Water molecule ionization by charged particles: *a short review*

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Water molecule ionization by charged particles: *a short review*

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Abstract. We present both singly differential and total cross sections for the direct ionization of water vapour by electrons as well as by ions (protons and alpha particles). An ab-initio calculation has been made by using the first Born approximation and an accurate molecular wave function proposed by Moccia [J. Chem. Phys. 40, 2186 (1964)]. The results of this model are compared to experimental data and to results obtained via semi-empirical models.

1. Introduction

Ionization of atoms and molecules by fast charged particles is of prime importance in a large number of areas including plasma physics, radiation physics and the study of penetration of charged particles through matter [1-3]. It has also been shown that experimental and theoretical data about the ionization of biological systems are needed in fundamental studies of charged particle interaction in biological matter (and more precisely in heavy-ion cancer therapy [4]). Moreover with the more and more regular use of ionizing radiations in medicine, it is today necessary to appraise the biological consequences of radiological examinations particularly to know, with the highest degree of accuracy, the energy deposits induced by all the radiations commonly used in radiotherapy and even in medical imaging (light and heavy ions, electrons and positrons, X-rays and γ-rays).

To describe the track-structure of a charged particle in the biological matter and then to quantify the full spectra of molecular damage radio-induced, Monte Carlo simulation is the preferential method. This latter consists in simulating, interaction after interaction, the history of each ionizing particle created during the irradiation of the biological matter. In this kind of study, all the projectile-target interactions are modelled by means of a large set of multi-differential and total cross sections to describe the complete kinematics of the collisions.

In these conditions, we clearly understand the necessity for the radiobiologists, the radiotherapists and the nuclear doctors to access to accurate differential and total cross sections to know the fine structure of the ionizing particle in the living matter, this latter being commonly described by water.

However, experimental measurements of ionization cross sections of water vapour by light and heavy charged particles are extremely scarce. Indeed, for electron as well as for light ion collisions, we essentially find in the literature singly differential and total cross sections (SDCS and TCS, respectively). Doubly and triply differential cross sections (DDCS and TDCS, respectively) are unfortunately more rare. We can then cite *i)* the experimental DDCS measured by Opal *et al.* [5] and by Bolorizadeh and Rudd [6] for water ionization by electron impact, *ii)* those reported by Rudd *et al.* [7-8], by Bolorizadeh and Rudd [9] and more recently by Gobet *et al.* [10] for protons and *iii)* the

extensive works given by Toburen *et al*. [11,12] and very recently the absolute DDCS reported by Ohsawa *et al.* [13] for He^{2+} ions.

Theoretically, the most recent study concerning the water ionization by electron impact has been published by Kim *et al.* [14-16] who developed a "binary-encounter-dipole (BED) model" which combines the binary-encounter theory of Vriens [17] with the dipole interaction of the Bethe theory [18] for fast incident electrons. The mixing ratios for distant and close collisions, and the interference between the direct and the exchange terms were determined by using the asymptotic behavior predicted by the Bethe theory for ionization and stopping power cross sections. The main inconvenience in the BED model is the knowledge of the optical oscillator strength data to describe the continuum, which is only available for a limited number of atoms and molecules. Later Kim *et al.* [14,16] have proposed an additional approximation in the so-called Binary-Encounter-Bethe (BEB) model. However, these two models (the BED and BEB models) give only a semi-empirical description of the ionization process and are moreover limited to singly differential and total ionization cross section calculations. More recently, Coimbra and Barbieri [19] have proposed an extension of the BEB model to calculate DDCS by reducing the number of adjustable parameters from 8 (in Rudd's model) to 3.

