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Electron Impact Single Ionization Cross Sections of Ar^+ Ion

Dr. Suresh Gupta[1]

ABSTRACT

Binary encounter approximation has been used for theoretical calculations of electron impact single ionization cross sections of singly ionized Ar atom at ground state in the energy range of 29.1eV to 2495.1 eV/amu. The cross sections for energy transfer given by Vriens' and quantum mechanical Hartree-Fock velocity distributions for target electron have been used in the calculation. The contributions in total single ionization cross sections from 3p and 3s subshells are observed higher than from 2p, and the contributions from 3p first increases with impact energy and then decreases with increase of impact energy whereas the contribution from 3s decreases with impact energy. About 69% of results have ratio factors ≤ 1.5 and 59% have values 1.25. Major contributions to the total ionization cross sections are from 3p and 3s for direct single ionization.

Key Words: Electron, Binary encounter approximation, Cross section of Ionization, Hartree - Fock velocity distribution, Single ionization.

1. INTRODUCTION

Single and multiple ionizations of atoms and molecules by ionizing particles like electrons and ions is one of the fundamental processes in atomic physics. Continuous data of ionization cross sections of respective processes have great importance in different fields of science. Knowledge of single and multiple ionization cross sections for atoms/ions by electron impact finds wide applications in plasma kinematics problems, plasma processes in comet, planetary atmospheres and biomedical applications, mass spectroscopy, gas lasers, upper atmosphere of Titan, astrophysics, and atmospherics physics. In the case of nuclear fusion research, knowledge concerning the behavior of impurities in the plasma is important. When neutral particles or ions being in low charge state are suddenly exposed to high electron temperature then processes of multi-ionization strongly influences the charge state evolution [1-6]. From an applied viewpoint multiple ionization processes are important in moderate and high temperature plasma and in all gaseous environments with all abundance of energetic electrons. Triple and higher multiple ionization processes start at increasingly higher energies and the corresponding cross sections are much smaller in magnitude compared to double ionization cross sections. Among different multiple ionization processes the double

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[1] Dr. Gupta is the Associate Professor of Physics, Patan Multiple Campus, TU

ionization is considered to be most important as the total ionization of the target depends on single and double ionization processes. The charge exchange processes contribute to the production of negatively charged ions which play an important role in accelerator technology, particularly in the design of tandem accelerator. A large number of elements both in neutral and ionic forms exist in upper atmosphere; the electron capture processes are particularly relevant and important in particle-atom collisions.

In the last decade, experimental work on multiple ionization ions by electron impact has received much attention. An interesting works on the multiple ionization of inert gas ion Ar^+ ($1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^5$) ions by electron impact has been carried out by D S Belic et al. (2010). They have observed that indirect processes significantly contribute to electron impact multiple ionization cross section of Ar^+. In the case of double ionization, they have considered small contribution from direct double ionization and large contribution from 3p ionization – autoionization. Difficulties with theoretical calculation for multiple ionization lie in the number of ionization mechanisms available in addition to the many body nature of the ionization process. Theoretical studies of electron impact double ionization cross sections are considered to be of much significance. Is it because of the contributions from different mechanisms i.e. simultaneous ejection of two electrons, inner shell ionization followed by Auger emission, resonant– excitation double auto-ionization process can be separately estimated at different impact energies. Complicated theoretical calculation of direct double ionization cross section becomes extremely difficult as it needs consideration of four charged particles in the final channel interacting through the long-range Coulomb potential. Hence, sophisticated calculations of the integrated double ionization cross section of atoms/ions are not available in the literature. However, in the past the semiclassical binary encounter approximation (BEA) has been used successfully by Roy and Rai (1973), Kumar and Roy (1978), Jha and Roy (2000, 2002, 2004, 2006), Gupta et al. (2015) and Gupta et al. (2017) in the in the calculations of charged particle impact single and double ionization cross section for several atoms and ions.

