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Proton and Alpha Particle Impact K- shell Ionization of Magnesium

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Abstract

K-shell ionization cross sections of Magnesium have been calculated in the Binary Encounter Approximation Effects of coulomb calculated results have been compared with theoretical cross sections of ECPSSR and the available experimental observations.

INTRODUCTION

Accurate cross-sections of charged particles impact inner shell ionization find application quantitative analysis of Auger Electron Spectroscopy (AES), Electron Probe Micro Analysis (EPMA) and Electron Energy Loss Spectroscopy (EELS)[1]. These cross sections are also useful in the fields of atomic physics, plasma physics, material and surface science and radiation chemistry[2]. Moreover, accurate values of ionization cross sections for inner shells (particularly K-shell) induced by heavy charged particles e.g., protons, alpha particles are required for trace analysis of many elements[3]. As experimental values of these cross sections are not always available at the desired impact energies theoretical studies of such processes become important. Moreover, these studies provide a test for suitability of different theories of charged particle impact direct ionization of atoms.

Plane Wave Born Approximation[4], Semi Classical Approximation[5]and Binary Encounter Approximation (BEA)[6] have been widely used for theoretical description of inner shell ionization process due to impact of heavy charged particle. Out of these, the BEA is simple, requires comparatively less computation but gives results comparable to those obtained from other approximations. In the present work we have performed calculations for K-shell ionization cross sections of Magnesium to impact of protons and alpha particles in the BEA.

We have incorporated the effects of two physical processes on the ionization cross section in the present investigation:

(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 and also changes the direction of velocity during collision. These two effects cause a reduction in the inner shell ionization cross section. Effects of Coulomb repulsion on the ionization cross section are found to decrease with increase in impact energy (see Brandt and Lapicki[7]).

(ii) Increase in binding of the target electron:
At low impact energies inner shell ionization occurs due to deep penetration of the incident positively charged particle into the atomic shell. The presence of the incident particle in the vicinity of the target electron causes an increase in the binding of the target electron. Under this condition, the electron response time is much smaller than the collision time. Hence the target electron adjust itself to the presence of the projectile and thereby decreases the probability of the ionization. As consequence ionization cross section is reduced at low impact energies and the effect gradually decreases with increase in the impact energy[7].

THEORETICAL CONSIDERATION

Following Thomas and Garcia[8] we have introduced the effect of the Coulomb interaction between the positively charged particle and the target nucleus on the ionization cross section analytically through the relation

$$\sigma(E_1) = \sigma(E'_1)\left[\frac{1}{2} + \frac{1}{2}\left(1 - \frac{Z_1 Z_{2k} e^2}{E_1 a_{2k}}\right)^{\frac{1}{2}}\right]^2 \qquad \text{……..(1)}$$

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

$$E'_1 = E_1 - \frac{Z_1 Z_{2k} e^2}{a_{2k}} \qquad \text{…….. (2)}$$

and $\qquad Z_{2k} = Z_2 - S_{2k}$

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

The effects of the increase in binding of the target electron is incorporated in the expression for ionization cross section 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, $\in$ is a correction factor given by Brandt and Lapicki[7]

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

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

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

and g is an impact velocity dependant factor given by[9]

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

where $x = \frac{V_1}{\left(\frac{1}{2}\theta_{2k}V_{2k}\right)}$, V_1 and V_{2k} are velocities of projectile and K-shell electron respectively

Vriens' expressions[10] for ionization cross section, incorporating the contributions from the above mentioned effects can be written as

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

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

$$4s'(s'-t) \le 1 \le 4s'(s'+t) \quad \ldots (6)$$

$$= 0; \qquad 1 \ge 4s'(s'+t) \quad \ldots (7)$$

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

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

and

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

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 momentum distribution for the target electron have been constructed using as the Hartree-Fock radial functions given by Clementi and Roetti[11]. The quantum mechanical values of K-shell energy reported by Clementi and Roetti[11] and the quantum mechanical values of the points of maximum radial probability reported by Desclaux[12] have been used as binding energy the shell radii. The screening constant for the K-shell has been taken equal to *0.3*.