Considering the direct ionization of water by proton impact, few theoretical models have been proposed. Thus, Senger *et al.* [20,21] have applied the plane-wave Born approximation (PWBA) starting from the well-known formula of Kuyatt and Jorgensen [22] for the ionization of atomic hydrogen by proton impact and its extension to the other L and M sub-shells by Khandelwal and Merzbacher [23,24] and Choi *et al.* [25]. More recently, Long and Paretzke [26] have shown that the plane wave Born approximation could be successfully employed to calculate doubly differential cross sections for proton energies above 200keV by using a dynamic and spatially screened Coulomb field interaction calculated in the local-density approximation of the density-functional theory. More recently, Olivera *et al.* [27] have used the continuum-distorted-wave-eikonal-initial-state (CDW-EIS) approximation (Fainstein *et al.* [28]) which represents the first order of a distorted-wave series by including the distortions due to the long-range Coulomb potential in both the initial and final channels.

For alpha particles, we essentially find two approaches: the Rudd's model and the HKS (for Hansen, Kocbach and Stolterfoht) model. The first approach, initially introduced for protons, is based on a binary encounter model modified to agree with the Bethe theory at high energies and with the molecular promotion model at low energies [29]. Relatively good agreements were then found between the experimental SDCS and the Rudd's results by means of a large number of fitting parameters. Thus, Uehara and Nikjoo reported in [30] that this model reproduced well the average energies of the secondary electrons ejected by He^{2+} ions for ion energies lower than 300keV/u, but that it underestimated them for greater energies (up to about 30% at 2MeV), what could be corrected by using suitable scaling factors (see [30] for more details). Furthermore, concerning the angular distributions for secondary electrons (namely the doubly differential cross sections, DDCS), Uehara and Nikjoo mentioned that ICRU [31] has recommended to use a semi empirical formula given by Hansen, Kocbach and Stolterfoht (see [32]) for determining the DDCS for electron emission by heavy ions. However, as underlined by the authors, these semi-empirical DDCS give only limited agreements with the experimental data. Under these conditions, Uehara and Nikjoo preferred to use a random sampling of ejected directions among the experimental data.

In these conditions, we have recently developed differential and total ionization cross section calculations [33-35] within the First Born Approximation framework (FBA), where the incident and scattered (fast) projectiles are described by a plane wave function whereas the ejected (slow) electron is described by a Coulomb wave function.

In fact, describing the ionization process at the multi-differential level needs sophisticated theoretical calculations that do exist for atomic targets but that remain scarce for molecules, and more particularly for water molecule. One of the basic difficulties in describing the ionization process in ion-molecule collisions at intermediate to high energies (*i.e.* the energy regime considered in this work) arises from the long range of the Coulomb interaction between all the charged particles. This

problem can be overcome by introducing distortion effects into the initial and final channels as implemented in the theoretical model reported by Olivera *et al.*, in order to calculate the contribution from the inner shell of water vapour to dose profile [27,36]. In that work, the authors calculated doubly differential cross sections for single ionization of vapour water by ion impact as a function of electron energy and angle by using the *continuum-distorted-wave-eikonal-initial-state* (CDW-EIS) approximation, initially developed by Fainstein *et al.* for protons traversing H, He and simple molecular targets [28,37]. Their model was a first order model of a distorted-wave series which introduced distortions (due to the long-range Coulomb potential in both the initial and final channels) as multiplicative factors to the initial and final continuum states of the molecular target [38]. In such a way, it was possible to account for two-centre effects which were not included in the first Born or plane-wave approximations. Furthermore, there is an additional difficulty in modelling the ionization process of molecule target namely the description of the molecular states of the target. There are different convenient ways to treat this problem: a first one, called Bragg's additivity rule, which consists in expressing each molecular cross sections (differential as well as total) as a linear combination of atomic cross sections weighted by the number of atoms in the molecule [36, 38] and a second one, called *complete neglect of differential overlap* (CNDO), where the molecular orbitals are written in terms of atomic orbitals of the atomic constituents [20,21]. However, as underlined by Galassi *et al.* [38], in both these models the calculated doubly differential cross sections exhibit unsatisfactory agreement with the experimental data at small angle regions. The authors linked these discrepancies to the fact that the electronic populations were not correctly reproduced in these two descriptions, especially for the calculations within the Bragg's rule framework. Finally, a third method to calculate the populations of the target is that of molecular orbitals constructed from a linear combination of atomic orbitals in a self-consistent field (MO-LCAO-SCF) [39], whose quality has already been highlightened by Galassi *et al.* [38] for low-Z molecule ionization by proton impact at intermediate and high energies. In previous works, we have used this kind of description, and more precisely that given by Moccia [40] who expressed molecular wave functions of small molecules like H_2O, NH_3 and CH_4 by linear combinations of Slater-type functions. Numerous studies have then been produced about ionization by electron impact in terms of multi-differential as well as total cross sections [33-35,41-43]. Very recently, we have extended our full-differential model to the water ionization by proton [34] and α-particle [35] impact, in a large impact energy range (0.1-10MeV) and provided differential and total cross sections which compared very satisfactory with a large set of experimental data.

