Electron impact single and double ionization of magnesium

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Abstract. Electron impact single and double ionization cross-sections for magnesium have been calculated in the binary encounter model using accurate expression for $\sigma_{\Delta E}$ (cross-section for energy transfer ΔE) as given by Vriens. Hartree-Fock velocity distributions for the target electrons have been used throughout the calculations. In case of double ionization contributions of inner shell ionization and Auger emission have been included in the present work. The results obtained in case of single ionization are excellent and at the same time the double ionization cross-sections show reasonably good agreement with the recent experimental observations. Substantiation of the viewpoint of Peach, and Boivin and Srivastava that a vacancy in the 2p shell of magnesium leads to double ionization is a remarkable feature of the present investigation.

PACS. 34.80.Dp Atomic excitation and ionization by electron impact

1 Introduction

Electron impact ionization of atoms and ions is one of the most fundamental collision processes in atomic and molecular physics. Knowledge of ionization cross-sections for these processes finds wide applications in plasma kinematics problems, mass spectrometry, gas lasers, upper atmosphere physics and astrophysics. Ionization rates for various atomic species found in astrophysical plasmas are also of great interest. From an applied viewpoint, multiple ionization processes are important in moderate and high temperature plasmas and in all gaseous environments with an abundance of energetic electrons [1]. Magnesium atom is considered to be astrophysically important since its emission spectra have been recorded by several groundbased and space craft-based instruments [2,3].

Experimental investigations of ionization crosssections for metals lead to several difficulties and have been carried out only by very few experimental groups for limited number of elements. Recently accurate experimental measurements of electron impact single, double and triple ionization of magnesium have been carried out by Boivin and Srivastava [4] using a crossed beam technique in the energy range from the respective thresholds to 675 eV. The experimental data obtained by Boivin and Srivastava [4] could not be compared with previous theoretical calculations of double ionization cross-sections due to non-availability of the same in the literature. Following the observations of Peach [5] in the calculations of single ionization cross-section of magnesium, Boivin and Srivastava [4] have mentioned that single ionization of 2p shell of magnesium leads to double ionization as a consequence of Auger emission. This means that ionization of 3s shell only contributes to single ionization of magnesium. In this context it would be interesting to calculate both single and double ionization cross-sections of magnesium in order to compare the theoretical predictions with the experimental data.

Quantal calculations of single ionization cross-section of magnesium are available in literature [5–7]. Rigorous theoretical calculation of the double ionization crosssections becomes quite complicated as it involves the consideration of the four charged particles in the final channel interacting through the long range Coulomb potential [8]. Sophisticated calculations of the integrated double ionization cross-sections of atoms/ions by electron impact are not available in literature. As a consequence of this, semiempirical and semi-classical approaches have been developed for calculation of double ionization cross-sections. Fisher et al. [9], on the basis of available experimental data, demonstrated scaling laws of electron impact multiple ionization cross-sections and proposed expressions for calculations of cross-sections. In this approach atomic radius R has been put equal to $\gamma \langle r \rangle$ ($\langle r \rangle$ being the expectation value of the distance of the atomic electron from the centre of the nucleus) and γ has been calculated from the best fit of Gryzinski's formula [10] to experimentally determined cross-sections. Nearly at the same time Deutsch et al. [11] extended the semi-classical Deutsch-Mark formalism [12] to study double and triple ionization. Later on Belenger et al. [13] reported semi-empirical formula for calculation of double ionization cross-sections

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for neutral atoms, positive and negative ions. In this approach the shape of the cross-section is described by analytical expression and approximation parameters (constants) are estimated by fitting the model cross-sections to reliable experimental data. Recently, using classical binary encounter approximation Gryzinski and Kunc [14] have derived general analytical expressions for electron impact double ionization cross-sections of atoms with atomic number $Z \gtrsim 20$ and s or d outer shells with two electrons. They have compared their calculations only with experimental data for Ca, Sr, Ba and Hg atoms and found satisfactory agreement. This model is consistent and convenient but it treats the process of double ionization in the "Statistical" way. However, this model is not applicable in case of magnesium. Here we would like to mention that the wave functions representing the bound electrons are the characteristics of the target atom but there is no consideration of wave functions in the above mentioned calculations.

