Electron Impact Ionization Cross Sections of Tungsten Atoms and Tungsten Ions*)

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Tungsten (W) and tungsten based materials have been recommended as the plasma facing component in the current fusion devices. The electron induced processes on these materials are of prime importance for the application purposes. Electron impact total ionization cross sections (TICS) are reported for the W atoms and W^+ ions. The TICSs have been calculated in the variants of distorted wave approximation (DWA) using Hartree-Fock wave functions and distorted potential with semi-classical exchange. Present TICS results have been compared with the available theoretical and experimental results. Reasonable agreement with the existing theoretical results have been obtained for the TICS of W atoms by present semi-relativistic distorted wave approach, however there are certain discrepancies for the TICS of W^+ ions. Differential cross sections (DCSs) have also been calculated at projectile energy 100 eV for the ionization of W atoms and W^+ ions and the DCSs have been found to be sensitive on the scattering angle.

Keywords: total cross section, DWA, ionization, Hartree-Fock potential, fusion plasma, differential cross section, TDCS, TICS

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1. Introduction

The ionization cross sections are essential in the modeling of plasma in fusion research. The electron collision processes on heavy atoms and their ions are important to study since they employ certain phenomena which are different from lighter targets. The tungsten (W) and tungsten based materials have been recommended as one of the materials to be used as plasma facing components for the International Thermonuclear Experimental Reactor (ITER) [1] and the Demonstration Power Station (DEMO) as these materials have thermophysical properties suitable for fusion application [2–4]. Tungsten is already in use as plasma facing components in tokamaks such as JET [5] and ASDEX-Upgrade [6]. In the fusion devices the tungsten and related materials may exhibit high melting temperature, strong resistance against sputtering and shorter penetration depth etc.

Electron induced processes such as excitation and ionization are prevalent in such magnetic fusion devices in a wide range of energies with significant variation of temperature and density [7]. A reliable data base is required for the electron impact ionization and excitation cross sections for W to model the electron induce interactions and to understand the spectroscopy involved. Detailed knowledge of electron tungsten interactions and W electronic structure is still scarce, however the W ions have been studied extensively. In earlier efforts, direct ionization cross sections of the W atom were calculated using semi-relativistic distorted-wave method [8] and electron impact single ionization cross sections were calculated for the W isonuclear sequence [9]. In later efforts electron induced ionization cross sections for W and W^+ ions have been reported [10]. Very recently electron impact integral cross sections [11] and electron impact single and double ionization cross sections [12] have been calculated for W atoms. Experimental data are available for the ionization of W^+ [13, 14], however no cross section measurements have been reported for ionization of W atoms.

We report in this communication the electron impact ionization cross sections for the W atoms and W^+ ions. The ionization cross sections have been calculated in the distorted wave approximation (DWA). We compare the results of present calculations with the available theoretical and experimental results. We also report the electron impact differential cross sections (DCS) for the ionization of W atoms and W^+ ions for which no earlier studies are available. The trends of DCS may give finer details of electron tungsten interactions which may be of help to understand the structure of target for application purposes.

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Brief theoretical formalism used to calculate ionization cross sections is described in next section.

2. Theory

In the electron impact single ionization process, an incident electron of linear momentum k_i and energy E_i ionizes the target (atom / ion) and the two emerging electrons are described by the linear momentum and energy (k_f, E_f) and (k_e, E_e), where the scattered (primary) electron is specified by subscript 'f' and the ejected (secondary) electron is specified by subscript 'e'. The energy conservation principle states;

$$E_i = E_f + E_e + E_b, \tag{1}$$

where E_b is the energy of the bound electron.

The triple differential cross section (TDCS) for the electron impact single ionization, which is the probability of single ionization, is expressed in atomic units as

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_f \mathrm{d}\Omega_e \mathrm{d}E_f} = (2\pi)^4 \frac{k_f k_e}{k_i} \sum_{av} |T(k_f, k_e, k_i)|^2. \tag{2}$$

The expression in Eq. (2) includes a sum over final and average over initial magnetic and spin state degeneracy. The T matrix in Eq. (2), which is the subject of approximation, includes interaction between the incident and target electrons and the nucleus. TDCS (eq. 2) for the ionization is written in terms of direct and exchange amplitude as