Electron impact single ionization of Ar^+ has been measured by Younger and Geo et al. using quantal Distorted Wave Born Approximation (DWBA). More recently Belic et al. (2010) have carried out the experimental measurements of absolute cross sections for electron impact single and multiple ionization of argon ions leading to the formation of Ar^{q+} (q=2-8). The experimental data of single ionization cross section of Ar^+ by Belic et al. (2010) have been compared with DWBA calculations of Younger et al. (1982) and Geo et al. (1997) and theoretical results obtained by Lotz (1967) semi-empirical formula. Results obtained by Lotz (1970) was better agreement with the experiment in comparison to the quantal calculations. Keeping in view the above mentioned facts and the success achieved by the binary encounter calculation, we have thought it worthwhile to carry out calculation of electron impact ionization cross sections for above mentioned target in BEA. This work will enable us to see the degree of success achieved in the different shells of the target.

2. METHODS AND THEORETICAL DETAILS

According to Thomson (1912) consider a situation of collision where the energy transfer in Coulomb collision between a particle of mass m_1 and charge $Z_1 e$ with initial kinetic energy E_1 and a particle of mass m_2 and $Z_2 e$ with initial kinetic energy $E_2 = 0$ (rest) In the case of binary encounter theory it is assumed that during the period of interaction between projectile and an orbital electron the other electrons and the nucleus play no role. The Thomson's energy transfer (ε) ionization cross section for electron –electron collision is given as:

$$\frac{dQ\ (\varepsilon)}{d\varepsilon} = \pi \frac{e^4 N}{E_1}\left[\frac{1}{U} - \frac{1}{E_1}\right] \tag{1}$$

For ionization $U \leq \varepsilon \leq E_1$; where U is ionization potential energy.

Thomas and William (1927) modified the formulation for more general case where $E_2 \neq 0$ (considered symmetrical distribution of velocity of target electrons), $m_1 \rangle\ m_2$ and $Z_1 \neq Z_2$ which is relevant to proton and alpha particle –atom collision. Energy transfer ionization cross section has been given as [Burgess et al. 1968]

$$\frac{dQ\ (\varepsilon)}{d\varepsilon} = \pi \frac{e^4 Z_1^2 Z_2^2 m_1}{m_2 E_1}\left[\frac{1}{\varepsilon^2} + \frac{4E_2}{3\varepsilon^3{}_1}\right] \tag{2}$$

In the binary encounter between the incident ion and the target electron the projectile transfers a part of its energy to the atomic electron so that it is ejected out. Classical theory of Thomas and Gryziniski (1965), classical model of ionization does not take into account the indistinguishability of the incident and bound electron (unsymmetrical collision model) and is not reliable for low incident energies. These difficulties are removed in the symmetrical collision model introduced by Vriens (1966). The computations with the Gryzinski model shows that choice of velocity distribution for the bound electron has very important effects on the calculated cross sections. For the same there used Hartree-Fock velocity distribution function for the bound electrons. Therefore, we have used symmetrical model of Vriens and Hartree-Fock velocity distribution function to obtain single ionization cross sections of Ar^+ by electron impact.

The expression of electron impact ionization cross section, including exchange and interference due to Vriens is given by,

$$Q' = \frac{\pi e^2}{E_1 + E_2 + U}\left\{\left(\frac{1}{U} - \frac{1}{E_1}\right) + \frac{2E_2}{3}\left(\frac{1}{U^2} - \frac{1}{E_1^2}\right) - \frac{\Phi' \ln\left(\frac{E_1}{U}\right)}{E_1 + U}\right\} \#(3)$$

where

$$\Phi' = \cos\left[\left(\frac{R}{E_1 + U}\right)^{\frac{1}{2}} \mathrm{In}\left(\frac{E_1}{U}\right)\right] \#(4)$$

In the above expressions E_1 and are kinetic energies of incident and particular bound electron of the target respectively and is Rydberg constant.

