© 2019 IJSRST | Volume 6 | Issue 6 | Print ISSN: 2395-6011 | Online ISSN: 2395-602X
Themed Section: Science and Technology
DOI : https://doi.org/10.32628/IJSRST

Double Capture Cross Sections of Magnesium by The Impact of Fast Proton

Akhilesh Kumar Gupta[1], L. K. Jha[2]
[1]Department of Physics, Patna Science College, Patna University, Patna, Bihar, India
[2]Department of Physics, B.R.A. Bihar University, Muzaffarpur, Bihar, India

ABSTRACT

Theoretical calculations of capture cross sections of magnesium by the impact of proton have been calculated using modified Binary Encounter Approximation (BEA). In the present calculation we have consider the impact energy range 90keV/amu-1000KeV/amu for which experimental data is available in the literature. The calculated results of capture cross-sections of Mg atoms are in good agreement with the experimental observations. We have used Hatree-Fock (HF) velocity distribution function in present calculation.

Keywords : Proton impact, Electron Capture, Double capture cross sections.

I. INTRODUCTION

When a positively charged particle incident on atoms or molecules there is a possibility that projectile capture an electron of the target atoms. The capture cross section is estimated in several cases for ion-atom collisions. [1-3]. The projectile with different impact energies interact with the target electron and the capture cross sections study suggests about different electronic states and the coupling of electrons. Charge transfer and exchange reaction in several kind of ionic/atomic collisions are of great importance due to their wide utility in controlled thermo-nuclear fusion, ion penetration in solids, radiation physics, astrophysics and many more. Apart from these charge transfer reactions are particularly important in influencing certain lines spectra in atmosphere. A theory proposed by Oppenheimer-Brikman-Kramers (OBK) for the calcution of electron capture cross-sections due to omission of nucleus-nucleus (n-n) interaction. The several approaches like continuum distorted wave (CDW), Belkie and Gayet Crothers and Todd and Crothers (1981), fixed scattered approximations by Roy and Ghosh (1979), the multi state perturbation stationary state approximation of Crothers and Hugges and impact parameter method of Morrison and Opik, were implemented for the study of electron capture processes.

An important method of healing and fueling a Tokomak Fusion Plasma is by injection of energetic H or D atmos, some cases helium in velocity range 3×10^8 cm/s -5×10^8 cm/s [4]. The application of charge changing process in the formation of vacuum Ultra-Violet radiation and X-Rays [5] and the investigations of solar corona [6] involved the electron capture processes [7]. Charge changing processes provide valuable information about design of radiation detector, radiation damage, production of negatively charged ions in applied accelerator technology particularly in design of accelerator and thermos-nuclear fusion. Charge changing process is particularly important in plasma diagnostics (see

McDowell and Ferendeci [8], Jochain and Post [9]). Owing to the large number of applications and interest of the workers in the field of collisional physics, the interest has rapidly grown in study of charge transfer phenomenon in recent decades. Electron captures, basic mechanism of rearrangement collision is rather a complicated problem and so its experimental and theoretical studies are a notable concern. Apart from different complexities intricate in the electron capture and charge changing mechanism due to the collision of different positively charged particles, several theoretical as well as experimental works have been done. In recent past Bates and McCarrol [10] Bransden [11], Bates and Kigston [12], Mapleton [13-16], Biswas et al. [17] , F. Fremon [18], Basu et al. [19], Amaya-Tapiya et al [20] etc. have reviewed the theoretical investigations of charge exchange processes in different quantal and semi quantal approximations.

Due to mathematical complexities and numerical challenges fully quantal and semi classical calculations of capture cross section are limited to the lighter target only. For this reason, it has been always a great matter of interest in thinking and developing for ion-atom collisions based on classical picture and model. These models are supposed to provide information about cross sections of moderate accuracy. Among the classical models, The Classical Trajectory Monte Carlo (CTMC) and Binary Encounter Approximation have been found in high degree of success for the theoretical investigation of ion-atom collision process.

Thomas [21] proposed a theoretical classical model in 1927 improved and extended by Bates and Mapleton [22] and Mapleton [13-16]. Two Binary Encounter theories (the original as good as modified), one between incident positive charge and the atomic target electron and next the interaction between ejected electron and target nucleus have been taken in consideration for electron capture. Original and modified model of Thomas [21] in found to give reliable estimate for electron capture cross-section from heavy atoms by energetic light nuclei. Bates and Snyder [23] proposed a classical model for electron capture involving single binary encounter between projectile (ionic) and target electron. Later on, a classical model for charge-changing with single binary encounter was proposed by Gryzinski [24] and in recent past Roy and Rai [25] given a new limit for energy transfer △E using Thomas [21] condition. In the present work, Modified Binary Encounter Approximation (BEA) is proposed for the calculation of electron capture from the atomic target. This method is based on Gryzinski Double Binary Encounter model and Thomas (1927) theory following the conditions for the electron capture in the estimation of electron capture cross-sections.