Now we would discuss the applications of the binary encounter approximation (BEA) in calculations of single and double ionization cross-sections. Gryzinski [10] carried out detailed investigations on applications of the BEA to different atomic collision processes. In context of electron impact ionization of atoms, he derived expressions for $\sigma_{\Delta E}$ and single ionization cross-section. Further, he proposed a double binary encounter model to describe the process of charged particle impact double ionization of atoms. According to this model the double ionization of atom may proceed via two alternative processes. In the first process the two electrons may be ejected from the atom by two successive encounters of the incident charged particle with the target electrons. Alternatively the incident particle may knock out only one atomic electron and the second electron is removed by the first ejected electron. The double ionization cross-sections corresponding to the two processes mentioned above are denoted by $Q_{\rm sc}^{ii}$ (scattered part) and Q_{ej}^{ii} (ejected part) respectively. Later on Vriens [15] found errors in Gryzinski's analytical expressions and obtained accurate expressions for $\sigma_{\Delta E}$ which are used frequently in calculations of single and double ionization cross-sections.

In the past the BEA has been used successfully in investigations of electron impact single ionization of atoms and ions [16,17]. In spite of certain unrealistic features in Gryzinski's [10] mathematical formulation for the process of double ionization, the idea of two double binary encounter processes has physical justification. These processes, in fact, correspond to the existence of correlation between the electrons of atoms and to the finite probability of the second Born process (see Vriens [18]). The model of Gryzinski was modified by Roy and Rai [19] with necessary corrections. Afterwards this modified model with some modifications was used in case of several atomic and ionic targets and satisfactory results were obtained [20–22]. Usually in these calculations Hartree-Fock and hydrogenic velocity distributions were used while considering the ejection of the first and the second target electrons respectively. Using this approach Chatterjee

et al. [23] reported double ionization cross-sections of magnesium only up to 200 eV impact energy. Gryzinski and Kunc [14] have discussed the works of Roy and coworkers [20, 22] in detail and pointed out their strengths and weaknesses. They have appreciated the estimation of the contributions of the p electrons from the next inner shell to double ionization of Ca, Sr and Ba atoms, prediction of acceptable magnitudes of the cross-sections for double ionization and appearance of the secondary peak in the cross-section. At the same time they have expressed the view that the use of hydrogenic velocity distribution while considering the ejection of the second electron, particularly from inner shells is physically not justified. Keeping the above mentioned facts in view, we have thought it worthwhile to apply the BEA using accurate expression for $\sigma_{\Delta E}$ and HF velocity distribution while considering ejection of the two electrons for calculation of direct double ionization cross-sections in the present investigation.

At this stage we would like to mention that correlation plays an important role in the double ionization process. Jha et al. [22] have discussed this aspect in detail with reference to calculations in the binary encounter approximation. One of the two binary encounter processes suggested by Gryzinski in which the first ejected electron knocks out the second electron partly takes into account electron-electron correlation (see Vriens [18]). Apart from this Hartree-Fock wave functions consider the electron-electron correlation to some extent through antisymmetrization (see Griffin and Pindzola [24]). Moreover, for fast projectiles the effect of electron-electron correlation may not be significant (see Deb and Crothers [25]). Undoubtedly the use of correlated wave function would be more accurate but in that case the aim of adopting a simplified approach will not be achieved. Thus the use of Hartree-Fock wave functions in the studies of direct double ionization processes using the BEA can be considered to be reasonable.

2 Theoretical methods

Electron impact double ionization cross-section including contribution from Auger emission can be written as

$$Q^{ii}(T) = Q_{\rm D}^{ii} + Q_{\rm A}^{ii}.$$
(1)

Here $Q_{\rm D}^{ii}$ denotes the contribution from direct ejection of the two electrons and $Q_{\rm A}^{ii}$ that from Auger emission. The expressions for the two processes leading to electron impact double ionization as given by Gryzinski [10] and modified by Roy and Rai [19] are

$$Q_{\rm sc}^{ii} = \frac{n_{\rm e}(n_{\rm e}-1)}{4\pi\bar{r}^2} \int_{U_i}^{E_q-U_{ii}} \sigma_{\Delta E} \\ \times \left[\int_{U_{ii}}^{E_q-\Delta E} \sigma_{\Delta E'} \,\mathrm{d}\left(\Delta E'\right) \right] \mathrm{d}\left(\Delta E\right), \qquad (2)$$

and

$$Q_{\rm ej}^{ii} = \frac{n_{\rm e}(n_{\rm e}-1)}{4\pi\bar{r}^2} \int_{U_i+U_{ii}}^{E_q} \sigma_{\Delta E} \\ \times \left[\int_{U_{ii}}^{\Delta E-U_i} \sigma_{\Delta E'} \,\mathrm{d}\left(\Delta E'\right) \right] \,\mathrm{d}\left(\Delta E\right).$$
(3)

