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Polarization of the $nf \rightarrow 3d$ ($n=4$, 5, 6) x-rays from tungsten ions following electron-impact excitation and dielectronic recombination processes

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ABSTRACT

Electron-impact excitation and resonant electron capture cross sections to the specific magnetic sublevels as well as the polarization of the strong $nf \rightarrow 3d$ ($n=4$, 5, 6) x-ray emitted from Ni-like through Ge-like tungsten ions have been studied systematically by using a fully relativistic distorted-wave method. We compare the polarizations for the same x-ray but from the above two different processes for the first time. It is found that the polarization degrees of x-ray following both the electron-impact excitation and the dielectronic recombination are totally different. Because the electron-impact excitation dominates in hot and dense plasmas and the dielectronic recombination plays a key role in low-density plasmas which are cooled and recombining by capturing continuum electrons, we hope that the specific plasmas conditions could be assessed by using these x-ray polarizations.

1. Introduction

Tungsten, because of its high melting point, low sputtering rate and low retention of tritium [1,2], has been used as plasma-facing materials in several magnetic fusion devices [3–5] and is the leading candidate material within the divertor region of the International Thermonuclear Experimental Reactor (ITER) tokamak [6,7]. Line radiations from highly charged tungsten ions can be used as diagnostic probes reflecting information about fusion plasmas. The Ni-like through Ge-like tungsten ions are arranged in a filled M-shell structure and expected to be present over a wide range of temperatures. The strong $nf \rightarrow 3d$ x-rays from those ions have great significance which are especially suitable for fusion plasma diagnostics since the inner-shell radiative transitions connecting the $3d$ subshell are very intense [8].

Until now, some experimental and theoretical studies for tungsten ions, for example, x-ray emission spectra and transition properties, charge state distribution, electron impact excitation (EIE) and ionization as well as dielectronic recombination (DR) processes have been performed. Extreme-ultraviolet (EUV) spectra in the wavelength range of 40–85 Å for Rb- to Cu-like tungsten ions have been recorded by Utter et al. [9] at the Lawrence Livermore National Laboratory (LLNL) electron beam ion trap (EBIT) facility. Neill et al. [10] measured M-shell spectra of Se- to Cr-like tungsten ions at the Livermore EBIT, the majority of lines in the spectra have been identified and assigned to the $4f \rightarrow 3d$ and $4d \rightarrow 3p$ transitions. Pütterich et al. [11] performed detailed investigations for the spectra in the wavelength range 4–14 nm of Cu- to Ag-like tungsten ions produced by the ASDEX Upgrade tokamak

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facility. Ralchenko et al. [12,13] studied the x-ray and EUV spectra of Br-like through Co-like tungsten ions with the EBIT at the National Institute of Standards and Technology (NIST). Biedermann et al. [14] investigated the soft x-rays originating from $3d \rightarrow 4f$ transitions around 0.56 nm from Cu- to V-like tungsten ions at Berlin EBIT. M-shell spectra and charge state distribution of highly charged tungsten ions have been studied by Clementson et al. [15,16] at the Livermore EBIT-I and SuperEBIT facility, these investigations covered energy measurements of $n=3 \rightarrow n=4,\ 5,\ 6$ transitions of the Co- to Zn-like tungsten ions. EUV spectra in the 4.5–6.5 nm region from low-density and high-temperature tungsten plasmas are produced and measured by Harte et al. [17] in the Large Helical Device at the National Institute for Fusion Science. Clementson et al. [18] measured the polarizations of E2 and M3 $(3d_{5/2}^{-1}4s)_{J=2,3} \rightarrow (3d^{10})_{J=0}$ transition lines of Ni-like tungsten ion using high-resolution crystal spectroscopy at the LLNL-EBIT facility.

On the theoretical front, fully relativistic *ab initio* calculations have been carried out for the wavelengths, oscillator strengths, and line intensities of Co- to Rb-like tungsten ions by Fournier [19]. A complete data set about the spectral lines and energy levels of H- to Hf-like tungsten ions was provided by Kramida et al. [20] using parametric fitting with Cowan's code. A comprehensive theoretical study of atomic characteristics for various tungsten ions is performed by Safronova et al. [21], in which excitation energies, oscillator strengths, radiative and autoionization rates, dielectronic satellite lines and dielectronic recombination rates are computed by using the relativistic many-body perturbation theory (RMBPT). Energy levels, wavelengths and radiative decay rates have been calculated for the $3p^n$ and $3d^n$ ground configurations of Co- to Rb-like tungsten ions as well as the $4p^n$ and $4d^n$ ground configurations of Ga- to Rh-like tungsten ions by Quinet et al. [22,23] using the fully relativistic multiconfiguration Dirac–Fock (MCDF) approach. Electron-impact ionization cross sections for the tungsten isonuclear sequence ions are calculated by Loch et al. [24] using a distorted-wave (DW) method. Das et al. [25] reported the M-shell EIE crosses and the linear polarizations of photon emissions of Zn- to Co-like tungsten ions. Ballance et al. [26,27] studied the EIE process and different collision parameters for Ni-, Cu-, and Zn-like tungsten ions using a fully relativistic R-matrix method including the contributions of radiation damping to the resonance. Behar et al. [28] performed relativistic calculations to the DR cross sections and rate coefficients of Ar-, Cu- and Ni-like tungsten ions. These works are intended not only to investigate design issues, plasma diagnostic and theoretical modeling of spectra for ITER operation but also to extend the reference data for energy levels and corresponding wavelengths of tungsten ions.

