -1/2 \end{bmatrix} F^k(ll') \\ & + \sum_k \frac{(2j+1)(2j'+1)\,\delta(k,1) - 3}{6j} \\ & \times \begin{bmatrix} j & k & j' \\ 1/2 & 0 & -1/2 \end{bmatrix}^2 \pi(l,l',k)\, G^k(ll') \Bigg], \end{aligned} \tag{2}$$

where

$$\pi(l,l',k) = \frac{\left[1+(-1)^{l+l'+k}\right]}{2}.$$

The collision-radiative model (CRM)[20,25] is used to describe the population distribution. The processes include collisional ionization (CI), three-body recombination, collisional excitation (CE), radiative recombination (RR), and dielectronic recombination (DR). For optically thin plasma, the spectral model CRM can be expressed as

$$\begin{aligned}\frac{{\rm d}N(n,g)}{{\rm d}t} = & N(n,g) N_{\rm e} S(T_{\rm e},n,g) \\ & - N(n+1,g) N_{\rm e} [\alpha(T_{\rm e},n+1,g) \\ & + N_{\rm e} R_{3{\rm b}}(T_{\rm e},n+1,g) + \alpha^{DR}(T_{\rm e},n+1,g)], \end{aligned} \tag{3}$$

where $N_{\rm e}$ is the density of electron, $N(n,g)$ is the population of ions in the fundamental state which has the ionization degree of n, S, α, $R_{3{\rm b}}$ and $\alpha^{\rm DR}$ are the CI, RR, three-body recombination, and DR rate coefficient, respectively. Under the stability approximation, the equation can be written as

$$\frac{{\rm d}N(n,g)}{{\rm d}t} = 0. \tag{4}$$

Equation (4) is difficult to calculate the rate coefficient.[26,27] The ionization equilibrium charge-state distribution can be obtained by using average rate coefficient and empirical formulas in Eqs. (3) and (4).[28–32]

$$\begin{aligned} S(n) = & \frac{0.9\times 10^{-5}\xi(n)(T_{\rm e}/I_n)^{1/2}}{I_n^{3/2}(4.88+T_{\rm e}/I_n)} \\ & \times N_{\rm e} \exp\left(-\frac{I_n}{T_{\rm e}}\right) \ ({\rm s}^{-1}), \end{aligned} \tag{5}$$

$$\begin{aligned} \alpha(n) = & 5.16966\times 10^{-14} \left(\frac{I_n}{T_{\rm e}}\right)^{1/2} N_{\rm e}, \\ & \times \left\{ 0.429 + \frac{1}{2}\ln\left(\frac{I_n}{T_{\rm e}}\right) \right. \\ & \left. + 0.469 \left(\frac{I_n}{T_{\rm e}}\right)^{-1/3} \right\} \ ({\rm s}^{-1}), \end{aligned} \tag{6}$$

$$R_{3b}(n+1) = \frac{2.97\times 10^{-27}\xi(n) N_{\rm e}^2}{I_n^2 T_{\rm e}(4.88+T_{\rm e}/I_n)} \ ({\rm s}^{-1}), \tag{7}$$

where $\xi(n)$ is the number of electrons in outer shell, I_n the ionization potential, $T_{\rm e}$ the electron temperature, and $N_{\rm e}$ the electron density. The Burgess–Merts formula is used to determine the DR rate

$$\alpha_{jk}^{\rm DR}(T_{\rm e}) = T_{\rm e} f(k,j) F_1 F_2 \exp\left(-\frac{\bar{E}}{T_{\rm e}}\right). \tag{8}$$

To obtain the population of each energy level, the equilibrium equation is solved. In this equation, we consider only the collisional excitation (CE), radiative transition, and dielectronic recombination (DR), so

$$\begin{aligned} & N_{C_i} \cdot X(C_i \to C_i') + N_{C_{i+1}} \cdot \alpha_{i+1}^{\rm DR}(C_{i+1} \to C_i') \\ & = N_{C_i'} \cdot A(C_i' \to C_i). \end{aligned} \tag{9}$$

In this equation, X_i represents the total electronic collisional excitation rate. As it is difficult to obtain the CE rate coefficient,[33] the empirical formula and average rate are used:

$$\begin{aligned} \bar{X}(C_{\rm g},C_{\rm p}) = & 1.6\times 10^{-5} \frac{\langle\bar{g}\rangle \bar{f}(C_{\rm g},C_{\rm p}) N_{\rm e}}{E_{C_{\rm p}C_{\rm g}}\sqrt{T_{\rm e}}} \\ & \times \exp\left[-\frac{E_{C_{\rm p}C_{\rm g}}}{T_{\rm e}}\right] \ ({\rm s}^{-1}), \end{aligned} \tag{10}$$

where $\langle g\rangle$ is Gaunt factor under the Maxwellian distribution, and[34]

$$\bar{f}(C_{\rm g},C_{\rm p}) = \frac{(E_{C_{\rm g}} - E_{C_{\rm p}})}{3} \frac{N_\alpha(g_\beta - N_\beta)}{g_\alpha g_\beta} 2[l_\alpha, l_\beta]$$

$$\times \begin{pmatrix} l_\beta & 1 & l_\alpha \\ 0 & 0 & 0 \end{pmatrix}^2 P^2_{\alpha\beta}.$$

Bauche's formula[24] is used to obtain the average transition rate coefficient. The electron population can be obtained by solving these equations, if the temperature and density of electron in the plasma are known.