In the present paper, we briefly present the theoretical model developed for calculating triply, doubly and singly differential and total ionization cross sections by electron impact as well as by light ion impact (protons and α-particles). Some results are reported in the following for comparison with experimental data and more details can be found in [33-35,41-43].

Atomic units are used throughout unless otherwise indicated.

2. Theory

Contrary to the existing models, the present work needs *neither experimental adjustments nor fitting parameters*. It is only based on quantum-mechanical developments performed in the *Born approximation* and appears as the first theoretical work dedicated to fully-differential as well as total cross section calculations for the water ionization by charged particles.

2.1. The cross section calculation

In the *first Born approximation* (FBA) the ejected electron is described by a Coulomb wave (we speak of FBA-CW model) while the incident and scattered particles are described by plane waves. In these conditions, the non relativistic triply differential cross section (TDCS), is simply given by

$$\frac{d^3\sigma}{d\Omega_e d\Omega_s dE_e} = M_p^2 * Z_p^2 * \frac{k_e k_s}{k_i} |T|^2, \quad (1)$$

where Ω_s and Ω_e represent the solid angles of detection for the scattered particle and for the ejected electron, respectively, M_p and Z_p the projectile mass and charge, respectively. The momenta $\vec{k}_i$, $\vec{k}_s$ and $\vec{k}_e$ are related to the incident and scattered particle energies (E_i and E_s, respectively) and to the ejected electron one (E_e). The matrix element T describes the transition of the system from the initial state to the final state (see [33] and [34] for details). The Coulomb wave used to describe the ejected electron can be written as

$$\varphi_c(\vec{k}_e,\vec{r}) = \frac{\exp(i\vec{k}_e.\vec{r})}{(2\pi)^{3/2}}\,{}_1F_1\left[-iz_e/k_e,-i(\vec{k}_e.\vec{r}+k_e r)\right]\times\exp\left(\frac{\pi z_e}{2k_e}\right)\Gamma(1+iz_e/k_e)\,. \tag{2}$$

In this model, z_e corresponds to the effective ionic charge and will be taken equal to 1.

2.2. The target description

To describe the water molecule in vapour phase, we have used the molecular description proposed by Moccia [40], who developed each of the 5 molecular wave functions in terms of Slater-like functions, centred at a common origin, namely upon the heaviest nucleus *i.e.* the Oxygen atom. Let us note that these functions refer, for a particular molecular orientation given by the Euler angles (α, β, γ), to the calculated equilibrium configurations, which agree well with the experimental data (see [43] for a summary). Under these conditions, the 10 bound electrons of the water molecule are distributed among 5 one-centre molecular wave functions $\upsilon_j(\vec{r})$ (with j ranging from 1 to 5) corresponding to the orbitals 1b1, 3a1, 1b2, 2a1 and 1a1 whose binding energy are 0.4954 a.u., 0.5561 a.u., 0.6814 a.u., 1.3261 a.u. and 20.5249 a.u., respectively. Each of them is expressed by linear combinations of Slater-type functions and is written as

