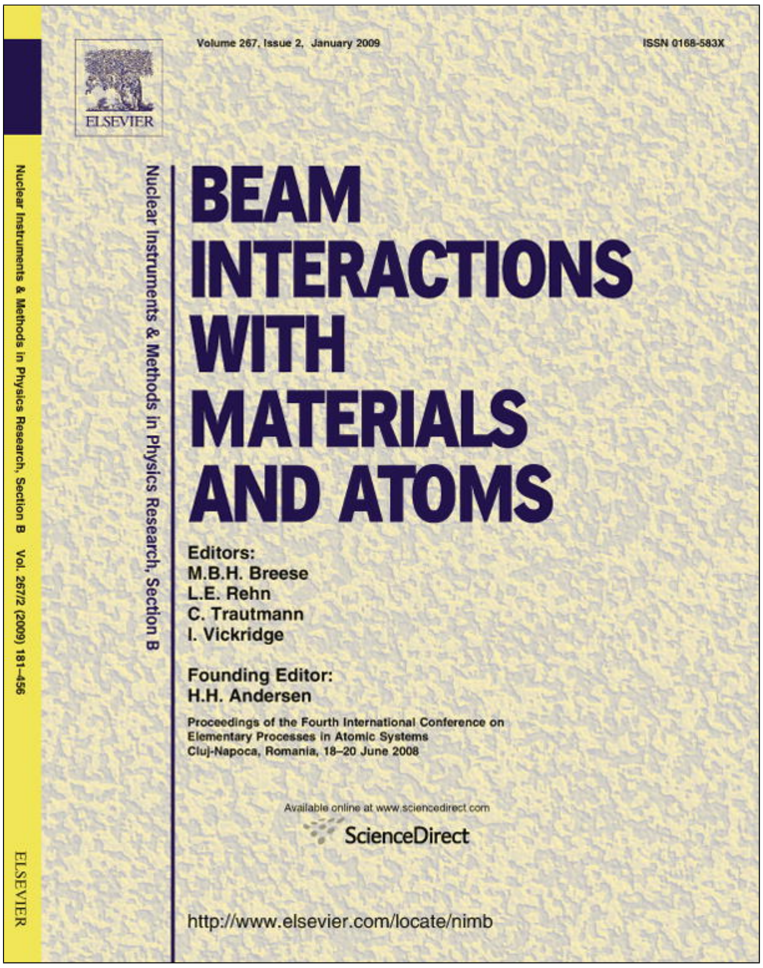
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Positron-impact ionization of atoms and molecules

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ABSTRACT

This paper presents the level of agreement between theory and experiment for positron-impact ionization of atoms and molecules. Distorted-wave theoretical models are able to reproduce the experimental integrated cross sections for atoms and diatomic molecules. The ECC phenomenon seen in the experimental triple differential cross sections can be obtained with a BBK-type model, but for very low impact energies the theory requires the inclusion of the coupling with the positronium formation channel.

1. Introduction

Positron interactions with matter play important roles in many physical processes of interest. Examples include the origin of astrophysical sources of annihilation radiation, the use of positrons in medicine (e.g. positron emission tomography); the characterization of materials; and the formation of antihydrogen, which is the simplest form of stable, neutral antimatter.

While the interactions of positrons with atomic targets have been studied for decades, this area is much less advanced, as compared, for example, with study of electron scattering processes, particularly at low energies. The reason for this is twofold. From an experimental viewpoint, positrons are much less common than electrons, and consequently techniques for using them to study scattering are less well developed. From a theoretical viewpoint, positron interactions with atoms and molecules are different in fundamental respects. In particular, the exchange interaction is absent, and a new process, the formation of positronium is believed to play an important role, either as an open or closed channel.

In this paper we are going to discuss the status of agreement between theory and experiment for positron-impact ionization of atoms and molecules. The earlier work dealt with the variation of the integrated cross sections with the positron-impact energy. Most results were reported for hydrogen, rare gas atoms and small molecules. Only recently has the intensity of the positron beams been sufficiently strong to perform triple differential cross sections (TDCS) measurements for the ionization of molecular hydrogen and helium.

