

## **Multiple ionization effect on $L_{\alpha}$ X-ray production cross sections of Dy, Ho and Er at 320 keV proton energy**

Manpuneet Kaur<sup>1, 2</sup>, Harsh Mohan<sup>3,\*</sup>, Arvind Kumar Jain<sup>3,\*</sup>, Parjit S. Singh<sup>2,\*\*</sup>, Santosh Kurra<sup>1</sup> and Bal Krishan<sup>1</sup>

<sup>1</sup>*Department of Physics, Guru Nanak Khalsa College, Yamuna Nagar, 135 001, HR, India*

<sup>2</sup>*Department of Physics, Punjabi University, Patiala 147 002, Pb, India*

<sup>3</sup>*Department of Physics, M. L. N. College, Yamuna Nagar, 135 001, HR, India*

\*, \*\* Present address:

\* Department of Physics (retired), M. L. N. College, Yamuna Nagar, 135 001, HR, India

\*\* Department of Physics (retired), Punjabi University, Patiala 147 002, Pb, India

### **Abstract**

In the present paper, L shell X-ray production cross sections for three elements ( $Z = 66, 67$  and  $68$ ) at single proton energy i.e. 320 keV have been investigated. Calculations are performed with ECPSSR model with two amendments 1) UA (United Atom) correction 2) Multiple Ionization (MI) effect. The resulting models are ECPSSR-UA and ECPSSR-MI. The resulting values from these two are compared with the available experimental values. Results with MI effect show the improvement over UA.

### **Introduction**

The passage of charged projectile in the target atom creates a vacancy in it. This vacancy can be filled via two independent processes: either by emission of X-rays or by ejection of Auger electrons. When the target is heavier then the probability of emission of X-rays becomes more [1]. These rays carry a lot of information about the target atom. In other words they carry the signature of the target atom. Study of X-rays has a significant role in various analytical techniques and attracted huge interest for last few decades [2-5]. One of these is PIXE (Particle Induced X-ray Emission) having applications in different fields such as medical, environmental, elemental analysis and material science [6-8]. Data published shows that a large portion of research is on K shell [9, 10]. Work is scanty for L shell especially with light projectiles like protons having low energy [11, 12]. This could be due to the fact that L shell consisting of three subshells, all having their different properties. Their way of ionization, decay of vacancy and their rearrangement processes are comparatively typical. The present research has been performed on L shells of three elements Dy, Ho and Er considering proton as the projectile having energy 320 keV. The aim of the present research is to motivate the researchers as well as enhance the data points at low proton energy.

### Theoretical methodology

In the year 1958, Merzbacher and Lewis [13] provided the Plane Wave Born Approximation (PWBA) for the calculation of ionization cross sections. This approximation was followed by the two classical theories named SCA (Semi Classical Approximation) [14] and BEA (Binary Encounter Approximation) [15-17]. But these theories fitted well only for the charged particles having high energies. At low energies, PWBA and BEA over predicted the cross sections. After that, Basbas *et al.* [18, 19] developed the PWBA by incorporating different effects like polarization, binding, Coulomb deflection (C) and relativistic motion of target electrons in the PSS (perturbed stationary state approximation). The inclusion of all these effects results to the CPSSR model [20]. Further inclusion of energy loss effect in this model gives the ECPSSR theory [21]. But the results of this theory were reliable only for K-shell. They show deviations for L-shell in the low projectile energy region. A modification termed as the united atom correction (UA) has been made in ECPSSR. The resulted model is ECPSSRUA [22, 23]. This model has been considered as the most relevant model for the calculation of K- and L-shell ionization cross sections for light ions. X-ray production cross sections have been extracted using ionization cross sections resulted from ECPSSRUA along with atomic parameters such as fluorescence yield and Coster-Kronig probability. It has been observed that even this model has not been efficient to obtain results at low energies [24-27]. Then the requirement to look over the parameters involved in the calculations has been realized. Keeping it in view, a phenomenon known as multiple ionization (MI) has been studied. The inclusion of this effect improves the results [28, 29]. Lapicki *et al.* [30] suggested a method to correct fluorescence yields and Coster-Kronig probabilities. It has been considered that with the impact of incoming projectile, fluorescence yields are altered by the creation of holes in the outer shells. This alteration has an equal probability for each shell which is calculated through the binary encounter approximation [31]. So, the equations for the corrected fluorescence yield and Coster-Kronig probability [32, 30] are given as

where,

$$\sigma_r^* = \frac{\sigma_r^0}{1 - (Z_1^2 / 2\beta v_1^2) [1 - (\beta / 4v_1^2)] (1 - \omega_r^0)} \quad f_r^* = f_r^0 [1 - Z_1^2 (1 - \beta / 4v_1^2) / 2\beta v_1^2]^2$$

$\sigma_s$  is the single hole fluorescence yield of the  $s^{\text{th}}$  (where,  $s = 1, 2, 3$ ) subshell.  
 $Z_1$  is the atomic number of the projectile.

