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Proton Impact K- Shell Ionization of Neon and Magnesium

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Abstract

In the present work, K-shell ionization cross-sections of Neon and Magnesium due to proton impact have been calculated through the Binary Encounter Approximation model. The effects of Coulomb deflection of the projectile under the influence of target nucleusand increase in binding energy of the target electron because of presence of the projectile inside K- shell of the target have been incorporated.The cross-sections have been averaged over Hartree-Fock momentum distribution for the target electron. The calculated cross-sections have been found in satisfactory agreement with the available experimental values and other calculated results.

Keywords: K-shell ionization, Binary Encounter Approximation, Proton impact, ECPSSR

1. Introduction

Study of ionization of atoms and molecules due to impact of charged particles is important because of its applications in the field of gaseous discharge, astrophysics, atmospheric physics, plasma physics, laser physics etc. Moreover accurate values of ionization cross sections for inner shells (particularly K-shell) of atoms induced by heavy charged particles e.g. protons, alpha particles are important for trace element analysis of many elements[1]. However, experimental measurements of cross sections are not always available at the desired values of impact energies and hence theoretical studies of such processes become important. Further these studies provide a test for suitability of the theories for charged particle impact direct ionization of atoms.

There are a number of theoretical methods for calculation of inner shell ionizationcross sections due to heavy charged particles e.g. Plane Wave Born Approximation[2], Semi Classical Approximation[3], Binary Encounter Approximation (BEA)[4]. Out of these, the BEA is simple and required less computational efforts but yields reasonable results.

2. Theoretical consideration

In the present work we have calculated K-shell ionization cross sections of atomic neon and magnesium due to impact of protons in the BEA. In the present calculations, we have incorporated the effects of the following two physical processes on the ionization cross sections.

(i) Coulomb deflection effect:

A positively charged particle coming close to the target nucleus experiences repulsion due to the target nucleus. This reduces the velocity of the incident particle as well as changes its trajectory during collision. These two changes cause a reduction in the inner shell ionization cross sections. In the present work the above effects have been incorporated following Thomas and Garcia[5] through the relation

$$\sigma(E_1) = \sigma(E_1{}') \left[\frac{1}{2} + \frac{1}{2}\left(1 - \frac{Z_1 Z_{2k} e^2}{E_1 a_{2k}}\right)^{\frac{1}{2}}\right]^2 \quad ; \tag{1}$$

where $\sigma(E_1{}')$ is the ionization cross section at the reduced energy.

$$E_1{}' = E_1 - \frac{Z_1 Z_2 e^2}{a_{2k}} \tag{2}$$

And $\quad Z_{2k} = Z_2 - S_{2k}$

Z_1 and Z_2 are the nuclear charges of the projectile and the target respectively, a_{2k} is radiation of K-shell of the target whereas S_{2k} is screening constant for K-shell.

(ii) Effect of increase in binding of the target electron:

For ejection of an electron from an inner shell, the projectile has to penetrate deep into the shell. This causes an increase in the binding energy of the target electron. Under this condition, the electron response time is much shorter than the collision time which allows the electron to adjust to the presence of the projectile and thereby increases the binding energy of the electron. This feature reduces ionization cross sections at low impact energies and the effect gradually decreases with increase in the impact energy[2].

The above described effect has been incorporated in the expression for ionization cross sections by replacing the unperturbed binding energy U_{2k} of the atomic K-shell by $U_c = \in U_{2k}$, U_c being the corrected binding energy, ∈ is a correction factor given by Brandt and Lapicki[2].

$$\in = 1 + \left(\frac{2 Z_1}{Z_{2k}\, \theta_{2k}}\right) g \tag{3}$$

θ_{2k} is the reduced binding energy for the K-shell and is given by

$$\theta_{2k} = \frac{U_{2k}}{Z_{2k}^2}$$

The factor g is an impact velocity dependent term and is given by[6]

$$g = \frac{1 + 5x + 7.14x^2 + 4.27x^3 + 0.947x^4}{(1+x)^5} \tag{4}$$

where

$$x = \frac{V_1}{\left(\frac{1}{2}\theta_{2k} V_{2k}\right)}$$

Vriens' expressions[7] for ionization cross section, incorporating the above mentioned effects can be written as

$$Q_I\ (s,t) = \frac{(s+s')^2 Z_1^2}{s^2 s'^2 U_c^2}\left[1 + \frac{2t^2}{3} - \frac{1}{4\left(s'^2 - t^2\right)}\right]\left(\pi a_0^2\right); \qquad 1 \le 4s'(s'-t) \tag{5}$$

$$= \frac{(S+S')^2 Z_1^2}{2S^2 s'^2 U_c^2\, t}\left[\frac{1}{4(s'+t)} + t + \frac{2}{3}\left\{2s'^3 + t^3 - \left(1+t^2\right)^{3/2}\right\}\right]\left(\pi a_0^2\right); \tag{6}$$

$$4s'(s'-t) \le 1 \le 4s'(s'+t)$$

$$= \quad 0; \quad 1 \geq 4s'(s'+t) \tag{7}$$

In the above equations s and t are dimensionless variables defined as

$$t^2 = \frac{V_{2k}^2}{V_0^2} \text{ and } s^2 = \frac{V_1^2}{V_0^2}$$

whereas,

$$(s')^2 = s^2 - \frac{1.058\, Z_1 Z_{2k}}{1836\, M\, a_{2k}\, U_c}$$

V_0^2 being corrected binding energy in Rydberg, while V_1, V_{2k} and M (mass of the projectile) are expressed in atomic units.