2. Theoretical models

2.1. Integrated cross sections

A number of distorted-wave Born approximation (DWBA) models were explored in the study of positron-impact ionization of atoms and molecules. Our initial work [1] studied the effects of screening and distortion in various channels of the ionization system, but in a subsequent paper [2] we found that in the case of positron-impact ionization two phenomena require special attention: (i) the distortion of the positron wave in the incident and scattered channel and (ii) the interaction between the positron and the ejected electron in the final state of the system.

We introduced the following models, which proved to be the most successful in all cases studied. Models CPE (Coulomb plus plane waves with full energy range) and CPE4, which use plane waves to represent the incident positron and plane waves or coulomb waves to represent the scattered positron and the ejected electron according to the target charges shown in Table 1. In that table k_e, E_e, Z_e are the momentum, energy and target charge seen by the ejected electron, while k_f, E_f, Z_f correspond to the scattered positron. As the table shows, Z_e and Z_f seen by the outgoing particles depend on which of the scattered positron or the ejected electron is the faster particle.

Model DCPE (distorted-wave CPE) is similar to CPE except that the incident and the fast scattered positron are not plane waves but distorted waves in the atomic static field and polarization potential. The same difference is between models DCPE5 and CPE4.

The integrated cross sections calculation is described in detail in our paper corresponding to positron ionization of helium [1]. This theory becomes more complex in the case of molecular targets. First, the ejected electron wave function must be orthogonalized

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Table 1
Target charges seen by the ejected electron (Ze) and by the scattered positron (Zf)

	Z_e	Z_f
CPE	-1 for $k_e < k_f$ -2 for $k_e > k_f$	0 for $k_e < k_f$ 1 for $k_e > k_f$
CPE4	$-(1 - E_e/E_{ef})$ for $k_e < k_f$ -2 for $k_e > k_f$ $E_{ef} = E_e + E_f - 2(E_e E_f)^{1/2}$	0 for $k_e < k_f$ 1 for $k_e > k_f$

to the target wave function. Secondly, the molecular orbitals are represented as linear combinations of Gaussian-type atomic orbitals and are expanded in a Legendre series for linear molecules [3] and in spherical harmonics for CH_4 [4].

2.2. Triple differential cross sections

The methods used for the calculation of integrated ionization cross sections fail to reproduce the electron capture to the continuum (ECC) peak in the triple differential cross sections. For this study we used a model representing the final state with 3 Coulomb wave functions, similar to the Brauner–Briggs–Klar (BBK) approximation [5]. Our paper on positron ionization of molecular hydrogen [6] shows that this approach has significant numerical challenges. Moreover, the calculations are complicated by the need to account for the experimental angular and energy resolution.

3. Results and discussion

3.1. Integrated cross sections

In the study of integrated cross sections for hydrogen and rare gas atoms [2] the best agreement with the experiments are obtained with the model DCPE5, followed closely by model CPE4. We illustrate this agreement in Figs. 1 and 2 corresponding to argon and krypton, respectively.

As expected for distorted-wave calculations, their agreement with the experiment is not as good at very low impact energies

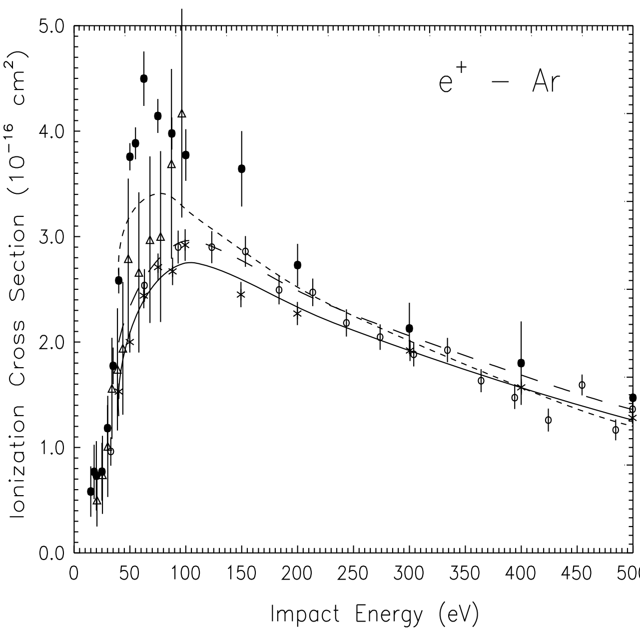

Fig. 1. Experiment: full circles [7]; empty circles [8]; triangles [9]; asterisks [10]. Theory: (—) DCPE5, (– – –) CPE4; (- - -) CPE [2].