RESULTS AND DISCUSSION

K-shell ionization cross sections for Magnesium due to impact of H^+ and He^{2+} have been calculated following the method outlined in section 2 and the results have been shown in tabular and graphical forms. The effects of interaction between the incident particle and the target nucleus and the increase in binding of the target electron in the presence of the projectile are shown separately. The experimental K-shell ionization cross section (σ_i) has been determined from the X-ray production cross section (σ_x) from the relation $\boldsymbol{\sigma_i = \sigma_x / \omega_k}$, where, ω_k is the fluorescence yield of the atomic K-shell which is taken equal to *0.03* (Lapicki[13]).

H^+ impact K-shell ionization cross sections

Cross sections have been calculated in the energy range 20KeV to 1.7MeV and the results have been presented in table 1 and figure 1. Experimental values of K-shell ionization cross sections have been obtained from the X-ray production cross sections as reported by Khan and Potter[14], Khan Et.al15, Brandt et.al[16] and Shima[17]. Our cross sections have been compared with these experimental observations and the calculated cross sections obtained in ECPSSR theory as reported by Lapicki[13]. These calculations use Plane Wave Born Approximation which has been modified to take account of the contributions from Coulomb interaction of the incident projectile with the target nucleus, increase in binding of the target electron in the presence of the projectile, capture of electron by the projectile, energy loss of the projectile and the relativistic nature of the K-shell electron to the ionization cross section.

Table 1: Proton impact K-shell ionization Cross sections of Magnesium

Impact Energy (KeV)	Expt. Ion. Cross section (10^{-26} cm^2) Ref:14	Expt. Ion. Cross section (10^{-26} cm^2) Ref:15	Expt. Ion. Cross section (10^{-26} cm^2) Ref:16	Expt. Ion. Cross section (10^{-26} cm^2) Ref:17	Cal. ECPSSR (10^{-26} cm^2)	Present calculation(10^{-26} cm^2)		
						A	B	C
20				2.00(0)	4.26(0)	2.61(1)	1.17(2)	2.60(2)
25		1.44(1)*		1.33(1)	1.94(1)	6.90(1)	2.94(2)	5.41(2)
30		5.10(1)		4.00(1)	5.80(1)	1.46(2)	5.95(2)	9.75(2)
35				1.00(2)	1.35(2)	2.69(2)	1.05(3)	1.59(3)
40		2.45(2)		2.00(2)	2.68(2)	4.49(2)	1.69(3)	2.41(3)
45				3.33(2)	1.35(2)	6.99(2)	2.55(3)	3.47(3)
50		7.57(2)		6.67(2)	7.79(2)	1.03(3)	3.64(3)	4.79(3)
60	1.17(3)	1.48(3)		1.67(3)	1.76(3)	1.98(3)	6.61(3)	8.26(3)
70		2.84(3)			3.38(3)	3.40(3)	1.08(4)	1.30(4)
80		6.17(3)			5.82(3)	5.37(3)	1.62(4)	1.90(4)
90		8.03(3)			9.22(3)	7.96(3)	2.30(4)	2.64(4)
100	9.33(3)	1.15(4)			1.38(4)	1.12(4)	3.12(4)	3.53(4)
125			2.77(4)		3.09(4)	2.28(4)	5.82(4)	6.40(4)
150	4.00(4)		5.00(4)		5.75(4)	3.98(4)	9.44(4)	1.02(5)
175			8.67(4)		9.45(4)	6.24(4)	1.39(5)	1.48(5)
200	9.33(4)		1.33(5)		1.42(5)	9.10(4)	1.93(5)	2.03(5)
300	3.13(5)				4.21(5)	2.61(5)	4.73(5)	4.88(5)
400	6.00(5)				7.93(5)	5.04(5)	8.24(5)	8.42(5)
500	7.67(5)				1.20(6)	7.95(5)	1.21(6)	1.23(6)
602		1.42(6)			1.61(6)	1.12(6)	1.61(6)	1.63(6)
686		1.50(6)			1.93(6)	1.38(6)	1.93(6)	1.95(6)
800		1.69(6)			2.31(6)	1.74(6)	2.34(6)	2.35(6)
900		1.92(6)			2.62(6)	2.04(6)	2.67(6)	2.68(6)
1000		2.14(6)			2.88(6)	2.32(6)	2.97(6)	2.98(6)
1100		2.42(6)			3.12(6)	2.58(6)	3.24(6)	3.25(6)
1200		2.58(6)			3.32(6)	2.81(6)	3.48(6)	3.49(6)
1310		2.93(6)			3.52(6)	3.05(6)	3.71(6)	3.73(6)
1400		3.15(6)			3.65(6)	3.22(6)	3.88(6)	3.89(6)
1500		3.43(6)			3.65(6)	3.39(6)	4.05(6)	4.06(6)
1600		3.57(6)			3.89(6)	3.54(6)	4.19(6)	4.20(6)
1700		3.80(6)			3.98(6)	3.67(6)	4.31(6)	4.32(6)