II. THEORETICAL CONSIDERATION

When a positively charged, particle is allowed to collides with target electron/ atomic electron it gets ejected providing the energy transfer ΔE greater thean the electronic binding energy. Taan and Lee (1981) based on Thomas (1927) second condition, proposed a theoretical framework for the calculation electron capture cross section by the impact of positively charged particle. This is shown that on the impact of positively charged particle to the target electron, ejected electron will be captured by the projectile satisfying the following condition.

$$F(\Delta \mathrm{E}, \theta) = (\Delta \mathrm{E} - \mathrm{U}) + \frac{1}{2}mV^2 - V[2m(\Delta E - U)]^{1/2}\, COS\theta - g < 0 \qquad (1)$$

Where $g = Ze^2/(\frac{rU}{V})$ and θ is the angle between impact velocity (V) and the velocity of the ejected electron. r is the shell radius, Ze represents charge on the projectile, m is electronic charge, U is given for the binding energy of the electron and $u = \sqrt{V^2 + v^2}$ where v is the velocity of the bound electron.

In case of $\Delta E > U$ and $F(\Delta E, \theta) > 0$ electron capture by the projectile will not take place but, the electron will be eject and left free directing to impact ionization. Following two conditions will be achieved during the ion-atom impact. Firstly, charge transfer and impact ionization both will take place if $\frac{1}{2}mV^2 > g$ in the energy transfer range $\Delta E_1 \leq \Delta E \leq \Delta E_u$ and $0 \leq \theta \leq \theta_m < \frac{\pi}{2}$. Secondly, impact ionization will take place only for energy transfer $U \leq \Delta E \leq \Delta E_1$ and $\Delta E_u \leq \Delta E \leq E$ where E being maximum energy imparted to the target bound electron by the projectile. ΔE_u , ΔE_1 and θ_m are expressed by (Tan and Lee 1981)

$$\Delta E_{1,u} = U + \frac{1}{2}mV^2 + g \mp V(2mg)^{\frac{1}{2}} \quad (2)$$

$$cos\theta_m = [1 - g/(\frac{1}{2}mV^2)]^{1/2} \quad (3)$$

For energy transfer $\Delta E_1 \leq \Delta E \leq \Delta E_u$, a correction fraction $C = \frac{1}{2}(1 - cos\theta_m)$ in case of charge transfer on the projectile impact. In this case the electron capture cross-section and impact ionization is given by

$$\sigma_{cap} = n_e C \int_{\Delta E_1}^{\Delta E_u} \sigma_{\Delta E}\, d(\Delta E) \quad (4)$$ and

$$\sigma_{ion} = n_e \left(\int_{U}^{\Delta E_u} \sigma_{\Delta E}\, d(\Delta E) + (1 - C) \int_{\Delta E_1}^{\Delta E_u} \sigma_{\Delta E}\, d(\Delta E) + \int_{\Delta E_1}^{\Delta E} \sigma_{\Delta E}\, d(\Delta E) \right) \quad (5)$$

where, $\sigma_{\Delta E}$ represents cross-section for energy transfer ΔE to the bound electron and n_e number of eqivalent electron in the shell.

The electron capture process may also take place in case of $\frac{1}{2}mV^2 < g$ even if $\triangle E < \triangle E_1$ (see Tan and Lee 1981) and therefore the capture cross section and impact ionization is given as

$$\sigma_{cap} = n_e \left(\int_{U}^{\Delta E_u} \sigma_{\Delta E}\, d(\Delta E) + \frac{1}{2} \int_{\Delta E_1}^{\Delta E_u} \sigma_{\Delta E}\, d(\Delta E) \right) \quad (6)$$

and $$\sigma_{ion} = n_e \left(\frac{1}{2} \int_{\Delta E_1}^{\Delta E_u} \sigma_{\Delta E}\, d(\Delta E) + \int_{\Delta E_u}^{E} \sigma_{\Delta E}\, d(\Delta E) \right) \quad (7)$$

