He^{2+} Impact K-Shell Ionization Cross-Sections: A BEA Calculation

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ABSTRACT: *K-Shell inoization Cross-sections for atoms due to impact of He^{2+} ions have been calculated in Binary Encounter Approximations. The effects of Coulomb deflection of the incident particles and increase in binding of the target electrons have been investigated. Hartree-Fock Velocity distributions for the target electrons have been used in the present calculations. The calculated Cross-sections have been compared with experimental results and other theoretical calculations wherever available. The present results give a good account of experimental observations.*

Keywords : *K-Shell ionization, Binary Encounter Approximation, Coulomb deflection, Increase in Binding, Hartree-Fock Velocity distribution.*

I. INTRODUCTION

The theoretical investigation of inner shell ionization of atoms by heavy charged particles impact is of fundamental importance and got attention before 1940. But this field received considerable attention in seventies mainly due to improvement in the experimental technique e.g. improved availability of accelerated heavy ions and much improved experimental counters on coincidence technique (see Hansteen[1], Burhop[2]).

The inner shell ionization and x-rays production by charged particles have been extensibly studied in last few decades, specially because of its importance for the particle induced x-rays emission (PIXE) in analytical studies. Theoretical studies of these processes are of much practical importance as they provide cross-sections for the emission of x-rays from various inner shells which can be used for the interpretation of experimental data (Sarter et al[3]). These Cross-sections are frequently applied to trace element analysis in environmental and biomedical samples and accurate determination of beam intensities in various particle accelerator experiment (Hardt and Watson[4]).

Ionization from an inner-shell of an atomic target takes place due to impact of heavy energetic structureless charged particles when the projectiles penetrate deep into the atomic inner shell. In case of deep penetration, major contribution to the ionization cross sections comes from the direct coulomb excitation of the target electron by the projectile.

Theoretical investigations of inner-shell ionization of atoms by incident charged particles involving direct coulomb excitation have been performed initially in the Plane Wave Born Approximation (PWBA) (see Merzbacher and Lewis[5]) and in the semi classical approximation (SCA) (see Bang and Hansteen[6]). In recent past, the Binary Encounter Approximation was developed by Gryzinski[7] and firstly used by Garcia[8] for description of inner-shell ionization. Specially, in case of inner shell ionisation, apart from its simplicity the BE Cross sections are competing with those obtained using SCA and PWBA and are in agreement with experimental results (see Bearse et.al[9]).

The theoretical values of inner shell ionization cross-sections due to heavy charged particles impact calculated in any one of the above mentioned approximations do not show agreement with the experimental observations. The discrepancy between the theory and experiment can be reduced to a large extent by incorporating mainly two out of various physical processes involved in inner shell ionization. The two processes are – Coulomb deflection of the projectile in the field of target nucleus and increase in binding of the target electron in the presence of the projectile (see Brandt et. al[10]). Garcia[8] has incorporated the effect of Coulomb deflection in BEA calculation. The effects of increase in binding of the target electron and Coulomb deflection of the projectile in BEA Calculations of heavy positively charged particle impact inner shell ionization Cross sections have been incorporated by Singhal and Singh[11], Kumar and Roy[12], Chatterjee et. al[13], Shrivastava and Roy[14]. Kumar and Roy[12] have used the correct expression for $\sigma_{\Delta E}$ (Cross-sections for energy transfer ΔE by the projectile to the target) as given by Vriens[15] in their calculations but the factor used by them for the increase in binding of the target electron is independent of impact velocity, which is not physically justified. Later on Shrivastava and Roy[14] used a velocity dependent correction factor incorporating the effects of increase in the binding of the target electron (see Basbas et al[16], Brandt and Lapicki[17]) in their calculations of heavy charged particle impact K-shell ionization cross-sections of atoms.

Inspired by the above mentioned facts, I consider it worthwhile to calculate K-Shell ionization cross–sections of atoms due to impact of -particles taking into consideration the physical processes properly along with the accurate quantum mechanical velocity distribution for the target electron (see Shrivastava and Roy[14]).

