Ultra Scientist Vol. 27(3)B, 214-220 (2015).

Benchmark Study for Positron (Electron) Impact Ionization of Noble Gas Atoms

KAMLESH K. SHARMA* and S. SAXENA

*Department of Physics, Invertis University, Bareilly (U.P.) -243 123 (India)
Department of Physics, Bareilly College, Bareilly (U.P.) – 243 005 (India)
E-mails: kamlesh.fphiiet@gmail.com,
sanjeev.sxn@gmail.com

(Acceptance Date 27th December, 2015)

Abstract

We have computed differential cross section (DCS) for ionization of noble gas atoms by impact of positron (electron) using truncated coupled state Born approximation (TCSBA). High quality Hartree-Fock Slater orbitals are used to model the target wave function. We have already computed some ionization results[1, 2, & 3] for noble gas series by impact of positron and electron as well, but in this paper, we are presenting for Ne, Ar, Kr & Xe atoms. We have compared DCS results with other available theoretical results as well as experimental data. It is observed that full orthogonalization of target wave function significantly improves present results and provides better agreement with experimental data for the noble gas series. Our present results are found in excellent agreement with other calculations. However some discrepancies suggested that more theoretical as well as experimental work is required in future to improve the data.

Key words : Cross Section, Ionization, Noble gas atom, Positron.

Introduction

The benchmark study of ionization of noble gas atoms by impact of charged particles continuously attracts a deep interest in collision physics for several reasons. But the collision processes have the paramount importance for understanding various branches of science and advanced technology. The collision of positron (electron) with noble gases, play a vital role in many emerging fields, e.g. in the initiation of plasma from neutral gases and medical field etc. On the account of various uses, we can say that noble gases are very fruitful for human life. Due to characteristics properties, noble atoms are used in lighting, photography and high powered gas lasers. On the practical side, reliable knowledge of ionization cross sections for above processes is very important for applications in plasma and discharge physics.

In recent years, much progress has been made in the theoretical as well as experimental treatment ionization processes.

During the last few years, Lohmann and co-workers have presented a set of measurements of fully differential cross section (FDCS) for electron impact single ionization of Argon at collision energies of 113.5eV and 200eV [4-9] which have turned out to be particularly challenging for theoreticians. Using the Breit-Pauli B-spline R-matrix method, Allan *et al*.[10] have calculated differential cross section (DCS) and Ballance *et al.*[11] studied about electron impact ionization cross section for Neon atom using R-matrix with pseudo states (RMPS) method. Most of the theoretical work on positron impact ionization of atoms is based on the distorted wave formalism. Using this approximation Moxom *et al.*[12] and Kara *et al.*[13] measured the cross section for Krypton by impact of positron. Marler *et al.*[14] studied positron impact ionization cross section for noble gases by using a qualitatively different method. McEachran and Stauffer[15] have been investigated positron impact ionization cross section by applying relativistic complex optical–potential method. Pindzola *et al.*[16] have reported the configuration average distorted wave calculations for electron impact ionization of Xenon. Recently, Montanari and Miraglia[17] described ionization cross section of rare gases by electron impact using continuum distorted wave and first Born approximation. Recently, Harris and Esposito[18] have calculated differential cross section for electron impact excitation as well as ionization of noble gas atom using first Born approximation and four body distorted wave models.

Theory : In the case of the positron (electron) impact ionization of a target atomic orbital, the truncated coupled state Born approximation is given by

$$d\sigma = \frac{4k'K^2}{kq^4}\left|\left(e^{-i\boldsymbol{q}.\boldsymbol{r}}\right)_{nlm\,K}\right|^2 d\Omega\, d\Omega_K dK \quad (1)$$

Where σ is the ionization cross section, $d\Omega$ and $d\Omega_K$ are elements of solid angle about the scattered and ejected electrons respectively. n, l and m are the usual orbital, angular and magnetic quantum numbers, $\boldsymbol{k}$ is the incident positron (electron) momentum (directed along the positive z axis), $\boldsymbol{k'}$ is the scattered electron momentum, $\boldsymbol{K}$ is the ejected electron momentum and $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k'}$ is momentum transfer.
The matrix element is given by

$$\left(e^{-i\boldsymbol{q}.\boldsymbol{r}}\right)_{nlm\,\boldsymbol{K}} = \int \psi_{\boldsymbol{K}}^{(-)^*} e^{-i\boldsymbol{q}.\boldsymbol{r}}\, \phi_{nlm} d^3r \quad (2)$$

Where ϕ_{nlm} is the target orbital wave function and $\psi_{\boldsymbol{K}}^{(-)}$ is the ejected electron wave function. To evaluate equation (1), all the momenta must be expressed in terms of the known variables and the integration variables[3].