Here $n_{\rm e}$ is the number of electrons in the shell under consideration, ΔE and $\Delta E'$ stand for energy transfer during the first and the second collisions respectively and \bar{r} denotes the mean distance between the electrons in the shell given by $\bar{r} = R/n_{\rm e}^{1/3}$ (*R* being the radius of the shell of the target atom). U_i and U_{ii} are the ionization potentials corresponding to ejection of the two electrons of the target. The symbol E_q represents the energy of the incident electron. Gryzinski obtained analytical expression for $Q_{\rm sc}^{ii}$ and $Q_{\rm ej}^{ii}$ by estimating the cross-section for the second collision for average value of energy transfer and assumed exponential velocity distribution for the target electron. These shortcomings have been removed in the work on double ionization by Roy and Rai [19].

In the present work we have used the accurate expression for $\sigma_{\Delta E}$ including exchange and interference as given by Vriens [15]. Following Catlow and McDowell [26], two dimensionless variables s and t defined by $s^2 = v_1^2/v_0^2$ and $t^2 = v_2^2/v_0^2$, where v_1 and v_2 are the velocities in atomic units of the incident and the target electrons respectively and $u = v_0^2$ is the ionization potential of the target in Rydbergs. All others energies involved have also been expressed in Rydbergs. Using these dimensionless variables $\sigma_{\Delta E}$ is given by (see Kumar and Roy [27])

$$\sigma_{\Delta E} = \frac{2}{(s^2 + t^2 + 1)u} \left[\left(\frac{1}{\Delta E^2} + \frac{4t^2u}{3\Delta E^3} \right) + \left(\frac{1}{(s^2u + u - \Delta E)^2} + \frac{4t^2u}{3(s^2u + u - \Delta E)^3} \right) - \frac{\phi}{\Delta E \left(s^2u + u - \Delta E \right)} \right]$$
(4)

where $\phi = \cos\{[1/(s^2u + u)]^{1/2} \ln s^2\}.$

The expressions for $Q_{\rm sc}^{ii}$ and $Q_{\rm ej}^{ii}$ have been integrated numerically over energy transfer and Hartree-Fock momentum distribution for ejection of the two electrons. Thus expressions (2,3) take the form

$$Q_{\rm sc}^{ii} = \frac{n_{\rm e}(n_{\rm e}-1)}{4\pi\bar{r}^2} \int_{t=0}^{\infty} \int_{U_i}^{E_q-U_{ii}} \sigma_{\Delta E} \\ \times \left[\int_{t=0}^{\infty} \int_{U_{ii}}^{E_q-\Delta E} \sigma_{\Delta E'} f(t) U_{ii}^{1/2} \,\mathrm{d}\left(\Delta E'\right) \mathrm{d}t \right] \\ \times f(t) U_i^{1/2} \,\mathrm{d}\left(\Delta E\right) \mathrm{d}t \times 8.797 \times 10^{-17} \,(\pi a_0^2) \quad (5)$$

and

$$Q_{\rm ej}^{ii} = \frac{n_{\rm e}(n_{\rm e}-1)}{4\pi\bar{r}^2} \int_{t=0}^{\infty} \int_{U_i+U_{ii}}^{E_q} \sigma_{\Delta E} \\ \times \left[\int_{t=0}^{\infty} \int_{U_{ii}}^{\Delta E-U_i} \sigma_{\Delta E'} f(t) U_{ii}^{1/2} \,\mathrm{d}\left(\Delta E'\right) \mathrm{d}t \right] \\ \times f(t) U_i^{1/2} \,\mathrm{d}\left(\Delta E\right) \mathrm{d}t \times 8.797 \times 10^{-17} \, (\pi a_0^2).$$
(6)

The symbol f(t) appearing in the above equations is the momentum distribution function for the target electron. Due to indistinguishability of electrons in the Vriens model $Q_{\rm sc}^{ii}$ and $Q_{\rm ej}^{ii}$ are exactly equal at all incident energies [27] and hence in order to obtain the double ionization cross-section, $Q_{\rm sc}^{ii}$ (or $Q_{\rm ej}^{ii}$) should be multiplied by two. In equation (5) u and s^2 have been replaced by U_i and E_q/U_i in expression for $\sigma_{\Delta E}$. In case of $\sigma_{\Delta E'}$ the corresponding replacements have been made by U_{ii} and $(E_q - \Delta E)/U_{ii}$ respectively. The only difference in equation (6) is that s^2 assumes the value $(\Delta E - U_i)/U_{ii}$ in expression for $\sigma_{\Delta E'}$.