3. Results and discussion

To compare with other calculation and experiment results, we calculate the X-ray spectra in a range of 4 Å to 7 Å, emitted from tungsten plasma with a temperature of 4.1 keV and density of 1.0 g/cm^3. The fraction abundances are shown in Fig. 1. The average ionization charge is 45.675 in this work at electron temperature $T_e = 4.08$ keV. Compared with Putterrich *et al.*'s work[10] in which it was reported that the average ionization charge is 45.391 at electron temperature $T_e = 4.1$ keV, the error is less in 0.63%. In Fig. 1, the ions in the plasma spread from V-like W^{51+} to Ga-like W^{43+}, showing a good agreement with that from V-like W^{51+} to As-like W^{41+} of Putterich *et al.*[10] and Fe-like W^{48+} to Kr-like W^{38+} of Neu *et al.*[11]

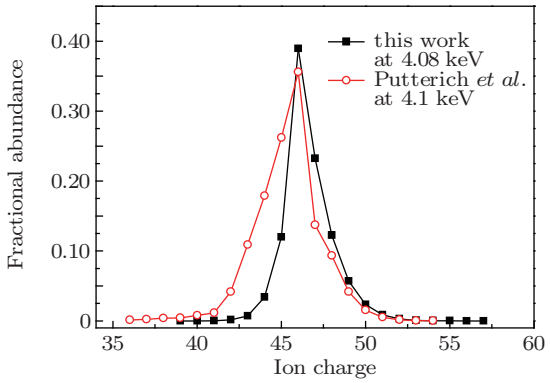


Fig. 1. (color online) Fractional abundances for tungsten plasma. (Our results are obtained at $T_e = 4.08$ keV and Putterich *et al.*'s[10] at $T_e = 4.1$ keV).

Table 1. Values of average ionization degree Z for electron density $N_e \sim 10^{24}$ cm^{-3} and electron temperature from 1 keV to 10 keV.

T/keV	1	2	3	4	5	6	7	8	9	10
Average ionization degree	35.59	43.09	44.71	45.59	46.70	48.19	49.92	51.60	53.08	54.36

The values of average ionization degree are listed in Table 1 with electron temperature ranging from 1 keV to 10 keV. The spectra of tungsten plasma in a region of 4 Å–7 Å at an electron temperature of 4 keV are given in Fig. 2. To compare with other's measured and calculated results, arbitrary unit is used, so that it can show some features of the real spectra.

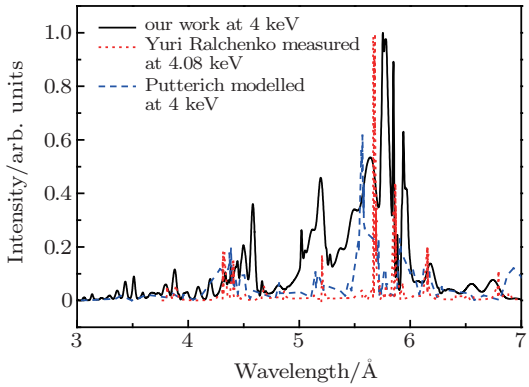


Fig. 2. (color online) Modeled spectrum for tungsten plasma at 4 keV comparing with measured spectra with microcalorimeter on NIST EBIT at 4.08 keV[9] and other's modeled spectrum at 4 keV.[10]

The line positions are plotted in Fig. 3 and the corresponding data are listed in Table 2. Our results and other calculation results[10] are both compared with experimental results.[9] It can be found that the results in this work are in good agreement with other's within a discrepancy of less than 1.26%. It means that it is appropriate to use subconfiguration energy level in stead of configuration energy level and that the collisional radiative model is effective. The spectrum fits well to the experimental results.

Table 2. Comparisons of partial line position between our results and cited experimental results.