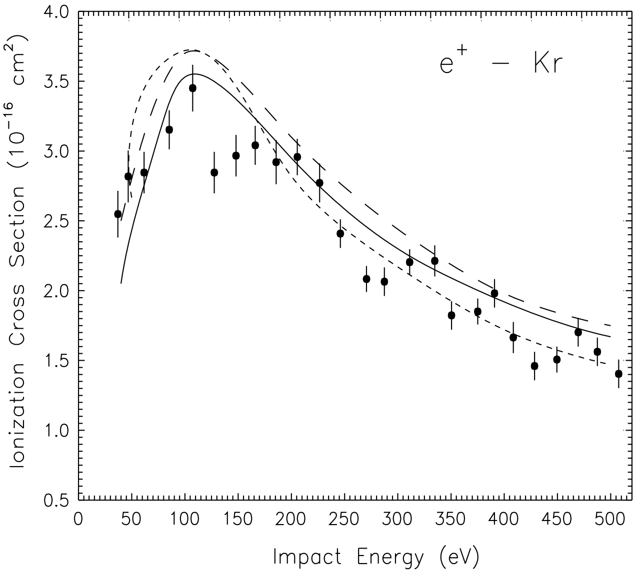

Fig. 2. Experiment: full circles [11]. Theory: (—) DCPE5, (– – –) CPE4; (- - -) CPE [2].

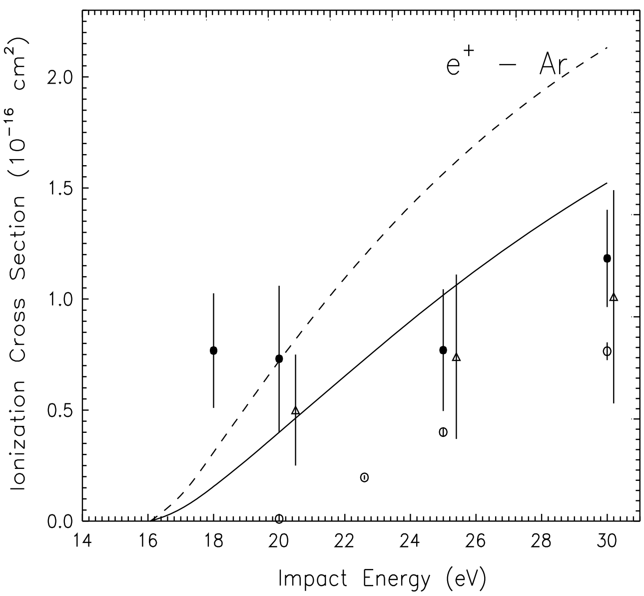

Fig. 3. Experiment: full circles [7]; triangles [9]; open circles [10]. Theory: (—) CPE4, (- - -) CPE [12].

[12]. Figs. 3 and 4 illustrate that CPE4 performs better than CPE even at very low impact energies.

Recently we employed our distorted-wave models in the study of the electron-impact ionization of atoms. We found that for electron-impact our distorted-wave models do not perform as well as for positron-impact ionization.

Fig. 5 shows the comparison of two of our models with the experiment for the electron-impact case. Our theory was modified to include the electron exchange [13]. This figure shows that the DCPE model overestimates the peak integrated cross sections, but does manage to predict the position of the peak. The CPE4 model does better than DCPE in terms of producing the correct size of the peak, but DCPE predicts better than CPE4 the position of the peak. Fig. 5 shows that the more elaborate theoretical approximations of [16,17] also overestimate the integrated ionization cross sections in the argon case.

