

# Electron Impact Double Ionisation of Lanthenum ( $\text{La}^{++}$ )

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**Abstract – The present paper provides extension of the binary encounter approximation calculations. In the case of +ve ions to the case of  $\text{La}^{++}$  ion.**

**Key Words : ION, Cross Section, Double Ionization, Binary.**

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## INTRODUCTION

As for as electron impact double ionization of positive ions are concerned. Cramdal [11] and Muller [12] have studied in laboratory and astrophysical plasma. The cross-sections are needed to determine the populations density of different atomic levels in a partially ionized Plasma (Burke and Taylor [13]). The systematic studies of electron impact ionization cross-section of ions provide valuable information about the influence of the unscreened field of the ionic charge on the cross-sections. Experimental observations indicate that in some cases due to significant contributions from single ionization of next inner shell following an Auger transition, the electron impact double ionization cross-section are of the same order of magnitude. So double ionization must also be considered in modeling and diagnostics of high atomic number elements (Achenbach et al.[14]).

Electron impact double ionization cross-section calculations using quantal methods are very complicated theoretically and are limited to a few lighter targets. Gryzinski's double binary encounter model has been suitably modified by Roy and Rai [2] Chatterjee et al. [10] has been used this calculations of electron impact double ionization of atoms. The result obtained have been found in reasonably good agreement with available experimental.

In this paper have extended the binary encounter approximation calculations in the case of positive ions, to the case of  $\text{La}^{++}$  ion.

The model proposed by Thomas and Garcia [3], an electron coming close to a positive ion would experience a coulombic attraction and consequently its impact parameter is reduced. The physical picture of this process has been shown in the figure as electron-ion collision geometry. Here the kinetic energy of the incident electron is increased and the

expression for increased kinetic energy  $E'_i$  can be given in terms of incident kinetic energy  $E_i$  net nuclear charge of target ion  $Z'e$  and collision radius  $\zeta$  as follows.

$$E'_i = E_i + \frac{Z'e^2}{\zeta}$$

Tomas and Garcia [3] have shown that the dependence of the collision radius  $\zeta$  on the distance of the bound electron from the nucleus  $r_A$  and also on the electron electron separation  $\rho$  such that an energy transfer  $\Delta E \geq U$  (binding energy of the target electron) may take place.

$$\sigma_i(E_i) = \sigma_i(E'_i) \left[ \frac{1}{2} + \frac{1}{2} \left( 1 + \frac{Z'e^2}{E_i \zeta} \right)^{\frac{1}{2}} \right]^2 \quad \dots(1)$$

In this way the expression for ionization cross section at increased energy  $E'_i$  multiplied by a factor

$$f = \left[ \frac{1}{2} + \frac{1}{2} \left( 1 + \frac{Z'e^2}{E_i \zeta} \right)^{\frac{1}{2}} \right]^2$$

gives the desired expression of ionization cross section for the ion. We define a dimensionless quantity  $s'$  as explained earlier corresponding to increased  $E'_i$  energy of the projectile in the form given as

$$S'^2 = S^2 + \frac{2Z'}{gU_i}$$

Where

$$S^2 = \frac{V_1^2}{U_i}$$

$V_1$  being the velocity of the incident electron and  $U_i$  is the first ionization potential of the target. In the above expression for  $S^2$ ,  $\zeta$  has been expressed in atomic unit and the energies are expressed in rydbergs. The factor  $f$ , in terms of dimensionless variables  $S$  and  $S'$ , reduces to the form

$$f = \frac{(S+S')^2}{4S^2} \quad (2)$$

To investigate electron impact double ionization cross section of positive ions, we have to calculate the value of  $Q_{SC}^{ii}$  as given by vriens [4, 5, 6] with  $S$  replaced by  $S'$  and have multiplied the results thus obtained by the factor  $f$ . This gives the contributions from the scattered electron to the direct double ionization cross sections. In order to obtain the direct double ionization cross section  $Q_d^{ii}$  of the shell under consideration, the value of  $Q_{SC}^{ii}$  (contributions from the scattered electron) has just been doubled as in case of atoms as discussed earlier. Hence the value of  $Q_d^{ii}$  takes the form

$$Q_d^{ii} = 2Q_{SC}^{ii} = 2f \frac{n_e(n_e-1)}{4\pi\bar{r}^2} \int_0^\infty \int_{U_i}^{E_i-U_{ii}} \left[ \frac{2}{(S'^2+t^2+1)U_i} \right. \\ \left. \left\{ \left( \frac{2}{(\Delta E)^2} + \frac{4t^2U_i}{3(\Delta E)^3} \right) + \frac{1}{(S'^2U_i+U_i-\Delta E)^2} + \frac{4t^2U_i}{3(S'^2U_i+U_i-\Delta E)^3} - \frac{\phi}{E(S'^2U_i+U_i-\Delta E)} \right\} \right. \\ \left. \times \left[ \frac{d f(t) U_i^{1/2} dt}{d(\Delta E)} \right] \right] d(\Delta E) [8.797 \times 10^{-17} (\pi a_0^2)] \quad (3)$$