Using equation (1), the DCS is given as

$$\frac{d\sigma}{d\Omega} = \frac{4k'K^2}{kq^4}\left|\left(e^{-i\boldsymbol{q}.\boldsymbol{r}}\right)_{nlm\,K}\right|^2 d\Omega_K dK \quad (3)$$

The incident and ejected electrons are identical particles, so allowance has been made in equation (1) for particle exchange. To compensate for this omission, the upper integration limit of the $\boldsymbol{K}$ momentum integration is taken to be $\sqrt{k^2/2 - E_0}$, which is the momentum of an electron ejected with half of the maximum possible energy. Further, the Born approximation always yields better results when, the effects of exchange are to reduce the cross section[19].

The Roothaan Hartree-Fock calculations of Clementi and Roetti[20] have been used to approximate the wave functions of occupied orbitals of the target atom. The wave function for a single atomic orbital is presented as a sum of Slater functions.

$$\phi_{nlm}(r,\theta,\phi) = \sum_{\mu} c_\mu A_\mu r^{n_\mu - 1} e^{-\lambda_\mu r} Y_{lm}(\theta,\phi) \quad (4)$$

where $Y_{lm}(\theta,\phi)$ is a spherical harmonic and

$$A_\mu = [(2n_\mu)!]^{-1/2}(2\lambda_\mu)^{n_\mu+1/2} \quad (5)$$

The outgoing scattered electron is described by a plane wave and the ejected electron is modeled by the hydrogenic Coulomb wave function, which is given by

$$\psi_K^{(-)} = \frac{1}{(2\pi)^{3/2}} e^{\pi/2K}\Gamma(1 + i/K)e^{i\boldsymbol{K}.\boldsymbol{r}} \times F_1(-i/K, 1, -ikr - i\boldsymbol{K}.\boldsymbol{r}) \quad (6)$$

Here Γ is the gamma function. F_1 is the confluent hyper-geometric function and $\boldsymbol{K}$ is the momentum of the ejected electron.

Results and Discussion

Using equation (3), we have computed differential cross section (DCS) for ionization of noble gases (*i.e.* Neon, Argon, Krypton and Xenon) at the incident energy 100eV by impact of electron as well as positron using truncated coupled Born approximation (TCBA) method. These computed results of electron (P_1) and positron (P_2) are compared with other available data.

The figure (1) shows DCS results for ionization of Neon using Hartree-Fock wave functions. We have compared the present electron results (P_1) with other theoretical results (DWBA) of Brunger[21] and available experimental data of Register *et al.*[22]. Our result P_1 shows a very good agreement with experimental data of Register *et al.* However the other available theoretical results DWBA do not match with either present result P_1 or experimental data and give higher cross section value. The positron impact ionization of Neon gives lower values of DCS. However variation of P_2 is almost same as that of experimental data and P_1.

The DCS results for ionization of Argon by impact of electron (P_1) and positron (P_2) have been plotted in the figure (2). Here, also the experimental results of Haynes and Lohmann[6] are also plotted. In this figure we observed that our results P_1 show a good agreement with experimental data whenever it is available. As usual the positron results give higher cross section with same trend as that of other results P_1. The two peaks can be observed at 30^0 and 120^0 for electron impact result.

The computed DCS of Krypton by electron as well as positron impact are shown in figure (3). Here we have compared the present results with other theoretical results (U) Guo *et al.*[23] using unitrized first order many body theory (UFOMBT). The only experimental data of Guo *et al.*[23] has also been plotted in this figure. The present results P_1 and experimental data both are in a good agreement. The other theoretical results (U) give higher cross section and show unmatched with experimental data as well as present results P_1. However the appeared dip is same in all the results in the angular range 80^0 to 100^0.

In the figure (4), we have shown the computed DCS results of ionization of Xenon by impact of electron and positron. Here DWBA results of Brunger[21] are also plotted. For comparison the present theoretical results, experimental data of Gibson *et al.*[24] is also plotted. As far as Xenon gas, a complicated variation of DCS with scattering angle can be seen in all theoretical results and experimental data. Our results P_1 give two sharp dip at about 30^0 and than 120^0. However this feature can also be seen in other theoretical result DWBA. The positron impact DCS P_2 also shows an abnormal feature. As scattering angle increases result P_2 decreases rapidly becomes constant and again decreases rapidly showing a dip at about 130^0. Further, it increases with increase of scattering angle.