II. THEORETICAL CONSIDERATION

Vriens[15] expressions for ionisation cross sections of atoms by α-particles impact have been used by incorporating the coulomb repulsion of the α-particles in the field of target nucleus as suggested by Thomas and Garcia[18] (See also Kumar and Roy[12]). The effect of Coulomb repulsion is introduced analytically through the relation (see Shrivastava et. al[19], Chatterjee et al[13]).

$$\sigma(E_1) = \sigma(E_1') \left[\frac{1}{2} + \frac{1}{2}\left(1 - \frac{Z_1 Z_{2k} e^2}{E_1 a_2 K}\right)^{1/2}\right] \quad \ldots\ldots (1)$$

Where $\sigma(E_1')$ is the ionization cross – section at the reduced energy

$$E_1' = E_1 - \frac{Z_1 Z_{2k} e^2}{a_2 K}$$

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

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

The effect of increase in binding of the target electron in the presence of the positively charged particle (α-particles) can be incorporated in the ionization expression for Cross – section by replacing the unperturbed binding energy U_{2k} of the atomic K-Shell by $U_C = \epsilon U_{2k}$ where U_C is the corrected binding energy and ϵ is a correction factor given by (see Brandt and Lapicke[17]).

$$\epsilon = 1 + \left(\frac{2Z_1}{Z_{2k}\theta_{2k}}\right) g \quad \ldots\ldots (2)$$

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

$$\theta_{2k} = \frac{U_{2k}}{Z_{2k}^2(13.6)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

The factor g is a velocity dependent term and for K-Shell it is given by (see Basbas et al[16])

$$g = \frac{(1+5\times+7.14x^2+4.27x^3+0.94x^4)}{(1+x)^5} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

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

Finally, Vriens[15] expression for ionization cross–sections incorporating the contributions of above mentioned effects, in terms of two dimensionless variable s and t (see Catlow and McDowwell[20]),

Can be expressed as

$$Q(s,t) = \left\{ \begin{array}{c} \frac{(s+s')^2 z_1^2}{s^2 s^{12} U_C^2}\left(1+\frac{2t^2}{3}-\frac{1}{4(s'^2-t^2)}\right)\pi a_0^2;\ 1 \le 4s'(s'-t) \\ \frac{(s+s')^2 z_1^2}{2s^2 s'^2 U_c^2 t}\left[\frac{1}{4(s'+t)}+t+\frac{2}{3}\left\{2s'^3+t^3-(1+t^2)^{\frac{3}{2}}\right\}\right]\pi a_0^2;\ 4s'(s'-t) \le 4s'^{(s'+t)} \\ O;\ 1 \ge 4s'(s'+t) \end{array} \right\} \ldots(5)$$

The two dimensionless variables have been defined

as $t^2 = \frac{v_{2k}^2}{v_0^2}$, $s^2 = \frac{v_1^2}{v_0^2}$

and $s'^2 = s^2 - (1.058\ Z_1\ Z_{2k}) / (1836\ Ma_{2k}U_c)$

v_0^2 is the corrected ionization energy in Rydbergs units of the Shell under consideration, $v_{1,}v_{2k}, v_0$ and M (Mass of the Projectile) are expressed in atomic units.

The resulting expression for ionization cross- sections have been integrated over Hartree-Fock velocity distribution for the bound electron, reduces to

$$Q(s) = ne\int_0^\infty Q(s,t)\, f(t)\, U_C^{1/2} dt \ldots\ldots\ldots\ldots\ldots\ldots (6)$$

Where n_e is the number of equivalent electrons in the shell under consideration and f (t) is the momentum distribution functions for the target electrons constructed by Hartree-Fock radial function which is given by Clement and Roetti[26] (see Kumar and Roy[12]). The binding energies of the target electrons have been taken from the table of Clementi and Roetti[21]. The quantum mechanical values of the points of maximum radial probability reported by Desclaux[22] have been used as Shell radii. For K-Shell, the Screening Constant has been taken equal to 0.30 (see Slater[23], Basbas et al[16], Langenberg[24]).