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_f \mathrm{d}\Omega_e \mathrm{d}E_f} = (2\pi)^4 \frac{k_f k_e}{k_i} \sum_{m=-l}^{l} \left(|f|^2 + |g|^2 - Re(f^* g) \right), \tag{3}$$

where

$$f = \left\langle \chi_f^{(-)}(k_f, r_f) \chi_e^{(-)}(k_e, r_e) \left| V_{fe} \right| \chi_i^{(+)}(k_i, r_f) \chi_b(r_e) \right\rangle, \tag{4}$$

$$g = \left\langle \chi_f^{(-)}(k_f, r_e) \chi_e^{(-)}(k_e, r_e) \left| V_{fe} \right| \chi_i^{(+)}(k_i, r_f) \chi_b(r_e) \right\rangle. \tag{5}$$

Here V_{fe} is the interaction potential between the incident and target electrons responsible for the ionization. The distorted wavefunction for the incident electron is represented by $\chi_i^{(+)}$. $\chi_f^{(-)}$ and $\chi_e^{(-)}$ represent the distorted wavefunctions for the two outgoing electrons and each is orthogonalized with respect to χ_b. χ_b is the target wave function, which is the ejected electron wave function before collision. The potentials are obtained from the Hartree-Fock functions of McLean and McLean [15] and localized version of potential is employed [16, 17].

Using partial wave expansion and performing angular integrations on eq. (2) the total ionization cross section is given by

$$\sigma(E_i) = \frac{16}{\pi E_i} \int_0^E \mathrm{d}E_e \sum_{l_i, l_e, l_f} (2L+1) |F|^2, \tag{6}$$

where l_i, l_f are electron orbital angular momentum quantum numbers in incident and final channels respectively, l_e is the ejected electron quantum number and L is the total orbital angular momentum. Energies obey the conservation defined in eq. (1)

F is the ionization amplitude, from eq. (3), it can be written as

$$|F|^2 = |f|^2 + |g|^2 - Re\,(f^* g)\,. \tag{7}$$

Performing the integrals over the angles in the eq. (4) and (5), the amplitude may be written as

$$F = \sum_{\lambda} f_\lambda (l_b l_i l_e l_f L) \left\langle \chi_b \chi_i \left| V_{fe} \right| \chi_e \chi_f \right\rangle_\lambda, \tag{8}$$

here f_λ is the angular factor. The Hartee-Fock target wave functions [15] have been used for the calculatins of TDCS. The total ionization cross sections for W atoms and W^+ ions have been calculated in two variants of distorted wave approximation (DWA) namely Cowan structure calculation [18] and HULLAC [19]. The Hartree-Fock target wave function and Hartree potential with semi-classical exchange [17] and correlation correction has been used for the semi relativistic DWA calculations with Cowan formalism [18]. Ionization cross sections using Cowan formalism have been calculated in fine-structure and configuration mode. The fine-structure mode includes the relativistic effects empirically in the calculations. The DWA cross section results using HULLAC [19] have been obtained with fully relativistic basis functions for target electrons. The basis function is obtained as a solution of the single-particle Dirac equation with a central-filed parametric potential which represents a nuclear field and a spherically averaged inter-electronic interaction. The parametric potential is optimized iteratively so that first-order configuration average energy of the total Hamiltonian for the ground state configuration with a given set of orbital functions becomes the minimum. Continuum basis functions are also calculated with the same parametric potential. The results and discussion is presented in next section.

3. Results and Discussion

The electron impact total ionization cross section (TICS) for W atom is plotted as a function of incident electron energy in Fig. 1. The present results calculated in the DWA are compared with other theoretical TICS results [11, 12] reported recently and no measurements are available to compare. The solid line is present TICS calculated using HULLAC [19] and the dashed and dotted curves are the present TICS calculated using semi-relativistic distorted wave Cowan formalism [18]. The dashed-dot curve represents the TICS for W atoms calculated in the semi-relativistic distorted wave approximation [12] and the dash-dot-dot curve is the TICS result for W atoms calculated through the electron-atom scattering process using a complex potential [11].

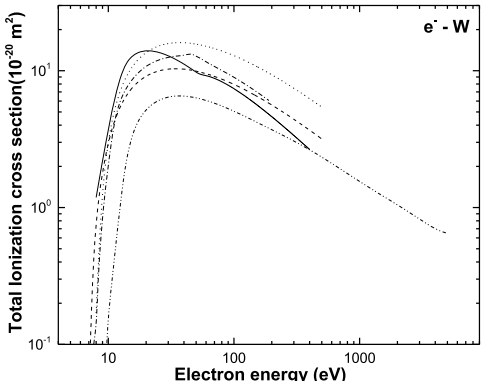

Fig. 1 Total ionization cross sections of W atoms plotted as a function of incident electron energy, solid curve: present DWA results in HULLAC [19], dashed and dotted curves: present DWA results in Cowan formalism with fine-structure and configuration mode; dash-dotted curve: results of [12] and dash-dot-dotted curve: results of [11].