$$\upsilon_j(\vec{r}) = \sum_{k=1}^{N_j} a_{jk}\Phi^{\xi_{jk}}_{n_{jk}l_{jk}m_{jk}}(\vec{r})\,, \tag{3}$$

where N_j is the number of Slater functions used in the development of the j^{th} molecular orbital and a_{jk} the weight of each real atomic component $\Phi^{\xi_{jk}}_{n_{jk}l_{jk}m_{jk}}(\vec{r})$ written as

$$\Phi^{\xi_{jk}}_{n_{jk}l_{jk}m_{jk}}(\vec{r}) = R^{\xi_{jk}}_{n_{jk}}(r)S_{l_{jk}m_{jk}}(\hat{r})\,, \tag{4}$$

where the radial part $R^{\xi_{jk}}_{n_{jk}}(r)$ is given by

$$R^{\xi_{jk}}_{n_{jk}}(r) = \frac{(2\xi_{jk})^{n_{jk}+1/2}}{\sqrt{(2n_{jk})!}}\,r^{n_{jk}-1}e^{-\xi_{jk}r}\,, \tag{5}$$

and where $S_{l_{jk}m_{jk}}(\hat{r})$ is the so-called real solid harmonic expressed by

$$\begin{cases} if\ \mathrm{m_{jk}} \neq 0: & S_{l_{jk}m_{jk}}(\hat{r}) = \left(\dfrac{m_{jk}}{2|m_{jk}|}\right)^{1/2}\left\{Y_{l_{jk}-|m_{jk}|}(\hat{r}) + (-1)^{m_{jk}}\left(\dfrac{m_{jk}}{|m_{jk}|}\right)Y_{l_{jk}|m_{jk}|}(\hat{r})\right\} \\ if\ \mathrm{m_{jk}} = 0: & S_{l_{jk}0}(\hat{r}) = Y_{l_{jk}0}(\hat{r}) \end{cases}. \tag{6}$$

3. Results and discussion

We only compare here the results of our model with experimental data for the SDCS and the TCS since the other theoretical models using fitting parameters can never be applied for the DDCS and the TDCS.

3.1. Proton and α-particle collisions

In Figure 1 we present a comparison between our theoretical results obtained in the FBA-CW model and experimental data available in the literature for water ionization by protons and He^{2+} ions.

Four values of proton energy have been considered: 1.5MeV [11], 0.5MeV [11], 150keV [9] and 100keV [9]. A good agreement is generally observed between the experiments and our results especially for ejected electron energies greater than 10eV. The semi-empirical model HKS [32] is also able to describe the experimental data if the energy of the ejected electrons is greater than 10eV, contrary to the Rudd's model [29] which largely overestimates the SDCS for low incident energies (E_{inc} = 100keV and 150keV in the present case). However, our model as well as the two semi-empirical models is unable to reproduce the decreasing of the SDCS for low ejected electron energies.

Considering now the alpha particles, four values of incident energy have been considered namely 1.2MeV [12], 24MeV [13], 40MeV [13] and 60MeV [13]. Good agreement is also observed between the experimental data and our theoretical results, except for ejected electron energies lower than 100eV where our model slightly overestimates the data of Ohsawa *et al.* [13]. In particular, the data of Toburen *et al.* [12] are perfectly reproduced by our model. We notice that the semi-empirical model HKS slightly underestimates the data of Ohsawa *et al.* [13] and perfectly reproduces the data of Toburen *et al.* [12]. Comparatively, the Rudd's model [44] reproduces with a relatively acceptable agreement the experimental data for high impact energies whereas it largely overestimates the SDCS for low incident energies, namely lower than 300keV/u. Finally, note that our theoretical results and both the semi-empirical results (Rudd's and HKS models) tend asymptotically to the same values.