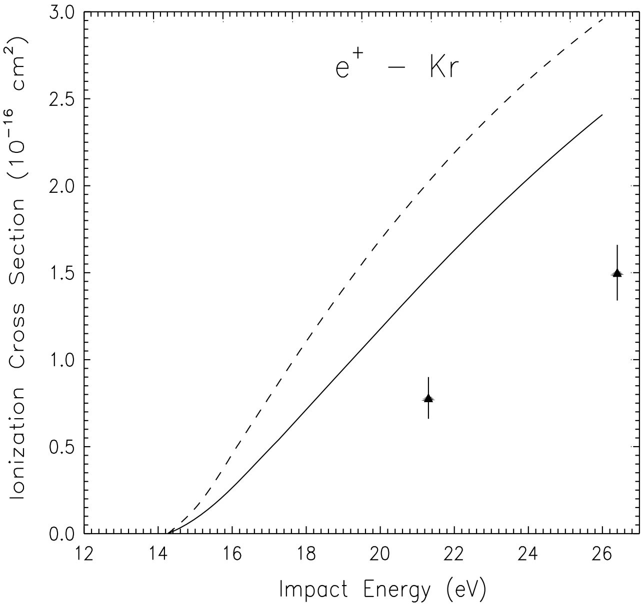

Fig. 4. Experiment: triangles [11]. Theory: (—) CPE4, (- - -) CPE [12].

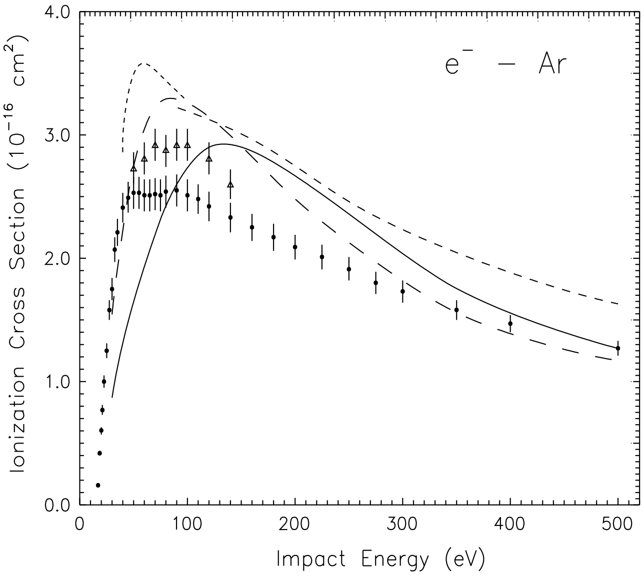

Fig. 5. Experiment: full circles [14]; triangles [15]. Theory: the solid line corresponds to CPE4, the long-dashed line to DCPE; the intermediate-dashed line corresponds to [16] and the shortest dashed line to [17].

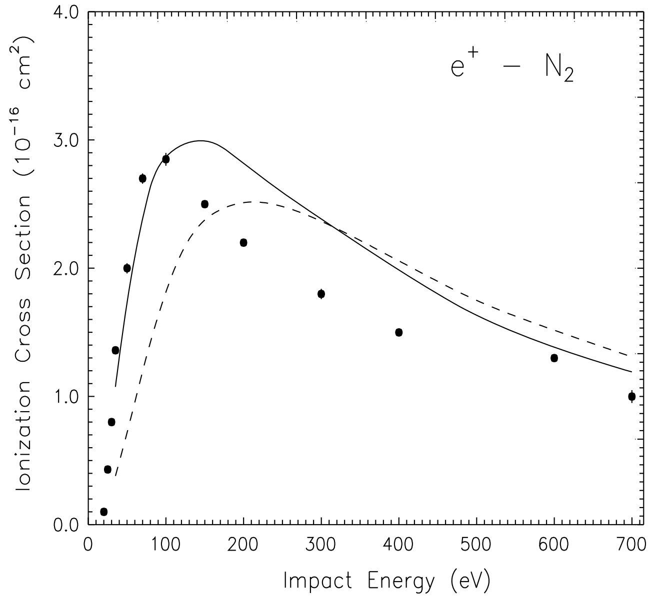

Fig. 6. Experiment: full circles [21]. Theory: (—) CPE, (- - -) CPE4 [19].