The details outline and theoretical description of calculation electron capture cross-section is provided by Roy and Rai [25] introducing two dimensionless variables s and t (See Catlow and Mc. Dowell) where, $s^2 = \frac{v_1^2}{v_0^2}$ and $t^2 = \frac{v_2^2}{v_0^2}$. $v_0^2 = U_i$ is the target binding energy in rydbergs v_1 and v_2 are the velocities of incident particle and target electron respectively in atomic units. The lower and upper energy limits for the electron capture can be given as

$$\Delta E_l = (s^2 + 1)U_i + g - 2s(U_i g)^{\frac{1}{2}} \quad (8)$$

$$\Delta E_u = (s^2 + 1)U_i + g + 2s(U_i g)^{\frac{1}{2}} \quad (9)$$

where $$g = {2zs}\Big/{r(s^2 + t^2)^{\frac{1}{2}}} \quad (10)$$

Corresponding to various values of E_l and E_u, the expressions for cross-sections denoted by $Q(s,t)$ can be determined by integrating Vriens expression for $\sigma_{\Delta E}$ (See Chatterjee and Roy [26] also Tan and Lee [27-28]).

Due to the angular divergence the correction factor for the solid angle is given as

$$c = \frac{1}{2}\left\{1 - (1 - \frac{g}{s^2 u})^{\frac{1}{2}}\right\} \quad (11)$$

The different conditions for the possibility of electron capture, energy transfer by the projectile to the atomic target limit E_l and E_u is explained by chatterjee and Roy [26] relative to the value of s , $4su(s-t)$ and $4su(s+t)$. The expression for the electron capture so obtained is integrated over Hartree-Fock (HF) velocity distribution for the target electron of the shell in considerations. Equation for the electron captures given as

$$Q(s) = n_e \int_0^\infty Q(s,t)\, f(t) U^{\frac{1}{2}} dt \qquad (12)$$

where $f(t)$ is momentum distribution function n_e is the number of equivalent electrons in the shell.

The final expression for the electron capture may be obtained by multiplying the expression of $Q(S)$ by solid angle correction factor C as

$$Q = Q(s) \times c \qquad (13)$$

Hartree-Fock (HF) radial function is given by Clementi and Roetti [29]. Also, Shell radii the quantum mechanical values of the maximum radial probability density reported by Lotz [30] and Desclaux [31].

III. RESULT AND DISCUSSION

The present theory is based on the method proposed by Tan and Lee [27-28] for calculation of electron capture cross-sections for atoms due to impact of fast light nuclei and the work of Chatterjee and Roy [26] on the BEA calculations of double electron capture cross-sections from atoms due to impact of light multi charged nuclei. The experimental result for double electron capture is reported by Shah et al. [32]. The double electron captures cross sections have been calculated due to proton impact energy range 90 KeV/amu-1000 KeV/amu. In the present calculation the contributions of the electron capture are considered from (3s, 3s), (3s, 2p) and (3s, 2s) shells respectively. The theoretical observation indicates that (3s, 2p) shells having major contributions in capture cross-sections. At the impact energies 90 KeV/amu, 110 KeV/amu, 130 KeV/amu and 150 KeV/amu the ratio of theoretical to experimental observation is 2.6, 1.89,1.62 and 1.55 respectively. In the intermediate energy range (170 KeV/amu-280 KeV/amu) the calculated results of double electron capture cross section is in agreement with experimental data. From the theoretical observation this is reflected that double electron capture process by the impact of proton with Mg atoms is prominent in intermediate energy range and the capture of both the electrons from the shell 3s and 2p dominates. At the higher impact energies, the capture cross section reduces and the ionization probability increases.

The double ionization process is supposed to take place via two successive encounters between incident ion and the target atom. In the first binary encounter the projectile with energy E_q transfers energy ΔE to one of the bound electrons; as a result of which the electron is emitted into free space leading to impact ionization. The projectile with remaining energy $(E_q - \Delta E)$ makes a second binary encounter with the residual target capturing one of its electrons.

In transfer ionization process by an ion incident on atomic target, after the ionization of the target in the first process, if the collision is slow, the target will get sufficient time for rearrangement and therefore for the second process the binding energy, the radius and momentum distribution function of the target ion can be used. However, in case of fast collision the target will not get sufficient time for rearrangement and the values of the binding energy, the radius and the momentum distribution function of the neutral atom would be proper choice.