$f_{st}$  is the single hole Coster-Kronig probability for subshells  $s$  to  $t$ .

$\beta$  is a parameter fixed from electron binding energies, it takes the value 0.9 for the L shell.

$v_1$  is the projectile ion velocity.

These modified parameters (using MI effect) are used for the extraction of X-ray production cross sections using ECPSSR ionization theory. These cross sections are then compared with their values extracted using ECPSSR-UA theory along with the parameters without MI effect. Numerous authors [33-35] have studied the MI effect for heavy projectile ions. Work is scarce with light ions. In this paper an attempt has been made to explore the work with protons having low energies.

### **Results and discussion**

In this paper,  $L_\alpha$  cross sections have been calculated at single proton energy i. e. 320 keV for three elements Dy, Ho and Er (see Figure). The calculations are performed into two sets. One set is accomplished with ECPSSR model including the MI effect. The other with the same model but using the UA correction. In both sets parameters recommended by Campbell [36, 37] are used. The obtained values are then compared with the experimental points [38]. The predictions with MI effect are represented by the solid line while those with UA are by dashed line. However, experimental values are denoted by the solid square. The cross sections are calculated in barns. From Figure, it is observed that the X-ray cross sections decrease with the increase of Z number. It may be due to the effect of nuclear charge which increases with the Z number. The figure shows that the MI effect improves the results. It fetches the values closer to the experimental points. The improvement is more for low Z numbers. As seen from the figure that the MI results are in good agreement with the experimental points. This improvement is more for Dy than that of Ho and Er. For example, in case of Dy, the difference between experimental and calculated values with UA correction was 8-9% and reduces to 0.03% with MI effect. In case of Ho, this difference reduces from 7.7% (UA correction) to 0.07% (MI effect). While for Er, from 14-15% (UA correction) to 5.5% (MI effect). All of these demonstrates that the MI effect is mainly prominent for low Z numbers impacted with low energy proton.

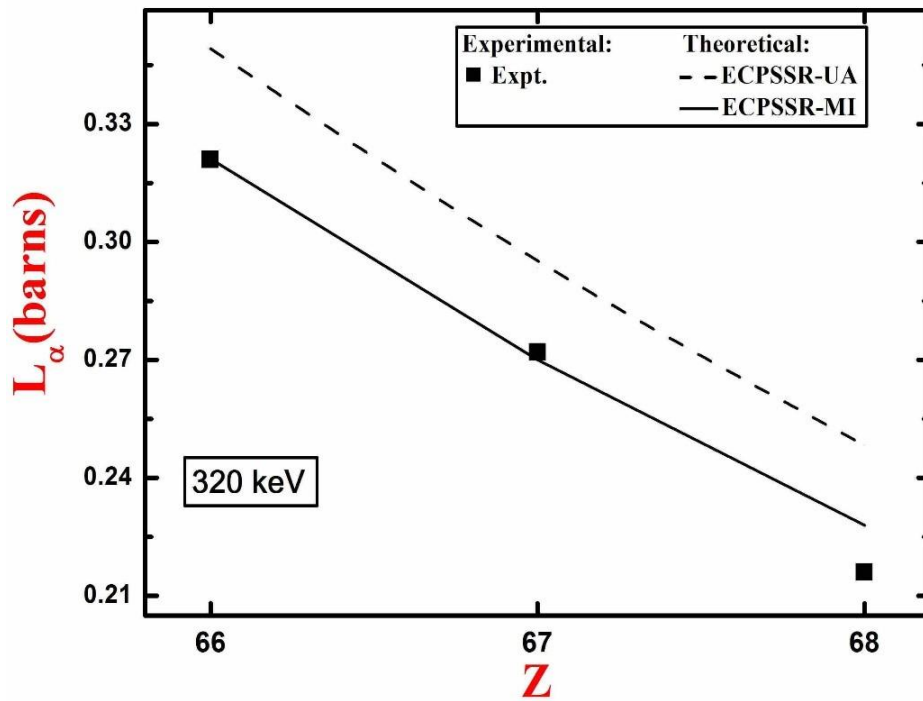


Figure:  $L_{\alpha}$  cross sections of low Z elements at proton energy 320 keV.

