W^{63+} and W^{64+} ionization by protons and photons

2015 J. Phys.: Conf. Ser. 583 012035

(http://iopscience.iop.org/1742-6596/583/1/012035)

Journal of Physics: Conference Series **583** (2015) 012035 doi:10.1088/1742-6596/583/1/012035

W^{63+} and W^{64+} ionization by protons and photons

S D López [1,3], J M Randazzo[2,3], R Della Picca[2,3] and F D Colavecchia[2,3]

[1] Instituto de Astronomía y Física del Espacio, Casilla de Correo 67 Suc. 28, C1428ZAA Ciudad Autnoma de Buenos Aires, Argentina.
[2] División Física Atómica, Molecular y Óptica, Centro Atómico Bariloche, 8400 S. C. de Bariloche, Río Negro, Argentina.
[3] Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina.

E-mail: sebastlop@iafe.uba.ar

Abstract. In this work we investigate the ionization by proton impact, and photo ionization, involving highly charged ions of W, in particular the Ne-like W^{64+} and Na-like W^{63+} which are more likely to appear in ITER plasma. Total cross sections are calculated in the continuum-distorted-wave-eikonal-initial-state (CDW-EIS) approximation for ion-impact, while two completely different methods are used for photoionization: a perturbative dipolar aproach and the recently introduced Sturmian model.

1. Introduction

Tungsten (W) is the material of choice for use as a key component in the divertor of the International Thermonuclear Experimental Reactor, ITER [1]. For this reason, the properties of tungsten, as a wall material and as an impurity within the plasma are of great interest. Also, data for radiative and collisional atomic processes involving tungsten ions interacting with the plasma are scarce, and need to be computed and measured. Among the variety of reactions within the plasma, we focus our attention in the ionization of highly charged tungsten ions by proton and photon impact. We investigate these collisions with the Ne-like W^{64+} and Na-like W^{63+}, which are the most common ionic states of Tungsten in ITER plasma [2, 3]. Singly differential and total cross sections are calculated in the continuum-distorted-wave-eikonal-initial-state (CDW-EIS) approximation for ion-impact [4, 5]. The initial bounded and final electronic wave functions are obtained with the Optimized Potential Model (OPM) presented by Talman [4].

2. Ionization by proton impact

Many perturbative theories have been developed to describe the single ionization produced by charged ion impact, being the distorted waves methods the most reliable and accurate at differential levels for intermediate to high impact energies. Particularly, the CDW-EIS model has proven to be very accurate for the ion-atom ionization collisions since early 80's [4]. This approximation is a two center approach, which includes the interaction of an active electron with both ions, the projectile and the target core, via Coulombic Distorted Waves. Moreover, the theory can accomodate modified Coulomb waves, which are solutions of a model potential that includes the screening effect of passive electrons [5]. This screening is included in the problem as a short range potential whereas keeping the long range interatiction for large distances between the electron and the residual dressed ionic core. The initial state considered is:

$$\chi_i(\mathbf{r}_T, \mathbf{r}_P) = \phi(\mathbf{r}_T) E_{-\mathbf{v}}(\mathbf{r}_P) e^{i\mathbf{K}_i.\mathbf{R}}, \tag{1}$$

where $\mathbf{r}_T$, $\mathbf{r}_P$ and $\mathbf{R}$ are the electron- target core, electron- projectile and projectile- target core coordinates respectively. Here, E represents an eikonal wave, with $\mathbf{v}$ the projectile velocity. We define $\mathbf{K}_i$ ($\mathbf{K}_f$) as the initial (final) projectile momentum relative to the target core. The wave function $\phi(\mathbf{r}_T)$ is the initial bound state of the electron:

$$\phi(\mathbf{r}_T) = R_{NL}(r)\, Y_{L,M}(\Omega). \tag{2}$$

The wave function proposal for the final state is:

$$\chi_f(\mathbf{r}_T, \mathbf{r}_P, \mathbf{R}) = \psi_{\mathbf{k}}(\mathbf{r}_T) D_{\mathbf{k}-\mathbf{v}}(\mathbf{r}_P) e^{i\mathbf{K}_f.\mathbf{R}}, \tag{3}$$

where k is the final electron momentum relative to the target core, D represents the usual Coulomb continuum distortion and $\psi_{\mathbf{k}}(\mathbf{r}_T)$ is the continuum wave function of the electron in the target core field

$$\psi_{\mathbf{k}}(\mathbf{r}_T) = \sum_{m,\ell} f_\ell(k, r)\, Y^*_{\ell,m}(\Omega_k)\, Y_{\ell,m}(\Omega). \tag{4}$$

As can be seen, the main problem to deal with, is to solve the eigen-states of the electron in the target core field. We use the Optimized Model Potential of Talman [6] to obtain effective central potentials for the active electron. With these potentials, we calculate radial wave functions $R_{NL}(r)$ ($f_\ell(k, r)$) for the bound (continuum) states, respectively, by solving a one active electron Schrödinger equation. The use of these radial functions leads to a CDW-EIS theory free of Post-Prior discrepancy [7].