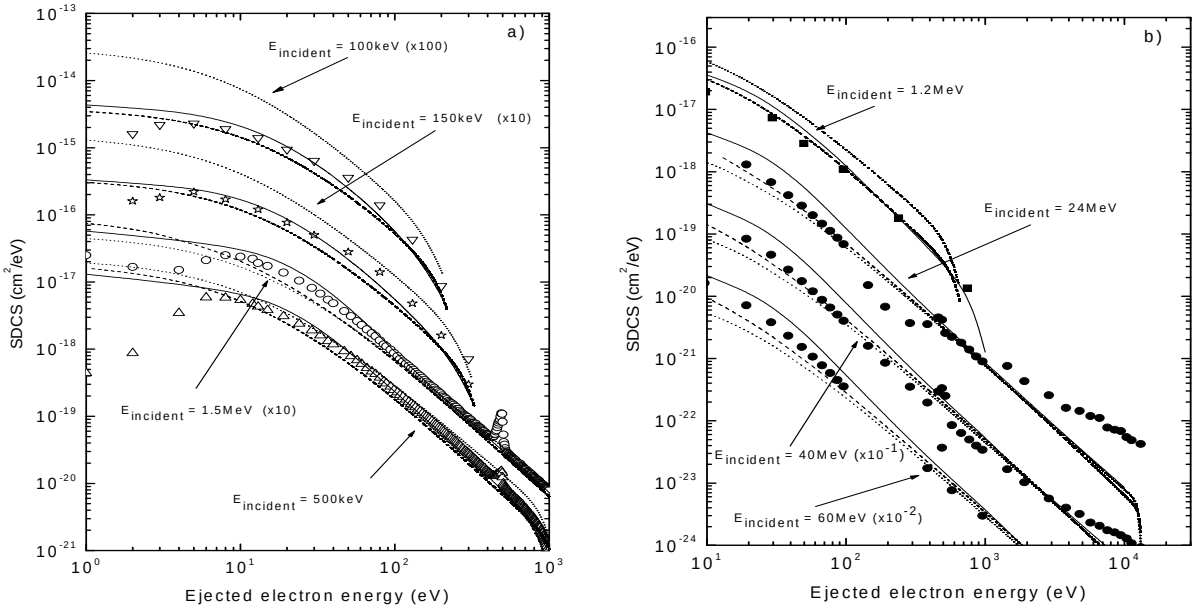

Figure 1. Singly differential cross sections for water vapour ionization by protons and α-particles (panel a and panel b, respectively). Comparison between our theoretical results (solid line) and those obtained in the HKS model (dashed line) and in the Rudd's model (dotted line). The experimental measurements are taken from different sources (see text for more details). Multiplicative factors have been used for clarity.

Figure 2 presents a comparison between our theoretical total cross sections obtained in the FBA-CW model and experimental data available in the literature for water ionization by protons and alpha particles. In the case of proton impact we observe that our model is able to reproduce with a good agreement all the existing experimental data taken from different sources [7,9,44] and also gives an excellent agreement with the theoretical results of Gervais *et al.* [45].

Fairly good agreement is also observed between our results and the experimental measurements for $^3He^{2+}$ (up triangles taken from [46]), and for $^4He^{2+}$ (circles taken from [12]). However, note that our FBA-CW model is not able to describe experimental data for proton energies lower than 100keV and for alpha particles energies lower than 200keV.