### Conclusion

The following are the main conclusions of the present research work:

1. For the comparison of calculated results, the values of a single experimentalist are available only.
2. It has been seen that the calculated results with MI effect are in better agreement with the experimental points than that of investigations with UA correction.
3. It is also perceived that the calculations with MI effect are in very good agreement for lower Z target's than that of the higher one.
4. The experimental work is limited for these elements in the low energy proton region. So there is a need to do experimental work for the present elements at the present proton energy.

## References

1. E. P. Bertin, *Principles and Practice of X-Ray Spectrometric Analysis*, Plenum Press, New York, 1975.
2. Z. Zhang, Y. Zhang, Y. Guo, X. Chen, L. Chen, Impurity element analysis of aluminum hydride using PIXE, XPS and elemental analyzer technique, *Nucl. Instr. Meth. B* **488** (2021) 1.
3. F. J. Ager, M. A. Respaldiza, S. Scrivano, I. Ortega-Feliu, A. Kriznar, B. Gómez-Tubío, Cultural heritage science at CNA (seville, Spain): Applications of XRF and IBA techniques to art and archaeological objects, *Radiat. Phys. Chem.* **167** (2020) 108324.
4. R. J. Chandrasekhar, B.G. Naidu, P. Sarita, S.Srikanth, G. J. Naga Raju, PIXE and ICP-MS Analysis of Andrographis Paniculata Medicinal Plant, *IOP Conf. Ser. Mater. Sci. Eng.* **225** (2017) 012235(1).
5. M. Oswal, R. Kaur, A. Kumar, K. P. Singh, S. Kumar, B. P. Mohanty, S. Kumar, Trace element analysis of aerosol samples using PIXE technique. *Int. J. PIXE.* **22** (2012) 271.
6. M. Vadrucci, A. Mazzinghi, A. Gorghinian, L. Picardi, C. Ronsivalle, C. Ruberto, M. Chiari, Analysis of Roman Imperial coins by combined PIXE, HEPIXE and  $\mu$ -XRF, *Appl. Radiat. Isot.* **143** (2015) 35.
7. N. T. Deoli, A. Mikolajczyk, Z. Fusilier, M. Zappi, H. J. Whitlow, Elemental composition of alligator eggshell and eggshell membrane using micro-PIXE, *Nucl. Instr. Meth. B* **502** (2017) 80.
8. W. Sudprasert, R. Meesata, H. J. Whitlow, H. Udeogu, A. B. De Vera, N. Deoli, Investigation of mercury pathways from dental amalgam by micro-PIXE, *Nucl. Instr. Meth. B* **450** (2017) 347.
9. H. Paul, K-Shell ionization by Light Ions: A graphical comparison of cross sections, *At. Data Nucl. Data Tables* **24** (1979) 243.
10. R. K. Gardner, T. J. Gray, Cross sections for K-shell ionization, X-ray production, or auger-electron production by ion impact, *At. Data Nucl. Data Tables* **21** (1978) 515.
11. J. Miranda, G. Lapicki, Errata and update to "Experimental cross sections for L-shell X-ray production and ionization by protons", *At. Data Nucl. Data Tables* **119** (2018) 444.
12. R. S. Sokhi, D. Crumpton, Experimental L-Shell X-Ray Production and Ionization Cross Sections for Proton Impact, *At. Data Nucl. Data Tables* **30** (1984) 49.
13. E. Merzbacher, H. W. Lewis, In: *Handbuch der Physik*, edited by S. Flugge (Springer- Verlag, Berlin) **34** (1958) 166.
14. J. Bang and J. M. Hansteen, Coulomb Deflection Effects on Ionization and pair-Production Phenomena, *Mat. Fys. Medd. Kgl. Dan. Vidensk. Selsk.* **31** (1959) 13.
15. J. D. Garcia, Inner-Shell Ionizations by Proton Impact, *Phys. Rev. A* **1** (1970) 280.