III. Result and Discussion

Calculations of K-Shell ionisation Cross-sections of neon, magnesium, chlorine and argon due to impact of α-particles have been performed along the lines discussed in sec. 2. Three sets of calculations have been done for every target atom. The effect of Coulomb interaction and the increase in binding are shown separately in figs along with the third one without taking the above mentioned two effects. The experimental K-shell ionisation cross-sections (σ_1) have been determined from the X-ray production cross section (σ_x) :

$\sigma_1 = \frac{\sigma_x}{w_k}$ where w_k is the fluorescence yield of the atomic K-Shell. For comparison with present calculations, the x-ray production cross-sections for these systems due to impact of α–particle measured by different group of workers as reported by Lapicki[25] in his review article and converted them into ionisation cross-sections as mentioned above, have been used. The present results of cross–sections have also been compared with the results of ECPSSR Calculation reported by lapicki[25]

The present calculated results of neon along with experimental observations of Harrison et al[26] and Langenberg and VanEck[27] have been shown in table-1 and Fig.-1. Cross-sections calculated in ECPSSR theory are also included in the table and fig. The results of Harrison et al[25] are available only at two impact energies on lower side i.e 116.KeV and 135.0 KeV whereas those of Langenberg and VanEck[27] are over an extended energy range (116.0 KeV – 1200.0 KeV). It has been observed that the present calculated results at all impact energies overestimate the experimental cross-sections. At low impact energies overestimation is high but the situation improves with increase in impact energy. Present results are always within a factor of two as compared to the results of ECPSSR calculations. As the alpha particle carries double the charge compared to Proton, the effects of corrections are more enhanced which is expected on physical grounds.

In case of magnesium, only one set of experimental observations of alpha particle impact K-Shell ionisation cross-sections have been reported by Lapicki[25]. The present calculated cross-section along with the experimental cross-sections of Sellers et al[28] and the results of ECPSSR Calculation have been presented in table-2 and fig.-2. The present results overestimate the experimental cross-sections but always within a factor of 1.5. This is expected because the experimental results are in high impact energy region in which the BEA is suitable for calculations of ionisation cross-section. The present results are also in satisfactory agreement with the ECPSSR calculations.

In case of He^{2+} impact K-Shell ionisation for chlorine, three sets of experimental results have been reported by Lapicki[24] in which Avaldi et al[29] have presented results over an extended energy range (800.0 KeV to 2800.0 KeV). The other two groups sellers et al[28] and Lewis et al[30] have reported their observations only at a few impact energies. The present calculated cross-sections along with experimental observations and results of ECPSSR Calculations have been presented in table-3 and fig.-3. The present results show reasonable agreement with experimental observations of Avaldi et al[29]. However the present calculations of cross-sections are always within a factor of 2 as compared to the experiments. Also, it is evident that the present calculations are reasonably in good agreement with the ECPSSR calculation.

Alpha particle impact K-shell ionisation cross sections of Argon have presented in table-4 & fig. 4. The present calculated results have been compared with the only one set of experimental results of Winter et al[31] (As reported by Lapicki[25]) along with the calculations of ECPSSR. Experimental results of cross-sections are available only at five impact energies. The present calculated results overestimate the experimental results but are always within a factor of two except at impact energy 800.0 KeV. Present results are also in reasonably good agreement with ICPSSR Calculations.

IV. Conclusions

A critical analysis of the results presented in Sec. 3 revealed that Binary Encounter Approximation (BEA) incorporating the corrections for two physical effects namely the Coulomb deflection of the projectile and increase in binding of the target electrons, gives a reasonable estimate of K-shell ionization cross-sections of atomic targets due to impact of α–particles. The present results, in general, overestimate the experimental cross-sections, which is more prominent at low impact energies. As the impact energy increases, the calculated cross sections come closer to the experimental observation. The present method is simple and gives results in reasonable agreement and complex calculations like ECPSSR. Hence the method is useful whenever fast calculations of such cross sections are required.