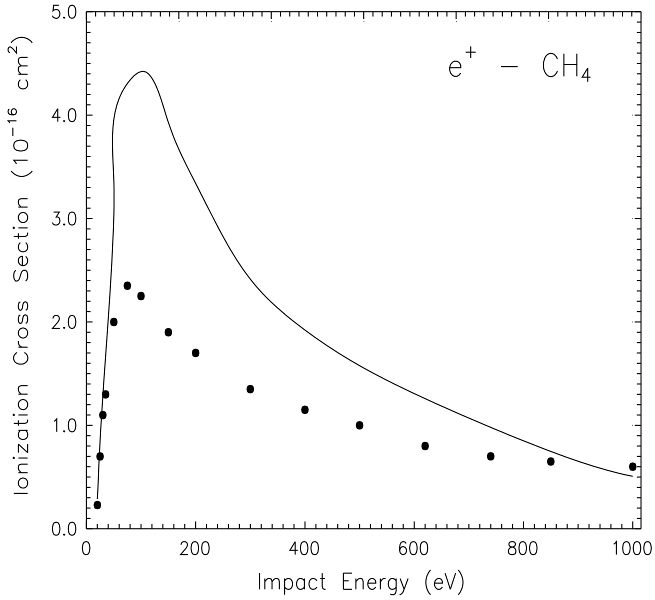

Fig. 7. Experiment: full circles [21]. Theory: (—) CPE [4].

Our distorted-wave models were also applied to the calculation of the integrated cross sections for positron-impact ionization of molecular targets. We obtained data for the following molecules: H_2 [3], O_2 [18], N_2 [19], CO, CO_2 [20] and CH_4 [4]. As in the case of atoms we obtained good agreement with the experiments for the diatomic molecular targets, but for the larger molecular targets our models failed to reproduce the experimental data.

Fig. 6 shows the level of agreement between our model calculations and experiment for N_2. Both models CPE and CPE4 are in fairly good agreement with the experiment, but CPE predicts the peak position much better than CPE4. It is interesting to note that for H_2 CPE4 produced data in better agreement with the experiment than CPE.

Fig. 7 illustrates the lack of agreement between our CPE model and the experiment in the CH_4 case. This kind of disagreement was also obtained for CO_2, which, unlike CH_4, is a linear molecule. It appears that for molecular targets larger than the diatomic molecules our approach using the CPE model and Gaussian representation of the target will significantly overestimate the integrated ionization cross sections.

3.2. Triple differential cross sections

We have studied positron-impact ionization of H_2 and He, two targets for which experimental data have recently become available. Figs. 8 and 9 illustrate the comparison of our MBBK (Molecular BBK) theoretical triple differential cross sections in the forward direction and the experimental data of Kover et al. [22,23] and Tokesi and Kover [24,25] for H_2. We also include the BBK data of Fiol et al. [27]. The experiments produced relative cross sections, while the theoretical curves correspond to data obtained after the convolution with the experimental angular and energy resolution. By

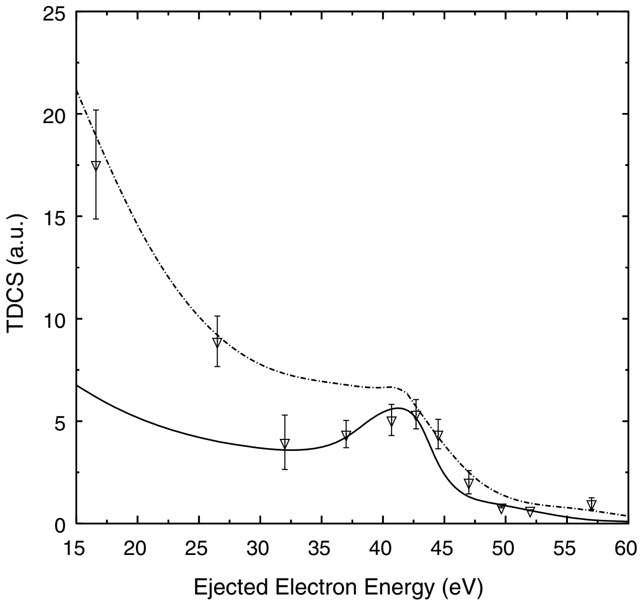

Fig. 8. TDCS for 100 eV incident energy. Experiment: triangles [22]. Theory: (—) MBBK [26], (---) BBK [27].