16. J. D. Garcia, X-ray Production Cross Sections, *Phys. Rev. A* **1** (1970) 1402.
17. J. D. Garcia., E. Gerjuoy, and J. E. Welker, Classical Approximation for Ionization by Proton Impact, *Phys. Rev.* **165** (1968) 66.
18. G. Basbas, W. Brandt, and R. Laubert, Perturbed-Stationary-State Theory of Atomic Inner-Shell Ionization by Heavy Charged Particles, *Phys. Rev. A* **7** (1973) 983.
19. G. Basbas, W. Brandt, and R. Laubert,  $Z_1$  dependence of K-shell X-ray production by heavy charged particles, *Phys. Lett. A* **34** (1971) 277.
20. W. Brandt, G. Lapicki, L-shell Coulomb ionization by heavy charged particles, *Phys. Rev. A* **20** (1979) 465.
21. W. Brandt, G. Lapicki, Energy-loss effect in inner-shell Coulomb ionization by heavy charged particles, *Phys. Rev. A* **23** (1981) 1717.
22. S. J. Cipolla, An improved version of ISICS: A program for calculating K-, L-and M-shell cross sections from PWBA and ECPSSR theory using a personal computer, *Comput. Phys. Commun.* **179** (2008) 616.
23. S. J. Cipolla, The united atom approximation option in the ISICS program to calculate K-, L- and M-shell cross sections from PWBA and ECPSSR theory, *Nucl. Instr. Meth. B* **261** (2007) 142.
24. H. Mohan, Investigation of L X-ray production from Au with protons in low energy region. *J. Phys.: Conf. Ser.* **194** (2009) 082011.
25. H. Mohan, A. K. Jain, G. Kaur, P. S. Singh, S. Sharma, Role of Fluorescence yields, Coster-Kronig transitions and ionization theories on L X-ray intensity ratios of Au. *Radiat. Phys. Chem.* **81** (2012) 1833.
26. H. Mohan, A. K. Jain, M. Kaur, P. S. Singh, S. Sharma, Cross section for induced L X-ray emission by protons of energy  $< 400$ . *Nucl. Instr. Meth. B* **332** (2014) 103.
27. A.K. Jain, H. Mohan, S. Sharma, Effect of vacancy de-excitation parameters on L X-rays of Pb using  $H^+$  beam, *Nucl. Instr. Meth. B* **268** (2010) 1790.
28. M. Kaur, H. Mohan, A. K. Jain, P. S. Singh, S. Sharma, Evaluation of multiple ionization effect in collision of low energy proton with Au, Pb, and Bi, *Radiat. Phys. Chem.* **151** (2018) 120.
29. M. Kaur, H. Mohan, A. K. Jain, P. S. Singh, S. Sharma, Influence of Multiple Ionization on L X-ray Intensity Ratio in Pt Induced by Proton, *Int. J. Pure and Appl. Phys.* **13** (2017) 71.
30. G. lapicki, R. Mehta, J. L. Duggan, P. M. Kocur, J. L. Price, F. D. McDaniel, Multiple outer-shell ionization effect in inner-shell X-ray production by light ions, *Phys. Rev. A* **34**(1986) 3813.
31. D. H. Madison, E. Merzbacher, In: B. Crasemann (Ed.), *Atomic Inner-Shell Processes*, Vol. I Academic Press, New York, 1975.

32. G. Lapicki, G. A.V. Ramana Murty, G. J. Naga Raju, B. S. Reddy, S. B. Reddy, and V. Vijayan, Effects of multiple ionization and intrashell coupling in L-subshell ionization by heavy ions, *Phys. Rev. A* **70** (2004) 062718(1).
33. H. R. Verma, L and M-shell X-ray production cross section measurements in  $^{73}\text{Ta}$  and  $^{78}\text{Pt}$  using  $\text{B}^{3+,4+}$  -ions of energies below and above the potential barrier, *Nucl. Instr. Meth. B* **449** (2019) 75.
34. H. R. Verma, Multiple ionization in  $^{67}\text{Ho}$  and  $^{71}\text{Lu}$  due to the impact of nitrogen- and silver-ions, *Radiat. Phys. Chem.* **150** (2018) 30.
35. M. Oswal, K. Kumar, U. Singh, G. Singh, K.P. Singh, D. Mehta, D. Mitnik, C.C. Montanari, T. Nandi, L X-ray production cross sections in high-Z atoms by 3-5 MeV/u silicon ions, *Nucl. Instr. Meth. B* **416** (2018) 110.
36. J. L. Campbell, Fluorescence yields and Coster–Kronig probabilities for the atomic L subshells, *At. Data Nucl. Tables* **85** (2003) 291.
37. J. L. Campbell, Fluorescence yields and Coster-Kronig probabilities for the atomic L subshells. Part II: the  $L_1$  subshell revisited. *At. Data Nucl. Tables* **95** (2009) 115.
38. P. S. Singh, , Experimental investigation of L X-ray emission phenomenon by low energy charged particles, Ph.D. Thesis (1989), Punjabi University, Patiala, Punjab.