Acknowledgement

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Table-1

He^{2+} impact K-Shell ionisation Cross-Sections of Ne

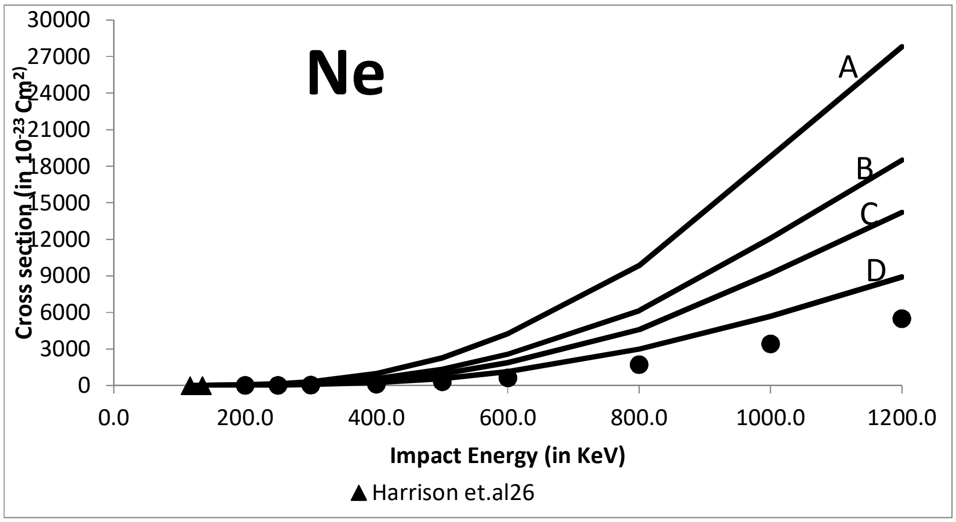
(in units of 10^{-23} Cm^2)

Impact Energy (KeV)	Harrison et.al[26]	Langenberg and VanEck[27]	Cal (Cm2) ECPSSR (D)	Present Cal (cm^2)		
				A	B	C
116.0	1.95		0.90	4.86	2.43	1.62
135.0	3.41		1.87	9.61	4.93	3.33
200.0		7.67	11.7	57.2	30.1	26.0
250.0		20.3	31.8	149.0	80.6	56.0
300.0		39.4	70.6	310.0	172.0	121.0
400.0		122.0	239.0	982.0	561.0	401.0
500.0		300.0	578.0	2280.0	1340.0	970.0
600.0		622.0	1140.0	4240.0	2570.0	1890.0
800.0		1720.0	2980.0	9840.0	6150.0	4590.0
1000.0		3430.0	5670.0	18800.0	12100.0	9180.0
1200.0		5480.0	8900.0	27800.0	18500.0	14200.0

Figure-1

He^{2+} impact K-Shell ionisation Cross-Sections of Ne

(in units of 10^{-23} Cm^2)



* A -Cal. without any effect.
B- Cal. with effect of culomb deflection.
C- Cal. with effect of culomb deflection and increase in binding.
D- Cal. ECPSSR

Table-2

He^{2+} impact K-Shell ionisation Cross-Sections of Mg

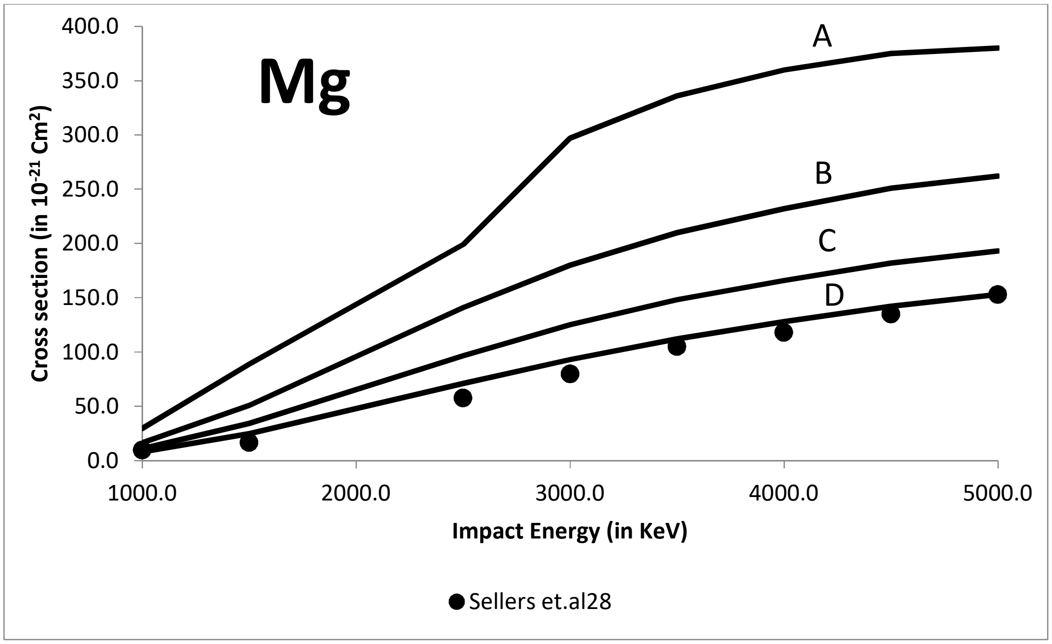
(in units of 10^{-21} Cm^2)