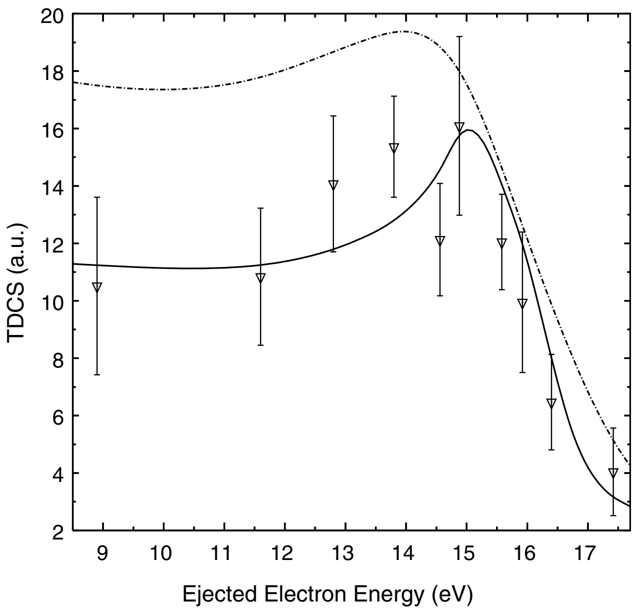

Fig. 9. TDCS for 50 eV incident energy. Experiment: triangles [23]. Theory: (—) MBBK [26], (---) BBK [27].

comparison to the BBK model used by Fiol et al., our MBBK model utilizes a Heitler–London type representation of the H_2 target.

Fig. 8 shows that for 100 eV incident energy our MBBK agrees best with the experiment for ejected electron energies higher than 30 eV, while BBK is in better agreement with the experiment at ejected electron energies lower than 30 eV.

Fig. 9 shows the results for 50 eV incident energy. In this graph the theoretical data was shifted by 1.6 eV to fit the position of the experimental peak. The most likely phenomenon responsible for the shift of the theoretical peak is the interaction between the direct ionization and the positronium formation channels, as suggested by Walters (see [29]). We did in fact get further support for this suggestion when we performed the same calculation in the helium case.

Fig. 10 shows our BBK calculations for He [28] compared to the relative experimental TDCS of Archidiacono et al. [29]. The full curve corresponds to a BBK calculation using an analytic fit to the Hartree–Fock helium wave function, while the dashed line corresponds to a hydrogenic representation of the helium atom. In the case of helium the theoretical curves were shifted by 2.66 eV to fit the position of the experimental peak. The larger shift in the helium case is due to the fact that the positronium formation has maximum probability for 45 eV positrons (which is very close to the 59 eV used in the ionization experiment), while in the case of H_2 it has maximum probability for 25 eV positrons.

All the above results correspond to zero ejected and scattering angles. Although there are no experiments measuring the TDCS at non-zero angles, we performed theoretical TDCS calculations at non-zero angles and we compared them against existing electron TDCS for the same energies and angles.

Fig. 11 presents a comparison of the TDCS data for positron and electron-impact ionization of H_2. The results shown in this figure correspond to coplanar asymmetric collisions. The MBBK electron data [30] are in excellent agreement with the relative experimental cross sections of [31]. Our MBBK positron data [32] are different from the electron data both in size and orientation. The binary peak corresponding to positron-impact is larger than the binary peak corresponding to electron-impact, while the opposite is true in the case of the recoil peaks. The explanation of this difference should be based on the changes in the electrostatic interactions in the ionization system. By replacing electron projectiles with positrons the electrostatic attraction between the projectile and the ejected electron increases the probability that the ejected electron escapes into the region of the binary peak and reduces the probability of escape into the region of the recoil peak.