The capture cross-sections by the impact of fast proton with Mg atoms have been estimated theoretically using method described in the previous section. For these calculations the binding energies and the momentum distribution function for the target electrons have been computed using the Hartree-Fock radial function given by Clementi and Roetti [29]. Shell radii the quantum mechanical values of the maximum radial probability density reported by Lotz [30] and Desclaux [31] have been taken into account. The calculated capture cross-sections for Mg atoms due to impact of proton and the experimental results of Shah *et al.* [32] have been compared and shown in Figure and Table.

Table : Proton impact double capture cross-sections of Mg in units of 10^{-17} cm^2

Energy (eV)	Contributions Of (3s, 3 s) shells	Contributions Of (3s, 2p) shells	Contributions Of (3s, 2s) shells	Total	Expt [32]
90	0.108	6.098	0.300	6.506	2.42±0.11
110	0.046	4.255	0.216	4.517	2.38±0.13
130	0.022	3.120	0.161	3.303	2.03±0.10
150	0.012	2.324	0.121	2.457	1.88±0.12
170	0.007	1.750	0.091	1.848	1.63±0.09
190	0.004	1.329	0.070	1.403	1.33±0.09
210	0.002	1.020	0.053	1.075	1.21±0.08
240	0.001	0.697	0.037	0.735	0.98±0.06
280	0.000	0.433	0.023	0.456	0.66±0.04
330	0.000	0.250	0.013	0.263	0.48±0.03
500	0.000	0.167	0.009	0.176	0.37±0.02
570	0.000	0.095	0.005	0.100	0.24±0.02
650	0.000	0.053	0.002	0.055	0.155±0.11
750	0.000	0.031	0.001	0.032	0.105±0.010
870	0.000	0.018	0.001	0.019	0.069±0.005
1000	0.000	0.003	0.000	0.003	0.012±0.001

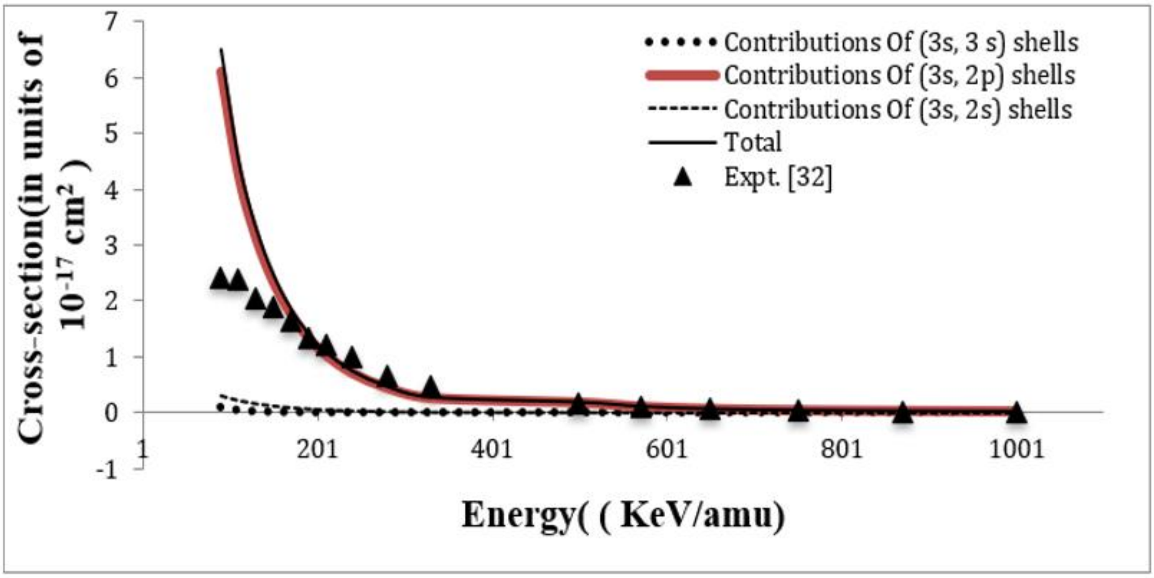

Figure : Double electron capture cross-section by impact of proton for Mg atoms.

Proton impact the present results and the experimental observations are in reasonably good agreement and it is observed that at low input energies the calculated cross-sections are higher than the experimental values. With the increase of energy values, the calculated cross-sections come closer to the experimental values. At impact energy 170 keV/amu, 190 KeV/amu and 120 KeV/amu the theoretical cross sections are 1.84 x 10^{-17} cm^2, 1.40 x 10^{-17} cm^2 the 1.0 x 10^{-17} cm^2 respectively, which is almost same as the theoretical results.