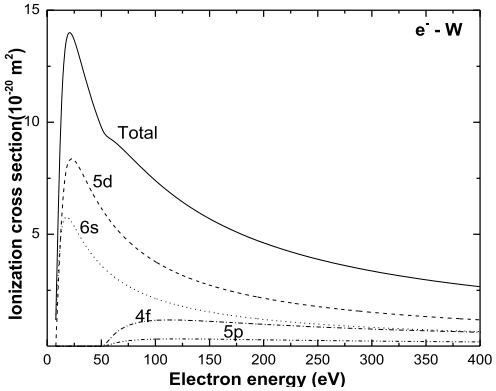

Fig. 2 Ionization cross sections of W atom subshells calculated in DWA using HULLAC [19], solid curve: total; dashed curve: 5d subshell; dotted curve: 6s subshell; dash-dotted curve: 4f subshell; dash-dot-dotted curve: 5p subshell.

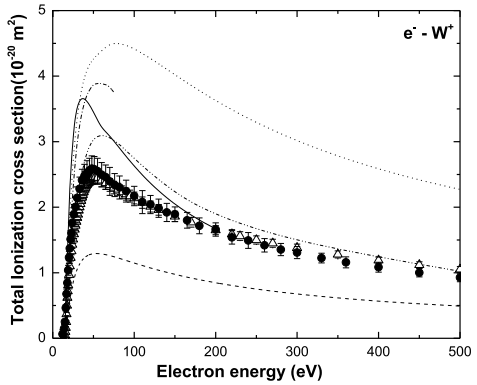

Fig. 3 Total ionization cross sections of W^+ ions plotted as a function of incident electron energy, dash-dot-dotted curve: results of [10]; dash-dotted curve: results of [8]; solid circles and hollow triangles: measurements [14] and [13]; other curves are the same as Fig. 1.

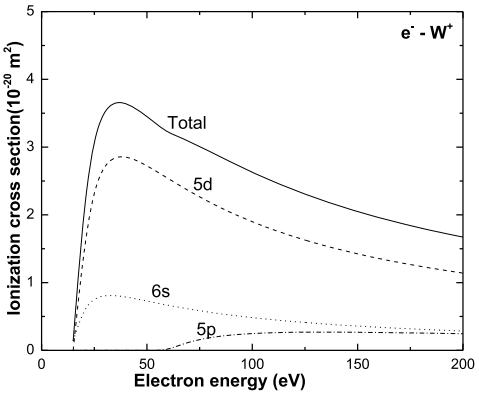

Fig. 4 Ionization cross sections of W^+ ion subshells calculated in DWA using HULLAC [19], solid curve: total; dashed curve: 5d; dotted curve: 6s; and dash-dotted curve: 5p subshell.

Present results with HULLAC [19], Cowan formalism with fine structure mode [18] and semi-relativistic distorted wave results of [12] give nearly same vales of TICS. Present results calculated in the configuration mode with Cowan formalism gives slightly higher and results of [11] with complex potential gives slightly smaller values of TICS for W atoms. Ionization cross sections calculated in the DWA using HULLAC [19] for the individual subshells 6s, 5d, 4f and 5p of W atoms are plotted in Fig. 2 along with the TICS.

The major contribution comes from the 6s and 5d subshells. The electron impact TICS results for the W^+ are presented in the Fig. 3. Present DWA results are compared with the semi-relativistic distorted wave [12] and Coulomb-Born [10] results. The theoretical TICS results are also compared with the available measurements [13, 14]. Present DWA results with HULLAC (solid curve) and Cowan formalism in configuration mode (dashed curve) gives higher values of TICS than the measurements, however the DWA results with HULLAC are less than the semi-relativistic distorted wave results of [12].

The Coulomb-Born results [10] are slightly higher than the measurements and the present DWA results calculated with fine-structure mode are almost 50% smaller from the measurements. Ionization cross sections calculated in the DWA using HULLAC [19] for the individual subshells 5d, 6s and 5p of W^+ ion are plotted in Fig. 4 along with the TICS. The major contribution comes from the 5d and 6s subshells.