Impact Energy (KeV)	Sellers et.al[28]	Cal (Cm2) ECPSSR (D)	Present Cal (cm^2)		
			A	B	C
1000.0	9.6	7.8	29.5	16.4	10.9
1500.0	16.7	24.9	88.9	50.8	34.3
2500.0	57.7	71.0	199.0	141.0	96.6
3000.0	79.7	93.1	297.0	180.0	125.0
3500.0	105.0	112.0	336.0	210.0	148.0
4000.0	118.0	128.0	360.0	232.0	166.0
4500.0	135.0	142.0	375.0	251.0	182.0
5000.0	153.0	153.0	380.0	262.0	193.0

Figure-2

He^{2+} impact K-Shell ionisation Cross-Sections of Mg

(in units of 10^{-21} Cm^2)



* A -Cal. without any effect.
B- Cal. with effect of culomb deflection.
C- Cal. with effect of culomb deflection and increase in binding.
D- Cal. ECPSSR

Table-3
He^{2+} impact K-Shell ionisation Cross-Sections of Cl

(in units of 10^{-23} Cm^2)

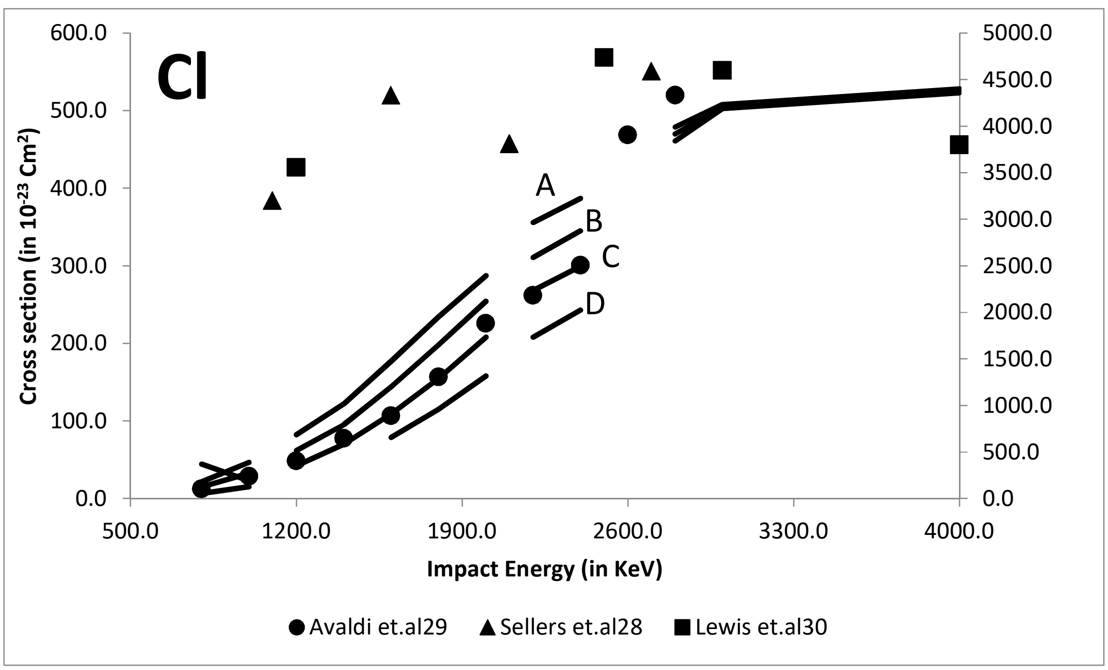
Impact Energy (KeV)	Avaldi et.al[29]	Sellers et.al[28]	Lewis et.al[30]	Cal (Cm2) ECPSSR (D)	Present Cal (cm^2)		
					A	B	C
800.0	12.8			6.67	21.7	15.1	44.4
1000.0	28.9			15.4	46.7	32.8	22.8
1100.0		3200.0					
1200.0	48.7		3560.0	29.9	82.3	61.9	42.4
1400.0	77.9				122.0	95.1	69.9
1600.0	107.0	4330.0		78.7	177.0	144.0	109.0