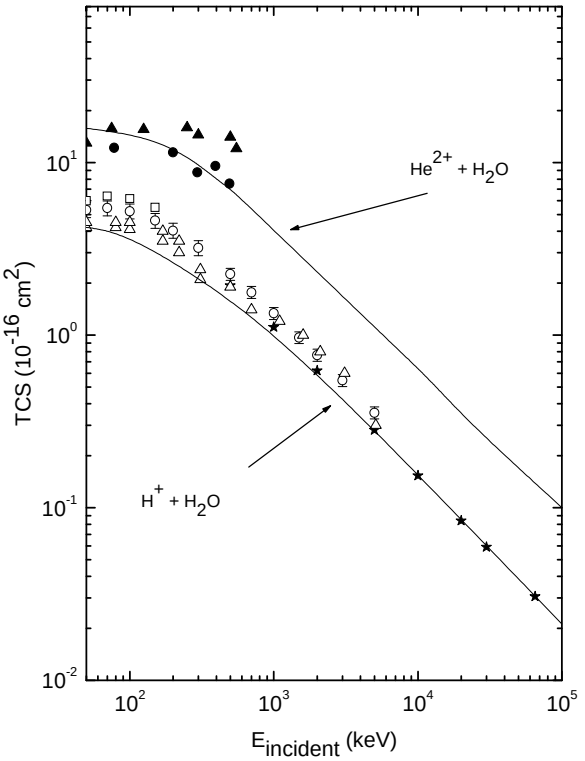

Figure 2. Total ionization cross sections of water vapour by protons and α-particles. Comparison between our theoretical results (solid line) and experimental data taken from different sources: solid up-triangles taken from [46] for $^3He^{2+}$ ions and solid circles taken from [12] for $^4He^{2+}$; for protons: open squares taken from [9], open up-triangles taken from [44] and open circles taken from [7]. The theoretical results of Gervais *et al.* [45] have also been reported for comparison (solid stars).

3.2. Electron collisions

In the figure 3, we have compared our theoretical results (solid line) to experimental data for three incident energy conditions: $E_{incident}$ = 100eV, 500eV and 1keV. We observe very good agreement between the experimental and the theoretical results, whereas large discrepancies may be observed (specially in the low incident energy range *i.e.* $E_{incident} \leq$ 100eV) between our results and the semi empirical ones (dashed line) given by Kim and Rudd [14,16] in the "binary-encounter-dipole" BED model (see Figure 3, panel a).

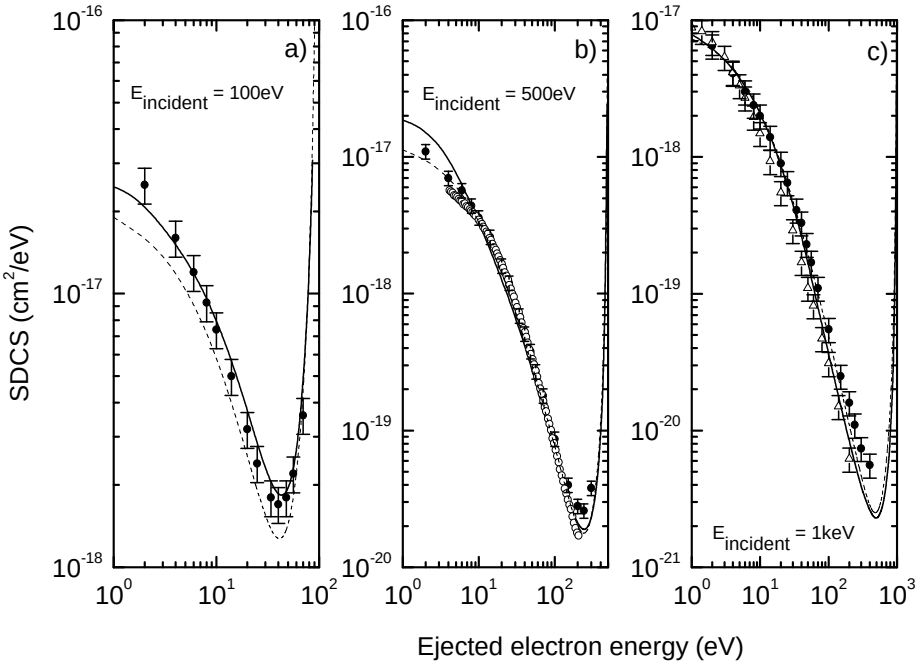

Figure 3. Singly differential ionization cross sections for water vapour by electrons. Panel a: $E_{incident}$ = 100eV. Panel b: $E_{incident}$ = 500eV. Panel c: $E_{incident}$ = 1keV. Comparison between our theoretical results (solid line) and those obtained in the BEB model (dashed line). The experimental data are taken from different sources: Opal *et al.* [5] (open circles), Bolorizadeh and Rudd [6,9] (solid circles) and Vroom and Palmer [47] (open triangles).