DIFFERENTIAL CROSS SECTION FOR NEON AT 100ev

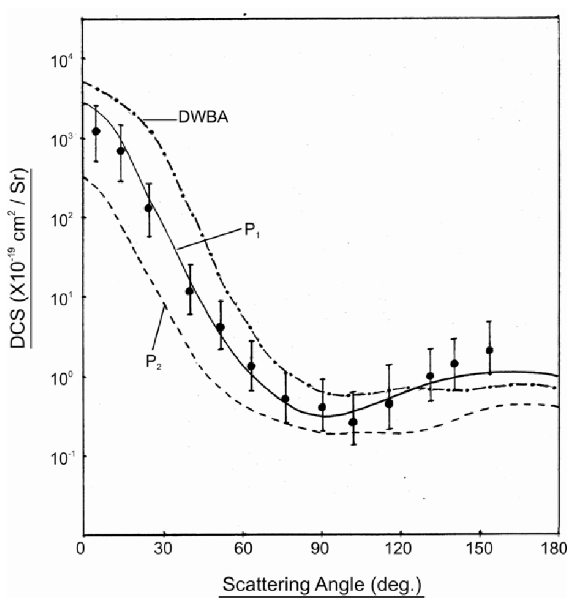

Figure (1)	:	**Differential Cross Section for Neon at 100eV.**
————————	:	Present results (P_1) for electron
— — — — — — —	:	Present results (P_2) for positron
— • — • —	:	DWBA of Brunger[21]
	:	Experimental results of Register *et al.*[22]

DIFFERENTIAL CROSS SECTION FOR ARGON AT 100eV

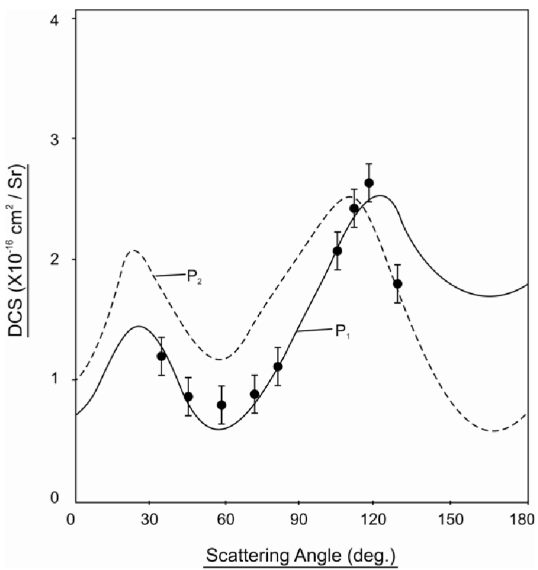

Figure (2) : **Differential Cross Section for Argon at 100eV.**

——————— : Present results (P_1) for electron

— — — — — — — — : Present results (P_2) for positron

(error-bar symbol) : Experimental results Haynes and Lohmann[6]

DIFFERENTIAL CROSS SECTION FOR KRYPTON AT 100eV

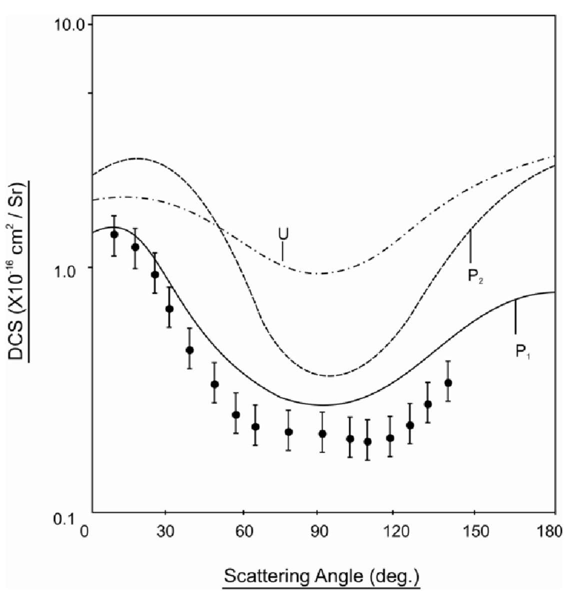

Figure (3) : **Differential Cross Section for Krypton at 100eV.**

——————— : Present results (P_1) for electron

— — — — — — : Present results (P_2) for positron

— • — • — : **(**U) Guo *et al* (UFOMBT)[23]

(error-bar symbol) : Experimental results of Guo *et al.*[23]