McDowell (1966) adopted two dimensionless variables s and t relating to the ratio of kinetic energy of incoming and orbiting electrons to the ionization potential energy U. Catlow and McDowell (1967) extended it to formulate the expression of ionization cross section of atoms in terms of the two dimensionless quantities and defined as:

$$s^2 = \frac{v_1^2}{v_0^2} \quad \text{and} \quad t^2 = \frac{v_2^2}{v_0^2}$$

where $U = v_0{}^2$ is the ionization potential of the shell under consideration expressed in Rydbergs and v_1 and v_2 are the velocities of the incident and the bound electrons respectively, in atomic units. All other energies have also been expressed in Rydberg. In terms of these dimensionless quantities, Vriens expression for electron impact ionization cross section takes the form

$$Q_i\,(s,t) = \frac{4}{(s^2 + t^2 + 1)}\left[\frac{(S^2 - 1)}{U^2 s^2} + \frac{2t^2(s^2 - 1)}{3U^2 s^4} - \frac{\phi'}{u^2(s^2 + 1)} \ln s^2\right] \pi a_0^2 \#(5)$$

where

$$\phi' = \left[\left(\frac{1}{s^2\ U + U}\right)^{\frac{1}{2}} \ln s^2\right] \#(6)$$

The expression (3) has to be integrated over continuous Hartree-Fock velocity distribution function for the bound electrons, and the final expression for ionization cross section becomes where n_e is the number of equivalent electrons in the shell under consideration and *f(t)* is the momentum distribution function for the bound electron which is defined as

$$f(t) = 4\pi t^2 U \rho_{\mathrm{nl}}\left(U^{\frac{1}{2}} t\right) \#(8)$$

Here

$$\rho_{\mathrm{nl}} = \frac{1}{2l+1} \sum_{m=-1}^{+1} [\psi_{\mathrm{nlm}}(\chi)]^2 \#(9)$$

where

$$\psi_{\mathrm{nlm}}(\chi) = \frac{1}{(2\pi)^{\frac{1}{2}}} \int \Phi_{\mathrm{nlm}}(r)\, e^{ik.r} dr \#(10)$$

is the Fourier transform of the one electron orbital. Complete wave function or Slater orbitals is given by

$$\Phi_{\mathrm{nlm}}(r) = N_{\mathrm{nl}} R_{\mathrm{nl}}(r) Y_{\mathrm{lm}}(\Omega) \#(11)$$

where $R_{\mathrm{nl}}(r)$ and N_{nl} are the analytical Hartree-Fock radial function and normalization constant given as

$$N_{nl} = [(2n)!]^{-\frac{1}{2}} (2\xi)^{n+\frac{1}{2}} \#(12)$$

and

$$R_{\mathrm{nl}} = r^{n-1} e^{-\xi r} \#(13)$$

Spherical harmonic $Y_{lm}(\Omega)$ have different form depending upon the value of quantum numbers ℓ, m. Inner shell electrons in heavy atoms have high velocity and they are relativistic in nature. Hence, relativistic effect plays an important role for such targets. In present work, ionization from valence shells and a few inner shells have only been considered and ignored relativistic effects for outer shell electrons of the atom. Keeping this fact in account we have used non-relativistic wave function in the present work.

In the present calculations, momentum distribution functions for the bound electrons have been constructed using Hartree-Forck radial functions reported by Clementi and Roetti (1974). For shell radii and binding energies of electrons, quantum mechanical value of radial distance of maximum probability given by Desclanx (1973) and quantum mechanical values of orbital energies given by Clementi and Roetti have, respectively, been used in the calculations.

3. RESULTS AND DISCUSSION

Computational calculation of equation (7) finally gives results of SICS for 3p, 3s and 2p under different selective constants of respective subshells. The expression of $Q_i(s,t)$ and $f(t)$ are taken from equation (5) and (8) respectively. The momentum distribution function $f(t)$ has been constructed from equations (9-13) for particular orbital electron of the target atom as discussed above. Integration over differential cross section $\sigma_{\Delta E}$ for energy transfer **(** ΔE **)** gives $Q_i(s,t)$ that represents ionization cross section due to a projectile of unit charge for a particular incident energy and particular bound electron. Theoretical investigation of direct single ionization has been carried out in the energy range of 29.1 eV/amu to 2495.1 eV/amu (Belic et al. 2010) using BEA. We compared the theoretical result of SICS with the experimental data of single ionization cross sections for corresponding impact energy. The calculated cross sections have been represented graphically in Fig.1. The calculated results of cross sections contributed from sub shells considered has been shown in Table 1 along with experimental values.

Table 1: Electron impact single ionization of **Ar**$^+$ in the unit of 10^{-17} cm^2.