In this frame, the total cross section (TCS) reads:

$$\sigma = (2\pi)^4 \mu^2 \frac{K_f}{K_i} \int |T_{fi}|^2 d\Omega_{K_f} d\mathbf{k}, \tag{5}$$

where T_{fi} is the transition matrix. Here μ is the projectile-target reduced mass and ε_i is the ionization energy of the target. Here we present results of the total cross section of the W^{+63} and W^{+64} ions as a function of the energy of the projectile, from the 3s, $2p^0$ and $2p^1$ levels of the W^{+63} ion and 2s, $2p^0$ and $2p^1$ of the W^{+64} ion, see Fig. 1. Cross sections were computed for impact energies between 150 keV and 3 MeV. For energies smaller than 150 keV, the CDW-EIS approximation is not correct, and for energies above 3 MeV, a simpler First Born Approximation could be used [4]. Overall all the cross sections present a similar behavior within the projectile energy range computed, not reaching any maximum in this region. To the best of our knowledge, these cross sections were never reported in the literature before.

3. Ionization by photon impact

We proceed now to evaluate photo ionization of the W^{+63} and W^{+64} ions considering the same initial levels that we use for ionization by proton impact. The cross section of photo ionization of q electrons from the shell NL due to the impact of photons with frequency ω is (see for example Eq. (3) of [8]):

$$\sigma = \frac{q(2\pi)^2}{2L+1} \alpha\omega k \sum_M \int d\Omega_k\, |\langle \psi_{\mathbf{k}} | \hat{\epsilon} \cdot \mathbf{r} | \phi \rangle|^2 = \frac{q(2\pi)^2}{3(2L+1)} \alpha\omega k \left[I_{L-1} L + I_{L+1}(L+1) \right] \tag{6}$$

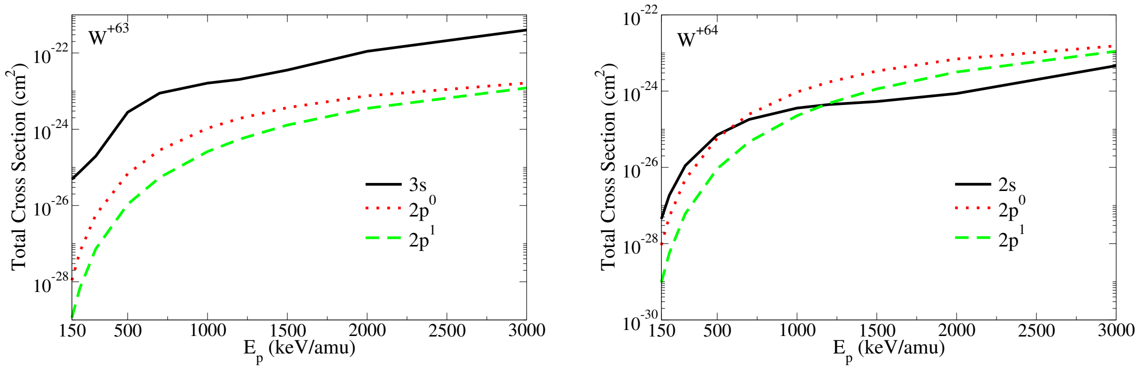

Figure 1. Total cross sections for the ionization from the $2p^0$, $2p^1$ and $3s$ level of the W^{+63} (left panel) and from the $2p^0$, $2p^1$ and $2s$ level of W^{+64} ions (right panel) as a function of the proton impact energy.

where the final electron momentum $\mathbf{k}$ is determined by the conservation of the total energy: $k^2/2 = \hbar\omega + E_{NL}$. The wave function ϕ is the initial state, Eq. (2), while $\psi_{\mathbf{k}}$ represents the one electron final state, Eq. (4). The radial integrals are defined by:

$$I_{L\pm1} = \int_0^\infty dr\, f^*_{L\pm1}(k,r)\, r^3 R_{NL}(r) \tag{7}$$

where f_L and R_{NL} are the radial part of final and initial electronic wave functions defined above.

We also make use of an alternative approach to evaluate the scattering wave function for a single photon absorption solution of the following non homogeneous equation:

$$\left[-\frac{1}{2}\nabla^2_{\mathbf{r}} + V(r) - E\right]\Psi^+_{V,sc}(\mathbf{r}) = \frac{1}{2}(\hat{\varepsilon}.\nabla_{\mathbf{r}})\Phi_0(\mathbf{r}) \tag{8}$$

in the velocity gauge, while in the length gauge $\nabla_{\mathbf{r}}$ must be replaced by $\omega\mathbf{r}$. This calculation can be performed using the Generalized Sturmian Functions model presented recently [9]. In this method, the wave functions $\Psi^+_{V,sc}(\mathbf{r})$ and $\Phi_0(\mathbf{r})$ are expanded in terms of a Sturmian radial basis set, and the equation (8) is solved for the coefficients of that expansion. The key role of the basis is that all its elements include the correct long-range boundary condition of the problem under scrutiny. The asymptotic behavior of the scattering wave functions must have the same behavior in both velocity and length gauges and has the form:

$$\Psi^+_{sc}(\mathbf{r}) \simeq A(\hat{\mathbf{r}})\frac{e^{i(kr-\frac{Z}{k}\log 2kr)}}{r}. \tag{9}$$