DIFFERENTIAL CROSS SECTION FOR XENON AT 100eV

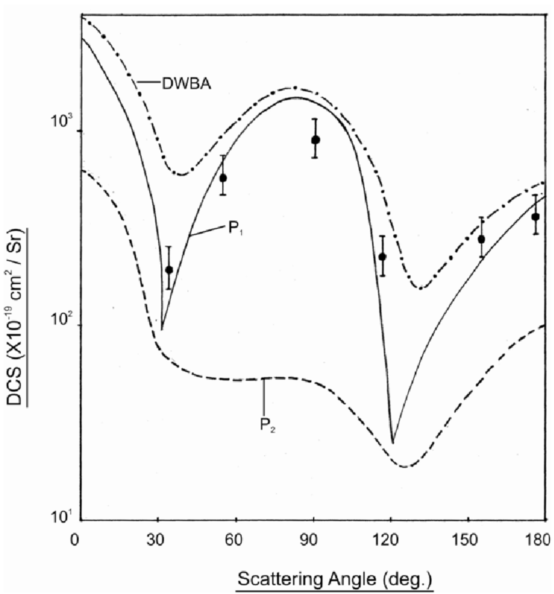

Figure (4) : Differential Cross Section for Xenon at 100eV.

———— : Present results (P_1) for electron

– – – – – : Present results (P_2) for positron

— • — • — : DWBA of Brunger[21]

(data point with error bar) : Experimental results of Gibson *et al.*[24]

Acknowledgement

One of us (KKS) wishes to thank Hon'ble Chancellor of Invertis University, Bareilly. We are also thankful to the Principal, Bareilly College, Bareilly (U.P.) for providing the necessary infrastructure.

References

1. Kamlesh K. Sharma and S. Saxena, *Acta Ciencia Indica,* Vol. XXXIX P, No. *2*, 57 (2013).
2. Kamlesh K. Sharma and S. Saxena, *Proceeding of 3rd International Conference on Current Developments in Atomic, Molecular, Optical and Nano Physics,* 156 (2011).
3. K. Kumar and S. Saxena, *Acta Ciencia Indica*, Vol. XXXVI P, No. *4*, 437 (2010).
4. M. A. Haynes and B. Lohmann, *J. Phys. B 33*, 4711 (2000).
5. M. A. Haynes and B. Lohmann, *J. Phys. B 34*, L131 (2001).
6. M. A. Haynes and B. Lohmann, *Phys. Rev. A 64*, 044701 (2001).
7. M. Stevenson, G. J. Leighton, A. Crowe, O. K. Vorov, and D. H. Madison, *J. Phys. B 38*, 433 (2005).
8. M. A. Stevenson and B. Lohmann, *Phys. Rev. A 73*, 020701(R) (2006).
9. M. A. Stevenson and B. Lohmann, *Phys. Rev. A 77*, 032708(R) (2008).
10. M. Allan, K. Franz, H. Hotop, O. Zatsarinny and K. Bartschat, *J. Phys. B 42*, 044009 (2009).
11. C.P. Balance, J.A. Ludlow, M.S. Pindzola and S.D. Loch, *J. Phys. B 42,* 175202 (2009).
12. J. Moxom, P. Ashley and G. Laricchia, *Can. J. Phys. 74*, 367(1996).
13. V. Kara, K. Paludan, J. Moxon, P. Ashley

and G. Laricchia, *J. Phys.* B *30*, 3933 (1997).

14. J.P. Marler, J.P. Sullivan C.M. Sukro, *Phys. Rev.* A *71*, 022701 (2005).
15. R.P. McEachran and A.D. Stauffer, *J. Phys.* B *43*, 215209 (2010).
16. M.S. Pindzola, C.P. Balance, J.A. Ludlow, S.D. Loch and D. C. Griffin, *J. Phys. B 43*, 025201 (2010).
17. C.C. Montanari and J.E. Miraglia, *J. Phys. B 47*, 105203 (2014).
18. A.L. Harris and T.P. Esposito, *J. Phys. B 48*, 215201 (2015).
19. M.R.H. Rudge, *Rev. Mod. Phys. 40*, 564 (1968).
20. E. Clementi and C. Roetti, *At. Data Nucl. Data Tables 14*, 177 (1974).
21. M.J. Brunger, *Ph.D. Thesis, The Flinders University of S. Australia* 5042 (1998).
22. D.F. Register, S. Trajmar, G. Steffensen and D.C. Cartwright, *Phys. Rev, A 29,* 1793 (1994).
23. X. Guo, D.F. Mathewst, G. Mikaelian, M.A. Khakoo, A. Crowe, I. Kanik, S. Trajmar, V.Zeman, K. Bartschat and C.J. Fontes, *J. Phys. B 33,* 1895 (2000).
24. J. C. Gibson, R.J. Sullivan, S.J. Buckman, V. Chan and P.D. Surrow, *J. Phys. B 29*, 3177 (1996).