The expression for single ionization cross-section Q^i is given by

$$Q^{i} = \int_{u}^{E_{q}} \sigma_{\Delta E} \,\mathrm{d} \,(\Delta E). \tag{7}$$

In terms of the dimensionless variables s and t discussed earlier, the expression for electron impact single ionization cross-section is given by (see Roy and Rai [16])

$$Q^{i}(s,t) = \frac{4}{(s^{2}+t^{2}+1)u^{2}} \left[\frac{s^{2}-1}{s^{2}} + \frac{2t^{2}}{3}\left(\frac{s^{4}-1}{s^{4}}\right) - \frac{\phi \ln s^{2}}{(s^{2}+1)}\right] (\pi a_{0}^{2}) \quad (8)$$

where $\phi = \cos\{[1/(s^2u + u)]^{1/2} \ln s^2\}.$

Expression (8) has been integrated numerically over the Hartree-Fock velocity distribution for the target electron and the final expression for the ionization crosssection reduces to

$$Q^{i}(s) = n_{\rm e} \int_{0}^{\infty} Q^{i}(s,t) f(t) u^{1/2} dt(\pi a_{0}^{2}).$$
(9)

In order to calculate Q_A^{ii} (contribution to double ionization cross-section from Auger emission) the expression (9) should be multiplied by a factor "a" (Auger yield of the shell under consideration). The momentum distribution function f(t) used in equations (5, 6, 9) is given by (see Catlow and McDowell [26])

$$f(t) = 4\pi t^2 u \rho_{nl}(t u^{1/2}). \tag{10}$$

Here

$$\rho_{nl} = 1/(2\ell + 1) \sum_{m=-\ell}^{m=+\ell} |\psi_{nlm}(\mathbf{x})|^2,$$

where

$$\psi_{nlm}(\mathbf{x}) = 1/(2\pi)^{3/2} \int \phi_{nlm}(\mathbf{r}) \mathrm{e}^{\mathrm{i}\mathbf{x}\cdot\mathbf{r}} \,\mathrm{d}\mathbf{r}$$

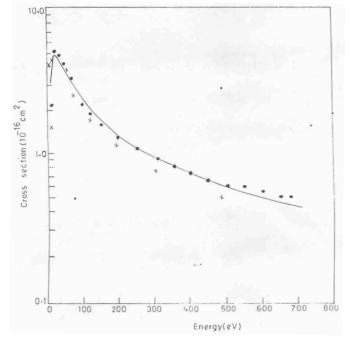


Fig. 1. Single ionization cross-section of Mg by electron impact (---) present results; (•) experimental data [4]; (×) calculations of Peach [5].

is the Fourier transform of the one electron orbital

$$\phi_{nlm}(\mathbf{r}) = N_{nl}R_{nl}(r)Y_{lm}(\Omega)$$

in which $R_{nl}(r)$ is the Hartree-Fock radial function. In equations (5, 6) f(t) has been constructed replacing u by U_i and U_{ii} for the ejection of the first and the second electron respectively.

We have considered total cross-section for electron impact direct double ionization as given by

$$Q_{\rm D}^{ii} = Q_{\rm D}^{ii} \left(3s, \, 3s\right) + Q_{\rm D}^{ii} \left(3s, \, 2p\right) + Q_{\rm D}^{ii} \left(3s, \, 2s\right) \qquad (11)$$

where $Q_{\rm D}^{ii}(3s, 2p)$ stands for the double ionization crosssection corresponding to one electron ejected from the 3s shell and the other from the 2p shell. The factor $n_{\rm e}(n_{\rm e}-1)/4\pi\bar{r}^2$ has been suitably modified for considering the last two modes of ionization. In these cases $n_{\rm e}(n_{\rm e}-1)$ has been replaced by $n_{\rm e1} \times n_{\rm e2}$ where $n_{\rm e1}$ and $n_{\rm e2}$ stand for the number of electrons in shells under consideration. In order to obtain the value of \bar{r} , the atomic radius has been replaced by the mean of the expectation values of radii of the shells. We have used orbital energies of shells of Mg $(2p^6 3s^2)$ and Mg⁺ $(2p^6 3s)$ as given by Clementi and Roetti [28]. The expectation values of radii reported by Desclaux [29] have been used as shell radii. Hartree-Fock radial wave functions given by Clementi and Roetti [28] have been used to construct the momentum distribution function f(t).

			single	ionization	$\operatorname{cross-sections}$	of
Mg in unit	$ts of 10^{-10}$	$^{6} {\rm cm}^{2}$.				