1800.0	157.0			115.0	234.0	198.0	155.0
2000.0	226.0			158.0	287.0	254.0	208.0
2100.0		3810.0					
2200.0	262.0			208.0	356.0	311.0	268.0
2400.0	301.0			243.0	387.0	345.0	299.0
2500.0			4740.0				
2600.0	469.0			328.0	439.0	428.0	397.0
2700.0		4590.0					
2800.0	520.0			394.0	479.0	470.0	461.0
3000.0			4600.0		508.0	504.0	503.0
4000.0			3800.0		528.0	526.0	523.0

Figure-3

He^{2+} impact K-Shell ionisation Cross-Sections of Cl

(in units of 10^{-23} Cm^2)



** In Figure-3 above, Sellers et.al[28] and Lewis et.al[30] are on the secondary Y-axis.

* A -Cal. without any effect.
B- Cal. with effect of culomb deflection.
C- Cal. with effect of culomb deflection and increase in binding.
D- Cal. ECPSSR

Table- 4

He^{2+} impact K-Shell ionisation Cross-Sections of Ar

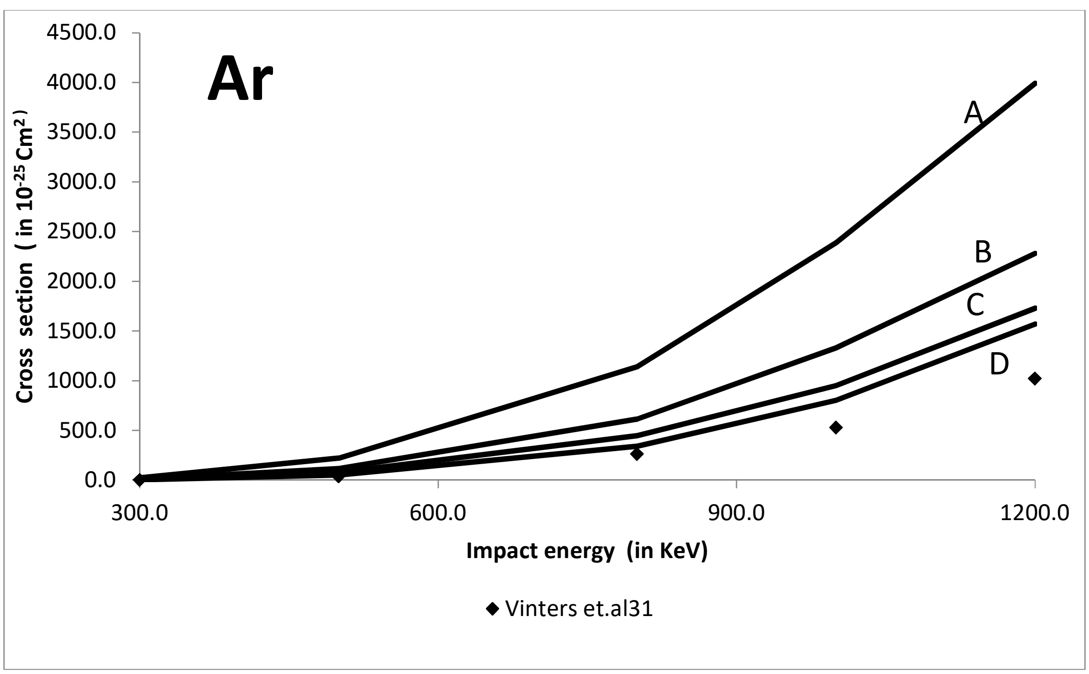
(in units of 10^{-25} Cm^2)

Impact Energy (KeV)	Vinters et.al[31]	Cal (Cm2) ECPSSR (D)	Present Cal (cm^2)		
			A	B	C
300.0	3.5	5.3	23.2	11.6	7.7
500.0	38.9	51.3	222.0	117.0	77.8
800.0	264.0	343.0	1140.0	616.0	449.0
1000.0	529.0	802.0	2390.0	1330.0	950.0
1200.0	1020.0	1570.0	3990.0	2280.0	1730.0

Figure- 4

He^{2+} impact K-Shell ionisation Cross-Sections of Ar

(in units of 10^{-25} Cm^2)



* A -Cal. without any effect.
B- Cal. with effect of culomb deflection.
C- Cal. with effect of culomb deflection and increase in binding.
D- Cal. ECPSSR

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