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Collisional-radiative model for the visible spectrum of W^{26+} ions

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ABSTRACT

Plasma diagnostics in magnetic confinement fusion plasmas by using visible spectrum strongly depends on the knowledge of fundamental atomic properties. A detailed collisional-radiative model of W^{26+} ions has been constructed by considering radiative and electron excitation processes, in which the necessary atomic data had been calculated by relativistic configuration interaction method with the implementation of Flexible Atomic Code. The visible spectrum observed at an electron beam ion trap (EBIT) in Shanghai in the range of 332 nm to 392 nm was reproduced by present calculations. Some transition pairs of which the intensity ratio is sensitive to the electron density were selected as potential candidates of plasma diagnostics. Their electron density dependence is theoretically evaluated for the cases of EBIT plasmas and magnetic confinement fusion plasmas.

1. Introduction

Tungsten (W) was chosen to be the cover material for the first-wall and divertor in the next generation magnetic confinement fusion (MCF) reactors, such as ITER, ASDEX, and EAST, due to its favorable physical and engineering properties such as low sputtering, high melting point, and low tritium retention rate [1,2]. However, tungsten impurity ions might inevitably be produced during the interaction between the edge plasma and cover material. These ions may be transported to the fusion core plasma, and be ionized further to produce highly charged W ions. These highly charged W ions will undergo radiative decay by emitting high energy photons. Consequently, large radiation loss could be caused by these highly charged impurity ions, which will lead to plasma disruption if the relative concentration of W ions in the core plasma is higher than about 10^{-5} [3]. Monitoring and controlling the flux of these highly charged W impurity ions will be important to retain the fusion [4]. Thus a thorough knowledge of atomic properties of tungsten ions will be helpful for MCF research. Nevertheless, tiny amount of tungsten impurity ions can also provide us with plenty of information about fusion plasmas such as electron density, electron temperature and ion temperature by their spectra. Thus, highly charged W impurity ions could be used for diagnosis of fusion plasmas. For the diagnostics with spectra, it is necessary to investigate the fundamental properties of W ions such as energy levels, radiative transition probabilities etc.

In the last three decades, extensive work had been performed on the atomic structure and radiative transition properties of highly charged W ions [5–9]. Most of experimental works have been carried out by using electron beam ion traps (EBITs) and fusion reactor facilities. An EBIT is a widely used device which can selectively produce and trap highly charged ions with specific ionization stage by using a mono-energetic electron beam. Since the ions can be trapped in an EBIT for relatively long time and the electron density in EBIT is relatively low, it is possible to observe weak transitions from those highly charged ions such as magnetic dipole (M1) or electric quadrupole (E2) transitions. Komatsu et al. [10] observed the visible spectrum of highly charged W^{8+-28+} ions by using an compact electron beam ion trap, called CoBIT, in Tokyo [11]. Several lines from M1 transitions among the ground state multiplets of corresponding ion were identified. The visible M1 transition of W^{26+} ions was firstly observed by them [12]. Yanagibayashi et al. [6] observed Extreme Ultra Violet (EUV) spectra in 2.6–3.2 nm range of highly charged W ions from JT-60U plasma at $T_e \approx 8$ and 14 keV which are identified to be of the $3p \rightarrow 3d$ transition from W^{47+} to W^{54+} ions. Z. Fei et al. [7] observed spectrum of the forbidden transition of W^{26+} with a compact electron beam ion trap in Shanghai (SH-Perm EBIT). Radtke et

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al. [8] observed the emission spectra of W ions with charge states 21 to 50 for the wavelength ranges 4.5–7.0 nm and 0.5–0.62 nm with the Berlin EBIT. Harte et al. [9] have studied the EUV spectra of tungsten with Large Helical Device (LHD) in National Institute for Fusion Science (NIFS), Japan. The spectra have been analyzed by using quasi-relativistic theory.

For theoretical study of the level structure and radiative transition properties of the highly charged tungsten ions, the inclusion of relativistic effect and the electron correlation effects is indispensable since tungsten ions are of the heavy and multi-electron system. Various theoretical methods were used to calculate the properties of highly charged W ions [7,13–16]. Z. Fei et al. [7] calculated the M1 transitions among the ground-state configuration of W^{26+} with multi reference relativistic many-body perturbation theory (MR-RMBPT). Gaigalas et al. [13,14] made a large-scale calculation using multi-configuration Dirac–Fock (MCDF) theory on the E1 and E3 transitions of W^{24+} ions in both relativistic and non-relativistic limits taking the valence–valence and core–valence correlation effects into account. Ralchenko et al. [15] measured the M1 transitions of $3d^n$ configurations in super EBIT, and the spectrum was analyzed by detailed collisional-radiative (CR) modeling. Xiao-Bin Ding et al. [16] calculated the M1 visible transitions among the ground state multiplets of the W^{26+} ion using MCDF method. Both valence–valence and core–valence correlation effects had been taken into account in the calculation of the energy level and transition probability. One of the M1 transition lines between $^3H_5 \to {}^3H_4$ has been assigned to the peak at 389.4 nm which was observed by Komatsu et al. [10]. Furthermore, strong transition lines between $^3H_6 \to {}^3H_5$ and $^3F_3 \to {}^3F_2$ have been predicted theoretically, which have been observed by the experiment with CoBIT at 464.4 nm and 501.9 nm, respectively [16].