λ/Å Exp.[9]	λ/Å Our work	Error/%	λ/Å Other's[10]	Error/%
3.80869	3.800	–0.23%	3.39353	–10.90%
3.89043	3.879	–0.29%	3.85239	–0.98%
4.3136	4.336	0.52%	4.38615	1.68%
4.40398	4.444	0.91%	4.47103	1.52%
5.20518	5.194	–0.21%	5.16579	–0.76%
5.6823	5.754	1.26%	5.56885	–2.00%
5.8631	5.849	–0.24%	5.90659	0.74%
6.15325	6.180	0.43%	6.12216	–0.51%

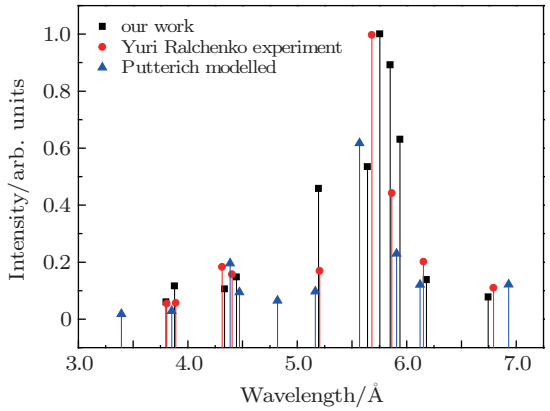


Fig. 3. (color online) Comparisons of line position among experimental results,[9] calculation results,[10] and our results.

There have three reasons for the difference of relative intensity in Fig. 2. First, we consider only CI, RR, three-body

recombination, and DR rate to obtain the fractional abundance of ions in CRM model. The effect of ionization balance caused by excited states is ignored. Second, to reduce the calculation, we choose empirical formulas to obtain CI, RR, three-body recombination, and DR rates. But the empirical formulas cannot always obtain good results especially under high temperature. The two reasons do not influence the fractional abundance of ions sharply, but seriously affect the population of each energy level. Because the average ionization degree is good, we think the ignoring of excited states is reasonable and we think that the CRM model is suitable and easy to obtain the ionization abundance. The third reason is that the intensity is calculated using SOSA model. The tungsten is treated as pure j–j coupling instead of both j–j coupling and l–s coupling. In our work, we focus on the X-ray emission spectra especially from M shell of high ionization tungsten. There have some spectral lines we cannot find in experimental spectra but exist in our work. That means that some transitions between subconfigurations do not really exist, wrong rate coefficients are used or subconfigurations are coupled by l–s rule. Besides the reasons mentioned above, the difference between our results and other's modeled results also come mainly from the different ionization stages. The rate equations adopt different rate coefficients, and the different electron densities are considered (W concentration is 10^{-5} in other work with respect to our 10^{0}). Above all, the method we use is suitable for high temperature tungsten. The results fit well to the experimental results in peak positions and it can give a general outline of the spectrum. We think that it is reasonable to use our method to obtain a reliable spectrum. The spectrum data at high temperature (1 keV–10 keV) for W have not been available before, now we show those results of our present work in Fig. 4.

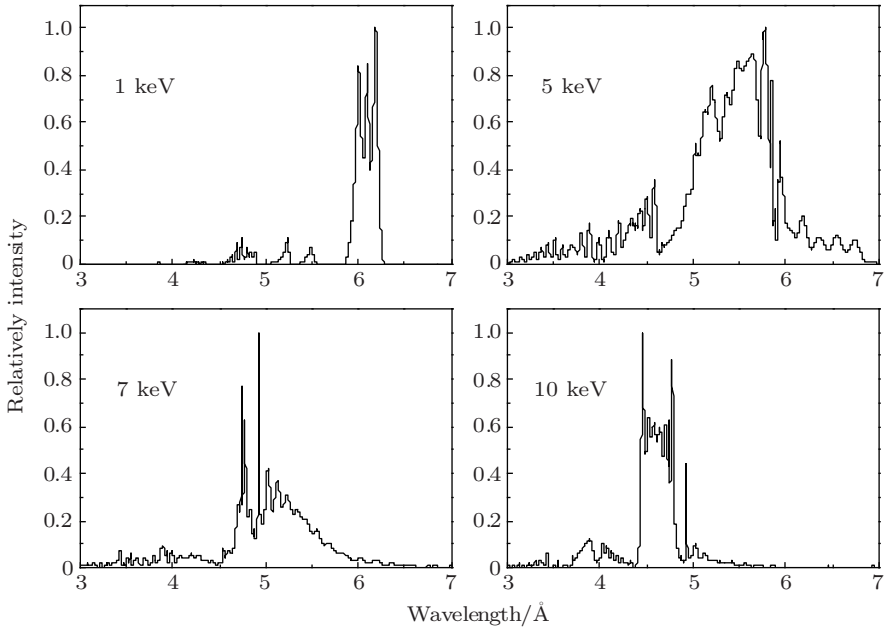


Fig. 4. Modelled spectra for tungsten plasma at 1 keV, 5 keV, 7 keV, and 10 keV.

4. Conclusions

The CRM model and SOSA method are used to obtain the atomic structure and the population of ionization states. The average ionization degree (45.675) and fractional abundances for tungsten plasma are obtained and the error is 0.63%. The line positions are in good agreement with other results with a discrepancy of less than 1.26%. The results fit well to the experimental results in line position, showing some features of the spectrum. We think that it is reasonable to use our method to obtain reliable spectra. The spectrum data at high temperature (1 keV–10 keV) for W are also reported.

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