The TICS results obtained from HULLAC [19] (solid line in Fig. 1) and fine-structure mode in Cowan formalism [18] (dashed line in Fig. 2) matches well for the W atoms. For the ionization of W^+, the HULLAC [19] results (solid line in Fig. 3) are higher from the available measuremnets however the Cowan [18] results in fine-structure mode (dashed line in Fig. 3) are smaller than the measurements. The configuration mode in Cowan formalism (dot-

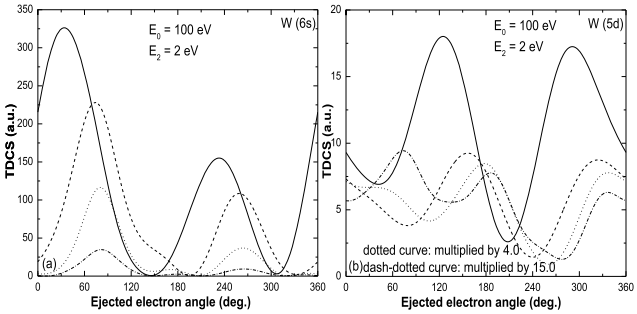

Fig. 5 TDCS for W atoms plotted as a function of ejected electron angle for different scattering angles, solid curve: 2^0; dashed curve: 5^0; dotted curve: 10^0; dash-dotted curve: 15^0.

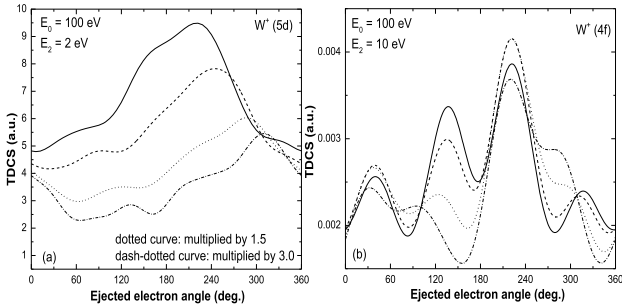

Fig. 6 TDCS for W atoms plotted as a function of ejected electron angle for different scattering angles, legends are the same as Fig. 5.

ted line in Fig. 3) gives nearly two times higher values of cross sections from the measuements. Further studies for the higher charged states of W may be required to decide about the suitability of better approach.

The electron impact triple differential cross section (TDCS) results are presented for the ionization of W (6s) atoms and W^+ (5d) ions in Figs. 5 - 6. The TDCS results have been calculated in the DWBA approach for the projectile energy 100 eV and ejected electron energy 2 eV at various scattering angles. The TDCSs for W atoms are plotted for scattering angles 2^0, 5^0, 10^0 and 15^0 in Fig. 5. A clear two peak structure, i.e binary and recoil peaks, is observed for the ionization taking place from 6s orbital of the W atom. The two peak structure also exist for the ionization from 5d orbital at smaller scattering angle however the TDCS for higher scattering angles show splitting of peaks.

The magnitude of TDCS decreases with increase in scattering angle and the position of the peaks also shift towards higher values of ejected electron angle. The electron impact TDCS for the ionization of W^+ (5d) and W^+ (4f) are plotted in Fig. 6. The trends of TDCS for the ionization of tungsten ions are different from the trends of TDCS for the tungsten atoms. The TDCS trends for the ionization of W^+ does not show the two peak structure, the TDCS observed for the W^+ ions require further efforts to understand the complex collision dynamics of the high Z target.

4. Conclusions

Electron impact ionization cross sections have been calculated for the W atoms and W^+ ions in the distorted wave formalism. Present distorted wave TICS results show nearly the same magnitude as obtained by semi-relativistic distorted wave results obtained earlier for the W atoms. The distorted wave TICS results for the W^+ ions overestimate the measurements and Coulomb-Born results, however, the distorted wave TICS calculated with fine-structure mode for W^+ ions show smaller values. The TICSs have been calculated in semi-relativistic approach in the Cowan formalism and in the fully relativistic approach in HULLAC. As the major contribution to cross section is from outer shells, present efforts should be capable to produce the reasonable TICS data. However higher degree of uncertainty is observed in the calculated TICS so further studies are required to obtain more accurate results. The differential cross sections for the W atoms and W^+ ions are found to be sensitive on the direction of momentum transfer i.e. scattering angle. Further efforts are anticipated for the calculation of ionization cross sections for tungsten atoms and ions which are important for the future fusion devices.

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