*1.44(1) stands for 1.44×10^1

The present method gives the total vacancy production cross section in the K-shell of the target due to impact of the projectile and hence it includes the contributions from electron capture by the projectile. In the impact energy range 20.0KeV to 45.0KeV our calculated cross sections over estimate the experimental result by a factor more than 2.0 but with increase in impact energy the agreement between the present result and our calculated values improves and they come very close. The discrepancy at low impact energy may be due to the assumptions in our approximation which are expected to be satisfied for fast collision. Beyond 60.0KeV impact energy the present calculations so close agreement with the cross section obtain in ECPSSR.

He^{2+} impact K-shell ionization cross sections

In case of He^{2+} impact K-shell ionization of Magnesium, calculations have been performed in the energy range 125.0K*eV* to 5.*0MeV* and the results along with the experimental observations of Brandt et.al[16], Seller et.al[18] and the calculations in ECPSSR as reported by Lapicki[13] are presented in Table 2 figure 2. Experimental observations of Brandt et.al[16] are available a narrow input energy range (128.0KeV to 200KeV). But the present results show a closer agreement with these observations compared to the ECPSSR results. Our results in energy range 1.0MeV to 5.0MeV are also very close to these experimental observations of Seller et.al[18] as well as calculations of ECPSSR.

Table 2: Alpha Particle impact K-shell ionization Cross sections of Magnesium

Impact Energy (KeV)	Expt. Ion. Cross section (10^{-24} cm^2) Ref:16	Expt. Ion. Cross section (10^{-24} cm^2) Ref:18	Cal. ECPSSR (10^{-24} cm^2)	Present Calculation(10^{-24} cm^2)		
				A	B	C
125	2.47		1.28	2.67	3.54(1)	4.44(1)
150	6.00		3.17	5.37	6.56(1)	7.90(1)
175	1.13(1)		6.63	9.61	1.09(2)	1.27(2)
200	1.97(1)		1.24(1)	1.58(1)	1.67(2)	1.91(2)
1000		9.60(3)	7.80(3)	3.61(3)	1.31(4)	1.34(4)
1500		1.67(4)	2.48(4)	1.08(4)	2.96(4)	3.00(4)
2500		5.77(4)	7.09(4)	3.40(4)	6.82(4)	6.86(4)
3000		7.97(4)	9.29(4)	4.74(4)	8.68(4)	8.71(4)
3500		1.05(5)	1.12(5)	6.07(4)	1.04(5)	1.04(5)
4000		1.18(5)	1.28(5)	7.35(4)	1.19(5)	1.19(5)
4500		1.35(5)	1.42(5)	8.54(4)	1.32(5)	1.33(5)
5000		1.53(5)	1.53(5)	9.62(4)	1.44(5)	1.44(5)

From the present investigations, it is concluded that our method gives K-shell ionization cross sections for atoms due to impact of H^+ and He^{2+} which are comparable to those obtained by ECPSSR theory but with comparatively much smaller computational effort and hence useful wherever such cross sections are needed for applications. Our results can be improved further by taking account of relativistic nature of K-shell electron. This can be done by use of relativistic wave functions.