Where

$$\phi = \cos \left[ \left( \frac{1}{(S'^2+1)U_i} \right)^{1/2} \ln S'^2 \right]$$

And

$$\alpha = \frac{4}{S_1^8 U_{11}^2} \left[ \left( \frac{S_1^2-1}{S_1^2} \right) \{ S_1^6 - 2S_1^4 + 8S_1^2 + 16 - 16(1+S_1^2)^{1/2} \} \right. \\ \left. + \frac{2(S_1^4-1)}{3S_1^4} \{ S_1^6 - 6S_1^4 + 24S_1^2 - 16 + 16(1+S_1^2)^{3/2} \} \right. \\ \left. - \frac{\phi'}{(S_1^2+1)} \ln S_1^2 \{ S_1^6 - 2S_1^4 + 8S_1^2 + 16 - 16(1+S_1^2)^{1/2} \} \right]$$

Where

$$\phi' = \cos \left[ \left( \frac{1}{(S_1^2+1)U_{ii}} \right)^{1/2} \ln S_1^2 \right]$$

In the above equations

$$t^2 = \frac{V_2^2}{U_i}$$

$V_2$  being the velocity of the target electron (in atomic units) and

$$S_1^2 = \frac{(E'_1 - \Delta E)}{U_{ii}}$$

where  $\Delta E$  is the energy transferred by the incident electron in the first ionization process and  $U_{ii}$  (in rydbergs) is the energy essential for the ejection of the second electron. The quantities  $n_e$  and  $\bar{r}$  are the number of equivalent electrons and average separation respectively. The value of  $\bar{r}$  is given by

$$\bar{r} = \frac{R}{n_e^{1/3}}$$

$R$  being the radius of the shell. In the equation (3)  $f(t)$  denotes the Hartree-Fock momentum distribution function which has been constructed according to the method explained earlier using Hartree-Fock radial functions for ions given by Clementi and Roetti [7]. The values of direct double ionization cross sections have been estimated by evaluating the integrals in equation (3) numerically over the energy transfer  $\Delta E$  and Hartree-Fock Velocity distribution for the bound electron. Further, to evaluate the total direct double ionization cross sections for the ion, the contributions from inner shell ionization have been taken into account. During the consideration of inner shells contributions, we have assumed that the first electron is always ejected from the valence shell whereas the second electron may be ejected from one of the inner shells.

In the present calculations, we have used the binding energy of the shells given by Lotz [8] and value of ionic radii have been taken from Hand Book of Chemistry and Physics, Chemical Rubber company, USA [9]. The inner shell radii of ions have been calculated using Bohr model of atom. For these calculations the effective nuclear charge has been obtained using Slater's rule.

## RESULTS AND DISCUSSION

In this paper we have calculated electron impact double ionization cross sections for La<sup>++</sup>. The

Calculated results have been compared with recent experimental observations Hirayama et al. [1].

The results of  $\text{La}^{++}$  have been presented in table 1. Experimental cross section curve has a single peak at about 500ev impact energy. The cross section at the peak is  $9.75 \times 10^{-19} \text{ cm}^2$ . No structure has been observed in the experimental cross section curve. Present calculation also shows as maximum at about 300ev impact energy. The value of maximum in the cross section curve is  $1.45 \times 10^{-18} \text{ cm}^2$ . Thus, although the position of the calculated peak is shifted towards the low impact energy side the magnitudes of calculated and observed cross sections overestimate the experimental results at low impact energies but the agreement between the calculated and experimental results improves with the increase in impact energy. The calculated results show reasonably good agreement with experimental observations. Discrepancies observed at low impact energies may partly be attributed to non-suitability of the binary encounter approximation under these conditions. More ever use of hydrogenic wave-function while considering the ejection of the second electron might partly be responsible for overestimation of cross sections at low impact energies. Use of Hartree-Fock velocity distribution for both the ejected electrons would lower the cross section at low impact energies leading to improved agreement with experiments.

**Table – 1**

**Electron impact double ionization of  $\text{La}^{++}$  (in units of  $\text{cm}^2$ )**

| Impact energy (ev) | Present Calculations | Experimental (Hirayama et al. <sup>12</sup> ) |
|--------------------|----------------------|-----------------------------------------------|
| 100.0              |                      | 1.6-30                                        |
| 125.0              | 0.12-20              |                                               |
| 130.0              | 0.36-19              |                                               |
| 135.0              | 0.90-19              | 0.90-19                                       |
| 170.0              | 0.81-18              | 9.69-19                                       |
| 200.0              | 1.66-18              | 6.9-19                                        |
| 250.0              | 1.92-18              |                                               |
| 300.0              | 1.62-18              | 9.0-19                                        |
| 500.0              | 1.16-18              | 8.6-19                                        |
| 650.0              | 0.36-18              |                                               |
| 700.0              | 0.38-8               | 7.6-19                                        |
| 900.0              | 0.68-18              | 5.6-19                                        |
| 950.0              | 0.62-18              |                                               |
| 1000.0             | 0.65-18              | 5.8-19                                        |

1.0-20 stands for  $1.0 \times 10^{-20}$

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