The above expressions have been averaged over Hartree-Fock velocity distribution for the target electron. The Hartree-Fock radial functions given by Clementi and Roetti[8] have been used to construct the momentum distribution for target electrons. The quantum mechanical values of K-shell energy given by Clementi and Roetti[8], have been used in the present work. The quantum mechanical values of the points of maximum radial probability reported by Desclaux[9] have been used as the shell radii. The screening constant for the K-shell has been taken equal to 0.3

Table 1: Proton Impact K-Shell Ionization Cross sections of Ne

INPUT ENERGY (keV)	**Calculated Ion. Cross section ($10^{-22}cm^2$)**			**Expt. Ion. Cross section ($10^{-22}cm^2$) Ref.:10**	**Expt. Ion. Cross section ($10^{-22}cm^2$) Ref.:11**	**Cal. ECPSSR ($10^{-22}cm^2$) Ref.:12**
	(A)	**(B)**	**(C)**			
48	3.26	1.67	0.68	0.78		0.69
58	5.56	3.28	1.31	1.48		1.52
68	8.58	5.56	2.23	2.60		2.85
77	11.90	8.23	3.32	4.35		4.85
97	21.50	16.30	6.89	9.94		10.50
116	33.30	26.60	11.80	18.30		19.20
125	39.70	32.40	14.70		17.80	24.50
135	47.30	39.30	18.20	30.00		31.50
150	59.90	51.10	24.50		31.70	42.40
200	110.00	98.20	51.80		69.40	92.50
300	230.00	216.00	131.00		177.00	225.00
400	360.00	345.00	228.00		313.00	366.00
500	483.00	469.00	330.00		391.00	492.00
600	594.00	581.00	427.00		465.00	601.00
700	691.00	679.00	517.00		533.00	601.00
800	773.00	763.00	596.00		583.00	763.00
900	842.00	833.00	664.00		667.00	884.00
1000	899.00	891.00	722.00		722.00	869.00

A- Without modification
B - Including Coulomb effect
C - Including Coulomb and Binding effect

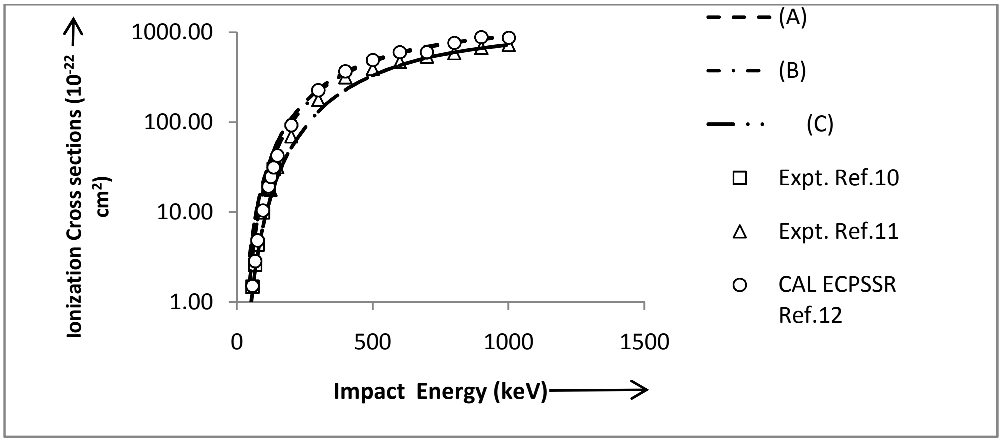

Figure1: Proton Impact K- Shell Ionization Cross sections of Ne.