Replacing electron projectiles with positrons has also an effect on the bending of the two peaks. For positron-impact the bending of both peaks is towards smaller ejected electron angles. More exactly, the bending relative to the momentum transfer direction occurs for both types of projectiles but in opposite directions. With the scattered angles very small, for positron projectiles the bending is in the forward direction and for electron projectiles in the backward direction.

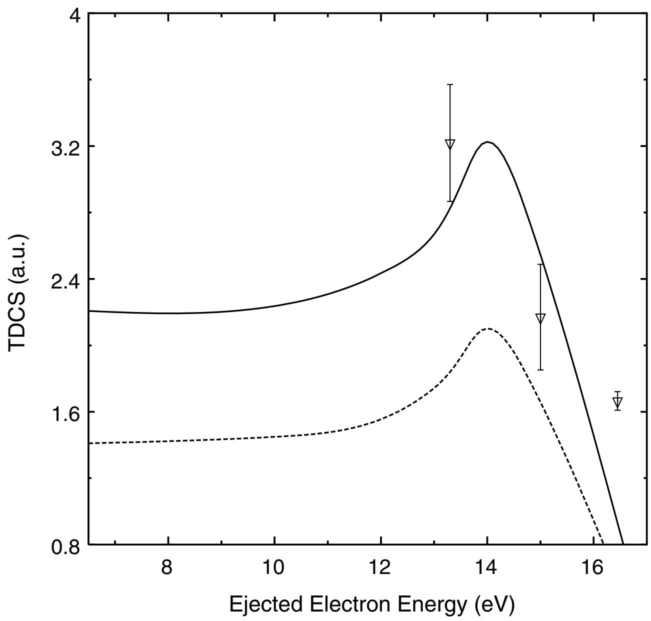

Fig. 10. TDCS for 59.16 eV incident energy. Experiment: triangles [29]. Theory: (—) Hartree–Fock helium wave function, (---) hydrogenic helium wave function [28].

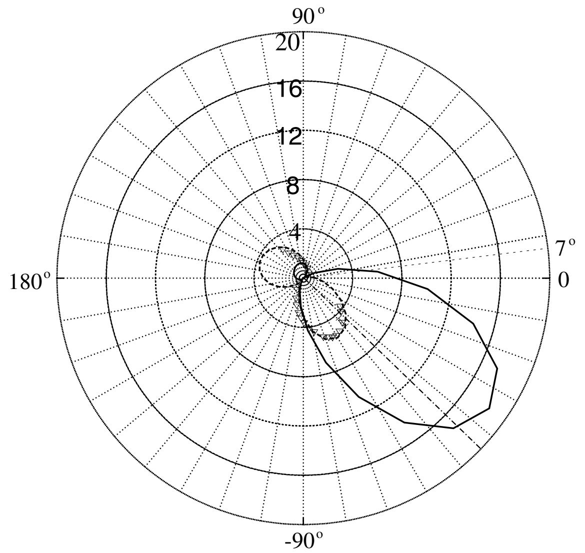

Fig. 11. TDCS for 59.16 eV incident energy, 4.5 eV ejection energy and 7° scattering angle. Experiment: [31]. Theory: (—) MBBK for positrons [32], (- - -) MBBK for electrons [30].

Fig. 11 predicts positron-impact TDCS data for non-zero scattering angles which are to be verified by experiments. These results can be used to calibrate future planned measurements [33].

4. Conclusions

We have performed calculations of integral and triple differential cross sections for positron-impact ionization of atoms and molecules for cases which were studied experimentally.

We conclude that our distorted-wave models produce integrated cross sections in reasonable agreement with the experiments for atomic and diatomic molecular targets. However, these models fail to produce good agreement with the experiments for electron-impact ionization of atoms and for positron-impact ionization of molecules containing more than two atoms.

Recent work on the triple differential cross sections for positron-impact ionization of H_2 and He showed that the use of a 3C model allows a good representation of the ECC phenomenon in the forward direction. A shift of the theoretical ECC peak for low positron-impact energies is most likely due to the absence of the coupling between the ionization and the positronium formation channels and this is a project that we plan to work on in the near future. Finally, we predict TDCS for non-zero scattering angles to be verified by future experiments.

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