Energy (eV)	Contributions of $3s$ shell	Contributions of $2p$ shell	Total	Experiment [4]
10.0	3.15		3.15	2.1
20.0	4.79		4.79	5.08
30.0	4.48		4.48	4.73
40.0	4.00		4.00	4.23
50.0	3.56		3.56	3.73
60.0	3.20		3.20	3.31
70.0	2.90	0.08	2.98	2.96
80.0	2.65	0.15	2.80	2.66
90.0	2.44	0.20	2.64	2.42
100.0	2.26	0.23	2.49	2.21
120.0	1.97	0.26	2.23	1.89
140.0	1.74	0.27	2.01	1.67
160.0	1.56	0.28	1.84	1.51
180.0	1.42	0.28	1.70	1.38
200.0	1.30	0.28	1.58	1.28
250.0	1.08	0.27	1.35	1.08
300.0	0.92	0.25	1.17	0.92
350.0	0.80	0.24	1.04	0.79
400.0	0.71	0.23	0.94	0.72
450.0	0.64	0.21	0.85	0.68
500.0	0.58	0.20	0.78	0.65
550.0	0.53	0.19	0.72	0.61
600.0	0.49	0.18	0.67	0.56
650.0	0.46	0.18	0.64	0.52
675.0	0.44	0.17	0.61	0.51

3 Results and discussion

First of all we would like to discuss the energy state of Mg⁺ $(2p^5 3s^2 {}^2P)$ in context of the present work. Slater [30] estimated the energy of this state relative to the ground state of Mg and obtained a value of 4.1 Rydbergs. Peach [5] observed that this state lies above the threshold of double ionization which is at 1.667 Rydbergs and concluded that single ionization of magnesium occurs purely by the removal of 3s electrons and the ejection of a 2p electron results in the following Auger effect:

$$Mg^+(2p^5 \, 3s^{2\,2}P) \to Mg^{2+}(2p^{6\,1}S) + e.$$
 (12)

In the present work we have obtained single ionization cross-sections by considering ionization of 3s shell only. Direct double ionization and Auger effect have been considered in our theoretical results of double ionization crosssections. These calculations have been performed from respective thresholds to 675 eV using the method given in Section 2. Our results of single ionization cross-sections, calculations of Peach using Ochkur approximation and the experimental data have been presented in Figure 1. The contributions of 3s and 2p shell ionization to single ionization cross-sections have been shown separately in the Table 1 for the sake of comparison with experimental observations. The single ionization cross-sections considering ionization of 3s shell only are in excellent agreement

	Direct double ionization cross-sections						
Energy (eV)	Contributions of $(3s, 3s)$	Contributions of $(3s, 2p)$	Contributions of $(3s, 2s)$	2p single ionization	Total	Experiment [4]	
25.0	0.15				0.15	0.05	
30.0	0.44				0.44	0.12	
35.0	0.61				0.61	0.24	
40.0	0.70				0.70	0.32	
45.0	0.72				0.72	0.36	
50.0	0.72				0.72	0.38	
55.0	0.71				0.71	0.44	
60.0	0.68				0.68	0.54	
70.0	0.61			0.84	1.45	0.74	
80.0	0.55	0.03		1.53	2.11	0.94	
90.0	0.49	0.33		1.97	2.79	1.13	
100.0	0.44	0.59		2.27	3.30	1.31	
120.0	0.35	0.84	0.00	2.60	3.79	1.61	
140.0	0.29	0.91	0.03	2.75	3.98	1.86	
150.0	0.27	0.91	0.04	2.78	4.00	1.97	
170.0	0.23	0.88	0.05	2.81	3.97	2.14	
180.0	0.21	0.86	0.05	2.81	3.93	2.20	
200.0	0.18	0.80	0.06	2.79	3.83	2.30	
250.0	0.13	0.67	0.06	2.67	3.53	2.41	
300.0	0.11	0.55	0.05	2.53	3.24	2.40	
350.0	0.09	0.46	0.04	2.40	2.99	2.36	
400.0	0.07	0.39	0.04	2.27	2.77	2.31	
450.0	0.06	0.34	0.03	2.14	2.57	2.26	
500.0	0.05	0.29	0.03	2.03	2.40	2.18	
550.0	0.05	0.26	0.03	1.93	2.27	2.09	
600.0	0.04	0.23	0.02	1.84	2.13	2.00	
650.0	0.03	0.20	0.02	1.76	2.01	1.92	
675.0	0.03	0.19	0.02	1.72	1.96	1.86	