The present paper is mainly focus on the emission spectrum and the intensity ratio of M1 transitions from W^{26+} ground state multiplets which might be used as potential candidate of diagnosis lines. A detailed collisional-radiative model was constructed to investigate the spectra from highly charged ions in EBIT and fusion plasmas by assuming the electron energy distribution function as a δ function and Maxwellian, respectively.

2. Theoretical method

The CR model has been used successfully in many previous studies to analyze and identify dozens of EBIT spectral lines from highly charged heavy ions in X-ray and VUV as well as optical regions [17,18]. In CR model the plasma was assumed to be optically thin and isotropic. The ground state of W^{26+} is in $4d^{10}4f^2$ configuration which have two electrons in the $4f$ subshell, and consequently have complex electron correlation effect. The atomic data, such as energy levels, radiative transition rates, and cross sections of collisional (de)excitation, which are necessary to construct the CR model, can be obtained in the framework of full relativistic configuration interaction (RCI) method with the implementation of Flexible Atomic Code (FAC) packages [19]. Based on these atomic data, a CR model code has been developed to investigate the spectra from EBIT.

The emission line intensity $I_{p,q}(\lambda)$ due to a radiative transition with wavelength λ from the upper level p to the lower level q in an optically thin plasma, can be defined as:

$$I_{p,q}(\lambda) \propto n(p)A(p,q)\phi(\lambda), \tag{1}$$

where $n(p)$ is the population of the ions in the upper level p, $A(p,q)$ is the transition probability or Einstein coefficient for transition from p to q, and $\phi(\lambda)$ is the normalized line profile. In this work, $\phi(\lambda)$ was taken as a Gaussian profile, which may include the effects of Doppler, natural, collisional and instrumental broadenings. The quantities $A(p,q)$ can be obtained from the experiments or accurate theoretical calculations. The populations $n(p)$, on the other hand, are determined by various atomic process such as spontaneous radiative transition, (de)excitation by electron collisions, radiative recombination, dielectronic recombination, ionization by electron impact, or three-body recombination, while the effect of radiative and dielectronic as well as three body recombination processes is expected to be negligible in the cases of current interest, because they scarcely affect the population of the low-lying levels that are relevant to the EBIT spectrum [20].

The temporal development of the population $n(p)$ in level p is described by the following rate equation:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}n(p) &= \sum_{q<p} C(q,p)n_e n(q) \\ &\quad - [\sum_{q<p} F(p,q)n_e + A(p,q) + \sum_{q>p} C(p,q)n_e]n(p) \\ &\quad + \sum_{q>p}[F(q,p)n_e + A(q,p)]n(q)\end{aligned} \tag{2}$$

where n_e is the electron density, $C(q,p)$ and $F(q,p)$ are collisional excitation and deexcitation rate coefficients from the level q to p, respectively. They can be calculated from the cross sections of collisional (de)excitation processes by assuming an appropriate free electron energy distribution. The electron energy distribution in the electron beam of an EBIT is mostly mono-energy under typical operation conditions [15]. Thus, in the present work for the EBIT case, the electron energy distribution function is taken as a δ function, while the Maxwellian distribution of the electron energy was assumed in the case of fusion plasmas. The first term in the righthand side of equation (2) refers to the population flux by the excitation processes from energy levels lower than p and the last term also represents the population flux by collisional deexcitation and radiative transition processes from the levels higher than p. The second term represents the depopulating flux of level p by both collisional excitation, deexcitation and radiative transition processes. A Quasi-Steady-State (QSS) equilibrium approximation was assumed, in which we set $\mathrm{d}n(p)/\mathrm{d}t = 0$ [12]. Under this approximation, $n(p)$ can be solved from the set of equations (2) to obtain the intensity $I_{q,p}(\lambda)$ by equation (1).

In order to construct the CR model for the W^{26+} ions, the configurations $4d^{10}4f^2$, $4d^{10}4f^1nl$ $(n = 5,6,7,8)$, $4d^{10}nln'l'$ $(n,n' = 5,6)$, $4d^94f^2nl$ $(n = 5,6,7)$ and $4d^94f^1nln'l'$ $(n,n' = 5,6)$ with l and l' from 0 to $n-1$ and $n'-1$ correspondingly, were included in the present calculation. All the energy levels, radiative transition probabilities and collision excitation cross sections among these levels were calculated. Most of the important configuration interaction effects were included in the present calculation.

3. Results and discussion

The level energies of the ground state $4d^{10}4f^2$ multiplets of W^{26+} have been calculated and are given in Table 1. The first column is the state designation in the LS coupling scheme. All the columns labeled as Cal(nl) are the level energies calculated from different electron correlation models. All the important configuration interaction contributions were included in a systematical way by constructing the interacting configurations from the single and double substitution from $n = 4$ subshells of W^{26+} ions to nl virtual orbits, where nl means the highest principle quantum number n $(n = 5,6,7,8)$ and angular quantum number l $(l = 0,1,\ldots,(n-1))$ of excited electron. The available calculated result by multi reference relativistic many-body perturbation theory (MR-RMBPT) and experimental observation by EBIT [7] were also provided. It can be inferred from the table that the level energies get converged by