E (eV/amu)	Total	Experiment			
	3p	**4s**	**2p**	**Total**	**Expt.**
29.1	1.47			1.47	1.20
31.1	4.57			4.57	3.00
33.1	6.58			6.58	5.10
35.1	7.97			7.97	6.40
37.1	8.98			8.98	7.70
40.1	10.03			10.03	9.20
45.1	11.08			11.08	10.1
55.1	12.01	1.28		13.29	11.2
65.1	12.33	1.80		14.13	11.8
75.1	12.42	2.02		14.44	12.3
85.1	12.39	2.12		14.51	12.5
95.1	12.31	2.17		14.48	12.6
115.1	12.06	2.21		14.27	12.4
135.1	11.75	2.19		13.94	11.9
155.1	11.42	2.15		13.57	11.4
195.1	10.78	2.04		12.82	10.3

245.1	10.05	1.90		11.95	9.20
295.1	9.42	1.76	0.28	11.38	8.40
395.1	8.37	1.52	0.51	10.40	7.10
495.1	7.55	1.34	0.58	9.47	6.10
595.1	6.89	1.19	0.6	8.68	5.40
795.1	5.90	0.98	0.61	7.49	4.30
995.1	5.17	0.83	0.59	6.59	3.70
1495.1	3.98	0.61	0.52	5.11	2.70
1995.1	3.25	0.48	0.46	4.19	2.20
2495.1	2.75	0.40	0.42	3.57	1.80

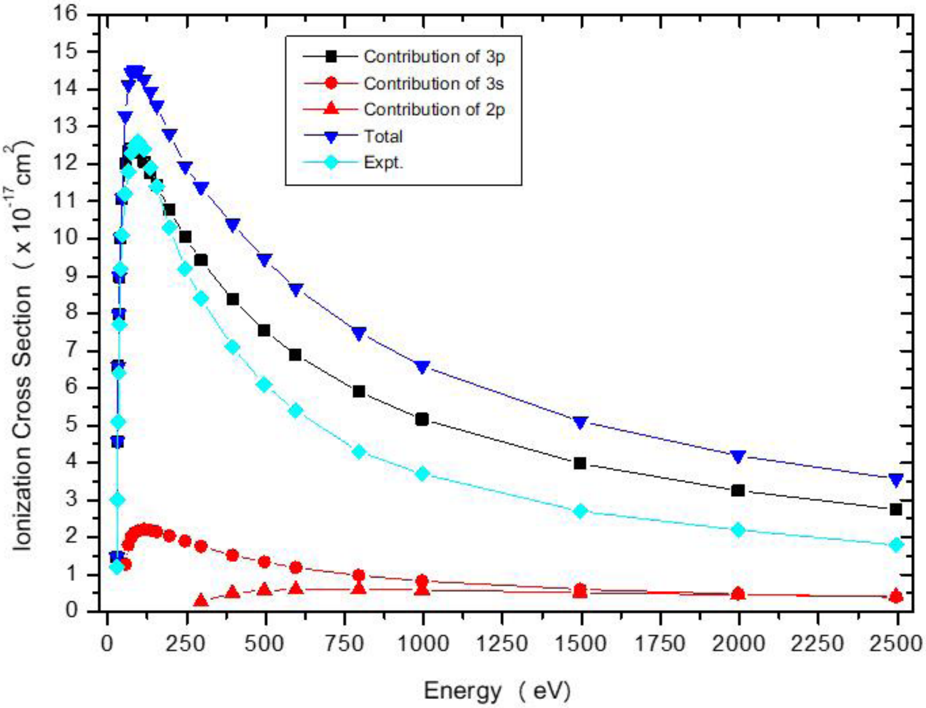

Fig.1: Variation of Cross section of 3p, 3s, and 2p subshells along with Total theoretical and Experimental values at different impact energy of electron.