Table 2. Electron impact double ionization cross-sections of Mg in units of 10^{-17} cm².

with experiment and are found to be better than the corresponding calculations of Peach [5] in the Ochkur approximation. The peaks which appear at the same impact energy 20 eV in our calculation and experiment are of magnitudes 4.79×10^{-16} cm² and 5.08×10^{-16} cm² respectively. It can be seen that the cross-sections considering the ionization of 3s shell only are in better agreement with experiment than those including ionization of 2p shell.

The results of double ionization cross-section along with the experimental data obtained by Boivin and Srivastava [4] have been shown in Figure 2 and Table 2. The contributions to direct double ionization from ejection of (3s, 3s), (3s, 2p) and (3s, 2s) electrons have been shown separately in Table 2. We have presented single ionization cross-sections of 2p shell in a separate column in order to show contributions of Auger emission. Keeping in view the dominant contribution of Auger emission and non-availability of the Auger yield in the literature, we have assumed the Auger yield to be unity. In low energy region close to threshold our calculations overestimate the cross-sections (being within a factor of 3.7) but in the region 45-60 eV the present results are within a factor of two of the experimental data. This can be regarded as success of the present method for theoretical calculations of direct

double ionization cross-sections. The discontinuity in the double ionization cross-section curve observed experimentally is obtained in our calculations at about 60 eV impact energy due to onset of Auger emission. Beyond 70 eV impact energy the contributions from Auger effect dominate and with increase in energy these contributions become larger and larger as compared to direct double ionization cross-sections. At energies higher than 450 eV it is found that the direct double ionization cross-sections are less than one fifth of the contributions of the Auger effect. It is clear from the Table 2 that our calculated results of direct double ionization cross-sections differ very much from the experimental data and the inclusion of the contributions of Auger effect brings the present results in reasonably good agreement with experiment.

A critical comparison of our calculated results with experimental observations shows that in the energy range 75–150 eV the present results differ from the experimental values by a factor slightly more than two. The maximum discrepancy is observed in the region 90–100 eV where our theoretical results and experimental observations differ by a factor of 2.5. Boivin and Srivastava [4] have observed a peak of magnitude 2.406×10^{-17} cm² at about 250 eV impact energy whereas a peak of

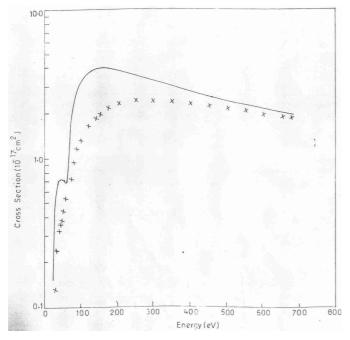


Fig. 2. Double ionization cross-sections of Mg by electron impact (--) present results; (\times) experimental data [4].

magnitude 4.00×10^{-17} cm² at about 150 eV is obtained in the present calculations. Thus the magnitude of the calculated peak shows a satisfactory agreement with that found in experiment but its position is considerably shifted towards low energy side. These discrepancies may be partly attributed to overestimation of 2p single ionization crosssections at low incident energies with respect to ionization threshold of 2p shell. Beyond 150 eV impact energy the calculated results are within a factor of 2 of the experimental data throughout the energy range investigated. We find that with increase in energy the agreement of our calculated results becomes better and better with experiment. It is remarkable that above 350 eV impact energy the calculated results are in excellent agreement with experimental data and lie within a factor of 1.25.

4 Conclusions

From the discussion given above it is apparent that electron impact single ionization cross-sections of magnesium are well explained by considering ionization of 3s shell only. It is also concluded that the present method gives reasonably accurate values of direct double ionization cross-sections. It has been found that the calculated results of direct double ionization cross-sections cannot explain the experimental observations in the energy region where indirect processes are effective. It is clearly observed that inclusion of contributions of Auger effect brings the calculated results in reasonably good agreement with experimental observations. Substantiation of the viewpoint of Peach [5] and Boivin and Srivastava [4] that a vacancy in the 2p shell of magnesium leads to double ionization is an interesting feature of our calculations.

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