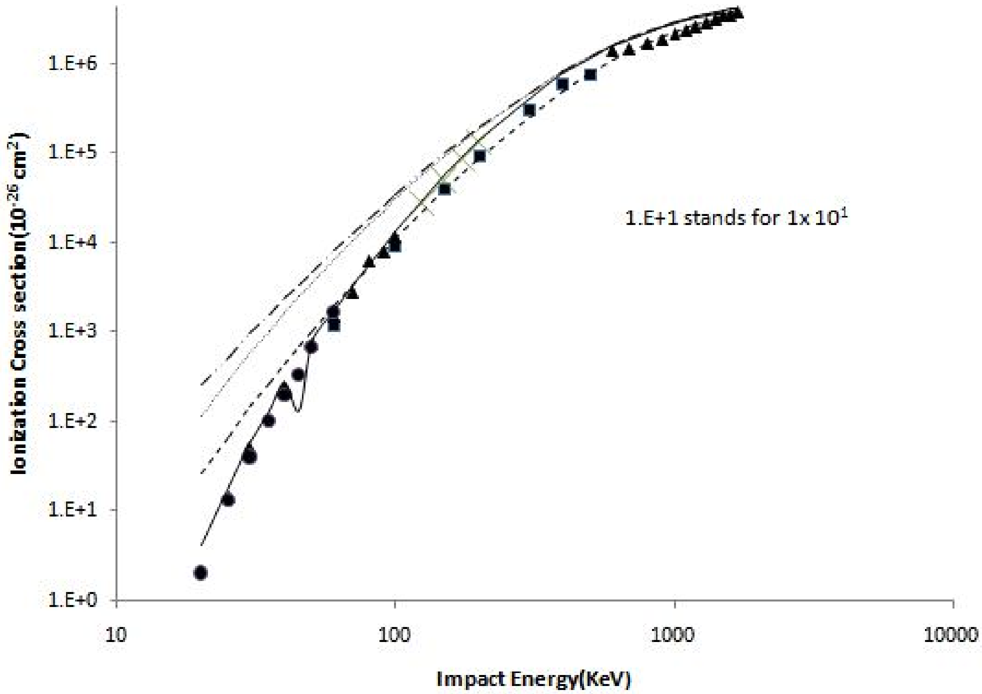

Fig. 1: Proton impact K-shell ionization Cross sections of Magnesium

– – – –	**A:** Present cross sections including both the processes
……….	**B:** Present cross sections including Coulomb effect only
▬ ▪▪ ▬	**C:** Present cross sections without any modification
────	ECPSSR cross sections

Experimental cross sections				
	■	(Ref. 14)	▲	(Ref. 15)
	✕	(Ref. 16)	●	(Ref.17)

Further, it is observed that inclusion of two physical processes described in section 1 lower the cross sections but this effect gradually decreases with increase in impact energy. The effect of increase in binding of the target electron in the presence of the projectile persists up to a higher value of impact energy compared to the effect of Coulomb interaction of the projectile and the target nucleus. These observations are as expected on the physical ground. Moreover, the present results due to impact of He^{2+} show a better agreement with experiments compared to those obtained due to impact of H^{+}. This observations may be due to the fact that our method is a semi classical approximations and He^{2+} being heavier compared to H^{+} it is expected to show more classical behavior compared to H^{+}.

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