Total ionization cross sections are reported in Figure 4 and compared to an extensive set of experimental data covering a large range of incident energies $E_{incident}$ = 20eV-10keV. The experimental ionization cross sections reported are those of Bolorizadeh and Rudd [6] (solid circles), Djuric *et al.* [48] (solid down-triangles), Schutten *et al.*,[49] (solid up-triangles), Khare and Meath [50] (open down-triangles), Straub [51] (open up-triangles) and Olivero [52] (open diamonds). Although close agreement exists between some of the measurements of ionization cross sections over part of the energy spectrum, there is considerable variation in the range 50eV to 1keV. We have excluded the sets of experimental data of Gomet [53] and Orient and Srivastava [54] which deviate greatly from the other measurements. Also, we have not included results from experiments that did not provide data on an absolute scale [55]. On the theoretical side, we have reported the Kim and Rudd results [14,16] (dashed line), which are in good agreement with ours, essentially at low ($E_{incident} \leq$ 20eV) and high ($E_{incident} \geq$ 1keV) incident energies, but display sensitive differences for intermediate incident energies. The FBA-CW results are in very good agreement with the experimental data sets reported, and the overall behaviour of the TCS theoretical curve is well reproduced. In particular, we observe the expected maximum located at $E_{incident} \cong$120eV, which is in good agreement with the experimental data.

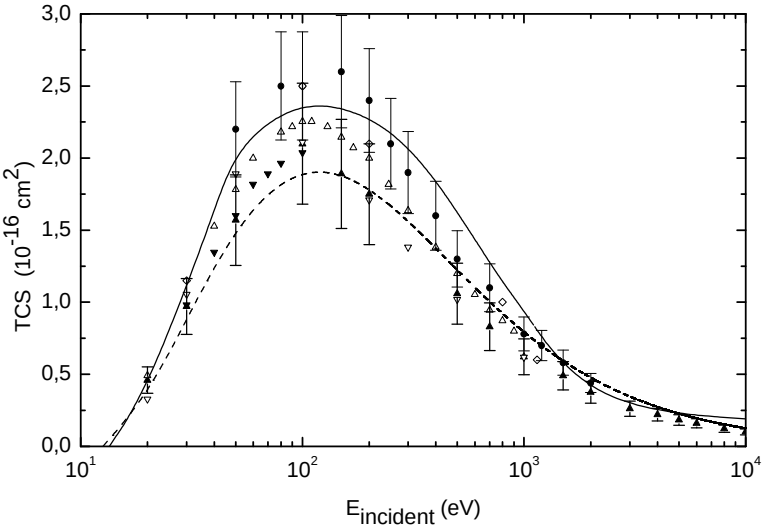

Figure 4. Total ionization cross sections of water vapour by electrons. Comparison between our theoretical results (solid line) and those obtained in the BEB model (dashed line). The experimental data are taken from different sources (see text for more details).

4. Conclusion

We have investigated in this work a full-differential theoretical approach to calculate doubly, singly differential and total ionization cross sections for electrons and light ions impinging a water molecule in its vapour phase.

Contrary to the simple analytical models available in the literature, our approach requires no experimental data for adjustment and is only based on a quantum-mechanical description of the charged particle-water interaction. In this kind of study, the water target is described by means of 5 molecular wave functions constructed from a linear combination of atomic orbitals in a self-consistent field (MO-LCAO-SCF).

Fair agreements are observed for the differential as well as the total ionization cross sections, for all the incident and ejected electron energies reported.

Finally, it is important to note that our theoretical approach may be easily introduced in numerical simulations such as Monte Carlo track structure code for electrons and light ions in water or in matter in general. Indeed, for these codes, multiple differential calculations represent useful input data to describe in detail all the ionizing events, in terms of energy deposits and angular distributions.

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