The cross section is a balance between the electronic flux $2i\, j_e = \Psi^{+*}_{sc}\nabla\Psi^+_{sc} - \Psi^+_{sc}\nabla\Psi^{+*}_{sc}$, and the photon flux j_s given by the Poynting vector associated to the electromagnetic wave:

$$\frac{d\sigma}{d\Omega} = \frac{j_e}{j_s} = \frac{2\mu_0 ck}{\omega}|A(\hat{\mathbf{r}})|^2. \tag{10}$$

We present results of the total ionization cross section of the W^{+63} and W^{+64} ions as a function of the energy of the ejected electron (which depends on the photon energy), from the 3s, $2p^0$ and $2p^1$ levels of the W^{+63} ion and 2s, $2p^0$ and $2p^1$ of the W^{+64} ion, see Fig. 2. Contrary to the proton impact case, there are non-dipolar full relativistic calculations of photoionization cross sections, recently reported by Trzhaskovskaya and collaborators [10, 11, 12]. We note that both methods presented here agree with each other. Furthermore, it is clear from the figure that our results deviates only a few percent from the relativistic ones in the high energy regime (beyond 30 keV of photon impact).

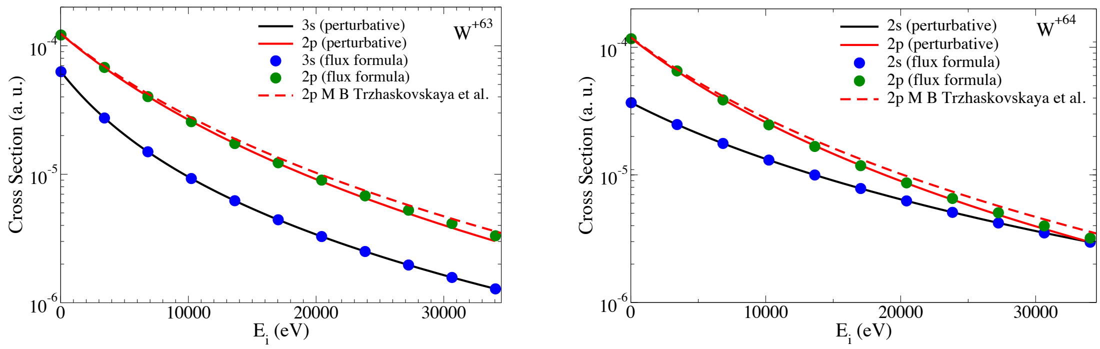

Figure 2. Total cross sections for the photo ionization from the 3s and 2p levels of the W^{+63} ion (left) and from the 2s and 2p levels of the W^{+64} ion (right) as a function of the energy of the emitted electron. Non-dipolar relativistic calculations (dashed lines) of Ref. [11, 12].

4. Summary and outlook

We have computed the total cross section of ionization of W^{+63} and W^{+64} ions by proton, which have not been considered before; and photon impact, that were presented this year in the literature. The total ionization cross sections for proton impact increase monotonically for all the sub-shells up to 3 MeV. The cross sections for photoionization agree well with their relativistic counterparts, suggesting that it is possible to consider a simpler dipolar approximation for these highly charged targets in the energy regime up to a few keVs. Further theoretical developments will be pursued along two directions: study other highly charged tungsten ions, and focus on multiple ionization processes.

Acknowledgments

We would like to thank the National Atomic Energy Comission of Argentina (CNEA), through the Integral Program of Controlled Nuclear Fusion. We also thanks the financial support of the National University of Cuyo, through the program 06/C424.

References

[1] www.iter.org
[2] Pütterich T *et al.* 2008 *Plasma Phys. Control. Fusion* **50** 085016
[3] Hirai T *et al.* 2013 *Fusion Eng. Design* **88** 1798
[4] Crothers D S F and McCann J F 1983 *J. Phys.* B **16**, 3229
[5] Gulyas L, Fainstein P D and Salin A 1995 *J. Phys.* B **28** 245
[6] Talman J D 1989 *Comp. Phys. Comm.* **54** 85
[7] López S D, Fiori M and Garibotti, C R 2011 *Phys. Rev.* A **83** 032716
[8] Della Picca R, Fainstein P D and Dubois A, 2011 *Phys Rev* A **84** 033405
[9] Gasaneo G *et al Adv. Quant. Chem.* **67** 153
[10] Trzhaskovskaya M B, Nikulin V K and Clark R E H 2008 *At Data Nucl Data Tables* **94** 71
[11] Trzhaskovskaya M B and Nikulin V K 2013 *At Data Nucl Data Tables* **99** 249
[12] Trzhaskovskaya M B and Nikulin V K 2014 *At Data Nucl Data Tables* **100** 986