The calculated results of single ionization cross sections of Ar^+ along with experimental data have been presented in Table1 and Fig.1. Contributions to single ionization from 3p, 3s and 2p shells have been also shown separately in the Table and Figure. The theoretical results slightly overestimate the cross sections at low impact energies. The ratio of theoretical to experimental cross section is 1.52 at 31.1

eV/amu and drop to 1.29 at 33.1 eV/amu. Beyond this energy the calculated cross sections remain within a factor of 1.25 of the experimental data in the energy region 35.1- 195.1 eV/amu. At higher energies the ratio of theoretical to experimental cross section becomes at 2495.1 eV/amu. The experimental maximum cross section is observed to be 12.6x $10^{-17}cm^2$ at 95.1 eV/amu. At this energy the ratio of theoretical to experimental cross section is 1.15. On the other hand the theoretical maximum cross section is found to be $14.5x10^{-17}$ cm^2 at 90.1 eV/amu which is slightly shifted on low energy side. The present results are seen to be in reasonably good agreement with the experimental data. Usually the calculations in the BEA overestimate the cross sections at low impact energies. At high energies the cross sections gradually become closer to the experimental and sometimes they become less than experimental data. The slowly increasing cross sections in high energy region observed in the present work need some possible explanation. According to Rudge (1968) theoretical results are supposed to be valid if ratio factor (ratio of theoretical to experimental) is less than 2. The obtained theoretical results have ratio factor below 2 and nature of variation of total theoretical and experimental curves are nearly same. About 69% of results have ratio factors ≤ 1.5 and 59% have values 1.25. Major contribution to the total ionization cross sections are from 3p and 3s for direct single ionization.

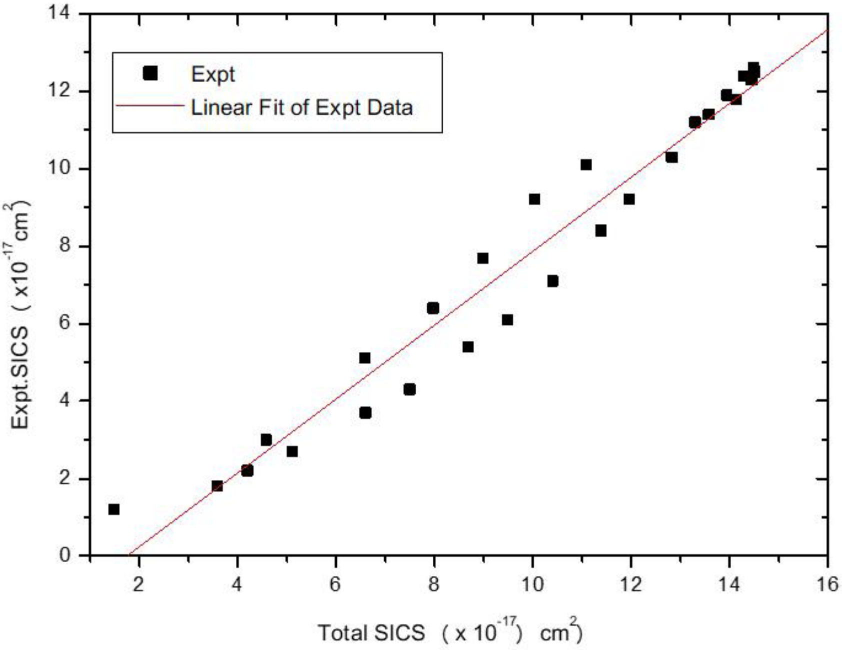

Fig.2: Linear Fit of theoretical values with the corresponding Experimental results.

The Figure above have coefficient of regression 0.9793 and standard deviation of 0.79136. It means about 97% of the theoretical data are in close agreement with the Experimental results.

4. CONCLUSIONS

The electron impact single ionization cross sections (SICS) of Ar^+ atom for the range of energies 29.1 to 2495.1 eV/amu have been theoretically calculated using the binary encounter approximation and Hartree-Fock velocities distribution. It is observed that the electron impact SICS of Ar^+ are well explained by considering direct ionization of 3p, 3s and 2p subshells. The obtained theoretical results have ratio factor below 2 and nature of variation of total theoretical and experimental curves are nearly same. About 69% of results have ratio factors ≤ 1.5 and 59% have values 1.25. Major contribution to the total ionization cross sections are from 3p and 3s for direct single ionization. Collision interaction at low energy is purely of quantum effect. The semi classical model does not include all physical insight of ionization in threshold range. Overall the results are in good and satisfactory agreement with the experimental observations for wide range of impact energies.

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