The existing work shows that linear polarization of x-ray provides important information of various physical effects [29–32] and detailed population mechanisms of excited states [33,34]. However, to the best of our knowledge, there are few work about the degree of linear polarization for the tungsten x-ray spectra interested in the studying of ITER fusion plasmas. In the present work, cross sections for EIE and resonant electron capture (REC) to specific magnetic sublevels of Ni-like through Ge-like tungsten ions have been studied by using a fully relativistic distorted-wave (RDW) method. Further, the degrees of linear polarization for the corresponding strong $nf \rightarrow 3d$ (n=4, 5, 6) x-ray emissions following both the EIE and REC processes are also calculated, respectively. The excitation and capture cross sections as well as the linear polarizations of the corresponding x-rays are discussed later.

2. Theoretical method

In the present work, the cross sections for electron-impact excitation to individual magnetic sublevels of Ni- to Ge-like tungsten ions are calculated by using a newly developed fully RDW program REIE06 [35], the target state wave functions are generated with the use of the atomic structure package GRASP92 [36] based on the MCDF method, and the continuum electron wave functions are produced by the component COWF of the Ratip package [37] by solving the coupled Dirac equation in which the exchange effect between the bound and continuum electrons are considered. It is convenient to choose the z-axis to be the direction of the motion of the incident electron, and then the z component of the incident electron orbital angular momentum is zero, namely, $m_{l_i}=0$. In this case the EIE cross section of the target ion from the initial state $\beta_i J_i M_i$ to the final state $\beta_f J_f M_f$ is given by [38,39]

$$\sigma_{\varepsilon_i}\left(\beta_i J_i M_i - \beta_f J_f M_f\right) = \frac{2\pi a_0^2}{k_i^2} \cdot \sum_{l_i, l_i', j_i, j_i', m_{s_i}, l_f, j_f, m_f} \sum_{J, J', M} (i)^{l_i - l_i'} [(2l_i+1)(2l_i'+1)]^{1/2}$$
$$\times \exp\left[i\left(\delta_{\kappa_i} - \delta_{\kappa_i'}\right)\right] C\left(l_i \frac{1}{2} 0 m_{s_i}; j_i m_i\right)$$
$$\times C\left(l_i' \frac{1}{2} 0 m_{s_i}; j_i' m_i\right) C(J_i j_i M_i m_i; JM)$$
$$\times C(J_i j_i' M_i m_i; J'M) C(J_f j_f M_f m_f; JM)$$
$$\times C(J_f j_f M_f m_f; J'M) R(\gamma_i, \gamma_f) R(\gamma_i', \gamma_f'), \quad (1)$$

here the subscripts i and f denote the initial and final states, respectively. The ε_i is the incident electron energy in Rydberg. a_0 is the Bohr radius. The C's and R's are Clebsch-Gordan coefficients and collision matrix elements, respectively. $\gamma_i = \varepsilon_i l_i j_i \beta_i J_i JM$ and $\gamma_f = \varepsilon_f l_f j_f \beta_f J_f JM$, where the J and M are the quantum numbers corresponding to the total angular momentum of the collisional system (target ion plus free electron), and its z component, respectively; the β_i represents all additional quantum numbers required to specify the initial states of the target ion in addition to its total angular momentum J_i and z component M_i, respectively, and the quantity β_f has a similar meaning for the final state. $m_{s_i}, l_i, j_i, m_{l_i}$ and m_i are the spin, orbital angular momentum, total angular momentum, and its z-component quantum numbers, respectively, for the incident electron ε_i; δ_{κ_i} is the phase factor for the continuum electron. κ is the relativistic quantum number, which is related to the orbital and total angular momentum l and j. k_i is the relativistic wave number of the incident electron and is given by

$$k_i^2 = \varepsilon_i\left(1 + \frac{\alpha^2 \varepsilon_i}{4}\right), \quad (2)$$