Table 2: Proton Impact K-Shell Ionization Cross sections of Mg

Input Energy (MeV)	Calculated Ion. Cross section ($10^{-22}cm^2$)			Expt.Ion. Cross section ($10^{-22}cm^2$) Ref.13	Expt.Ion. Cross section ($10^{-22}cm^2$) Ref.14	Expt.Ion. Cross section ($10^{-22}cm^2$) Ref.15	Cal. ECPSSR Ion. Cross section ($10^{-22}cm^2$) Ref.12
	(A)	**(B)**	**(C)**				
0.05	0.48	0.36	0.10	0.07	0.07		0.08
0.06	0.83	0.66	0.20	0.15	0.16	0.12	0.18
0.07	1.30	1.08	0.34	0.28			0.34
0.08	1.90	1.62	0.54	0.62			0.58
0.09	2.64	2.30	0.80	0.80			0.92
0.10	3.53	3.12	1.12	1.15		0.93	1.37
0.15	10.20	9.44	3.98			4.00	5.75
0.20	20.30	19.30	9.10			9.33	14.20
0.30	48.80	47.30	26.10			31.30	42.10
0.40	84.20	82.40	50.40			60.00	79.30
0.50	123.00	121.00	79.50			66.70	120.00
0.60	160.00	160.00	111.00	142.00			162.00
0.69	195.00	193.00	138.00	150.00			193.00
0.80	235.00	234.00	174.00	169.00			232.00
0.90	268.00	267.00	204.00	192.00			262.00
1.00	298.00	297.00	232.00	214.00			288.00
1.10	325.00	324.00	258.00	242.00			314.00
1.20	349.00	348.00	281.00	258.00			333.00
1.30	371.00	369.00	303.00	293.00			352.00
1.40	389.00	388.00	322.00	315.00			364.00
1.50	406.00	405.00	339.00	343.00			375.00
1.60	420.00	419.00	354.00	357.00			390.00

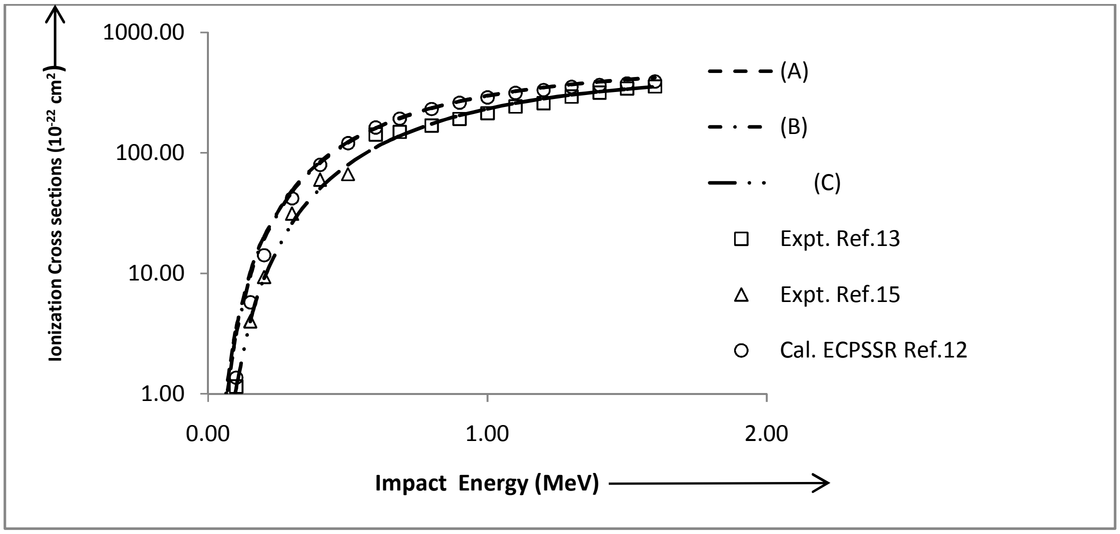

Figure 2: Proton impact K- shell ionization cross-sections of Mg

3. Results and Discussion

3.1 Proton impact K – shell ionization cross sections of Neon

We have calculated K – shell ionization cross sections of Neon due to impact of protons in the energy range from 48.0 keV to 1000.0 keV and the results have been shown in the table 1 and figure 1. Experimental values of two sets have been reported, one set due to Harrison et. al.[10] is limited to low energy range (48.0 keV to 135.0 keV) whereas the other set due to Langerberg and van Eck[11] in the energy range from 125.0 keV to 1000.0 keV. We have presented a comparison of our results and the experimental observation and the theoretical calculations in ECPSSR[12]. At low impact energies our results are slightly underestimate the experimental values but with increase in impact energy the agreement improves. This is a general trend of BEA cross sections. Overall agreement of our results with the experiments is satisfactory; they are always within a factor of two. The present results are also in reasonable agreement with the values of cross sections obtained in ECPSSR theory.

3.2 Proton impact K – shell ionization cross sections of Magnesium

We have calculated K – shell ionization cross sections for Magnesium due to impact of proton in the range from 0.05 MeV to 1.7 MeV and the results have been shown in the table-2 and figure-2. Results obtained have been compared with the available experimental results of Khan et. al[13], Shima[14], Khan and Potter[15] and calculations of ECPSSR[12]. Experimental results due to Shima[14] have been reported only for two impact energies (0.05 MeV and 0.06MeV) whereas those of Khan and Potter[15] are over a limited energy ranges (0.06 MeV to 0.50 MeV).Observations of Khan et. al[13] are available over an extended energy range (0.05 MeV to 1.60 MeV). Our calculations overestimate the experiments but the agreement improves with increase in the impact energy. Present results are also in reasonably good agreement with ECPSSR[12] calculations.

4. Conclusion

A critical study of the results presented in section 3 leads to the conclusion that the present method gives reasonable values of proton impact K- shell ionization cross sections of Neon and Magnesium with very small computational effort. The present results are also in close agreement with the cross sections obtained using more improved method namely ECPSSR.

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