IV. CONCLUSION

The theoretical calculation of proton impact electron capture cross-section of Mg atoms is in very good agreement with the experimental observation throughout. In intermediate energy range theoretical result is becoming more and more prominent. This is also noted that BEA having high degree of success in the theoretical study of charge changing processes and also give viable theoretical description for the justification of experimental observations.

V. REFERENCES

[1] F. P. Ziemba, G. J. Lockwood, G. H. Morgan, and E. Everhart, Phys. Rev. 118, 1552 (1960)

[2] G. J. Lockwood and E. Everhart, Phys. Rev. 125, 567 (1962)

[3] P. R. Jones, P. Costigan, and G. Van Dyk, Phys. Rev. 129, 211 (1963)

[4] M. Purkit, S. Sounda, A. Dhara, C. R. Mandal, Phys. Rev. A 74, 042723 (2006)

[5] A.V. Vinogradov and I.Sobelman, Sov.Phys JEPT 36, 115(1973)

[6] J. E. Bayfield and G.A. Khayrallah, Phys. Rev. A 11, 920(1975)

[7] D. Basu and S.C. Mukherjee and D. P. Sural, Phys. Reports 42C,145(1978)

[8] M. R. C. McDowell and A. M. Ferendeci, Atomic and Molecular Processes in controlled thermonuclear fusion (Plenum, London, 1980).

[9] C. J. Jochain and D. E. Post, "Atomic and molecular Physics of controlled thermonuclearfusion", (Plenum, London, 1983).

[10] D. R. Bates and R. McCarroll, Adv. Phys. 11, 39 (1962)

[11] B. H. B. Ransden, Advan, Atom. Molec. Phys. 10, 1923 (1977)

[12] D. R. Bates and A. E. Kingston, Advan. Atom. Molec. Phys. 6, 269. (1970)

[13] R. A. Mapleton, Phys. Rev. 122, 528 (1961)

[14] R. A. Mapleton, Phys. Rev. 164, 51 (1967)

[15] R. A. Mapleton, Air Force Cambridge Research Lab. Report No. AFCRL 67-0351, P.263 (1967)

[16] R. A. Mapleton, "Theory of Charge Exchange", (New York, Wiley Interscience, 1972)

[17] S. Biswas, K. Bhadra and D. Basu, Phys. Rev. A 15, 1900 (1977)

[18] F. Fermont J. Phys B. At. Mol. Opt. Phys, 49, 6 (2016)

[19] Basu, S. C. Mukherjee and D. P. Sural, Phys. Reports. 42C, 145 (1978)

[20] A Amaya – Tapia, R. Hernandez – Lamoneda and H. MartineZ, J. Phys. B: At. Mol. Opt. Phys. 34, 5 (2001)

[21] L. H. Thomas, Proc. Roy. Soc. A 114, 561 (1927)

[22] D. R. Bates and R. A. Mapleton, Proc. Phys. Soc. 87, 657 (1966)

[23] D. R. Bates and R. Synder, J. Phys. B: At. Mol. Phys. 6, 642 (1973)

[24] M. Gryzinski, Phys. Rev. A 138, 336 (1965)

[25] B. N. Roy and D. K. Rai, J. Phys. B: At. Mol. Phys. 12, 2015 (1979)

[26] S. N. Chatterjee and B.N. Roy, J. Phys. B: At. Mol. Phys. 18, 4283 (1985)

[27] C. K. Tan and A. R. Lee, J. Phys. B: At. Mol. Phys. 14, 2309 (1981)

[28] C. K. Tan and A. R. Lee, J. Phys, B: At Mol. Phys. 14, 2409, (1981)

[29] E. Clementi and C. Roetti, At. Data Nucl. Data Tables 14, 177 (1974)

[30] Lotz, C. Opt. Soc. Am 58, 236 (1968).
[31] J. P. Desclaux, At Data Nucl. Data Tables 12, 325 (1973)
[32] M.B.Shah, P. McCallion, Y. Itoh and H.B. Gilbody, J. Phys. B: At. Mol. Opt. Phys. 25, 3693(1992).

Cite This Article :

Akhilesh Kumar Gupta, L. K. Jha, "Double Capture Cross Sections of Magnesium by The Impact of Fast Proton ", International Journal of Scientific Research in Science and Technology (IJSRST), Online ISSN : 2395-602X, Print ISSN : 2395-6011, Volume 6 Issue 6, pp. 408-414, November-December 2019.
Journal URL : https://ijsrst.com/IJSRST121655