

Investigation of Screening Effect on L- sub shell X-ray Production Cross-Sections by Low Energy Proton for PIXE Application

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Abstract— PIXE (Proton induced x-ray emission) by proton beam is important technique to find out qualitative and qualitative analysis of element present in the specimen. Quantity of the element directly related to x-ray production cross section. Many literature shows discrepancy between theoretical and experimental x-ray cross section. In this work, x-ray production cross section calculated by ECPSSR theory with 25% variation of screening constant for L sub- shell and compared with experimental measured data. Variation of screening constant suggested in literature and we have seen almost no effect in L shell x-ray cross-section.

Keywords-PIXE, X-ray cross-section, ECPSSR, Screening Constant, Ionization cross-section

I. INTRODUCTION

The ionization of the inner atomic shells by ion impact is an important field of physics of atomic collision from theoretical as well as experimental point of view. The study of inner-shell ionization involves measurements of the x-ray production cross-sections for the target atoms. The accurate knowledge of x-ray production cross-sections by ion impact is necessary due to importance of this phenomenon for developing more reliable theoretical (ECPSSR) models. The precise knowledge about the x-ray cross section data for various projectiles and target is needed for analysis of the PIXE data, because PIXE is a very useful technique for elemental characterization of a given sample. PIXE is well known and useful technique for finding out qualitative and quantitative analysis of various samples (taken from environment).PIXE can analyzed a sample that contains about 30-50 elements together with concentration of about 1ppb [1]. The concentration of various elements determined by using the relationship between the net area of an element's characteristic K or L x-ray photo peak line in the x-ray spectrum and the amount of element present in the sample. It has vast applications in various fields of research. In PIXE technique low Z elements are analyzed by x-shell characteristics x-ray, and high Z elements are analyzed by Lshell characteristics x-ray. In order to get precise quantity of element, precise knowledge of x-ray cross section is important.

The ion-atom collision is very complex phenomena, in first order approximation, direct ionization of the inner (K and L) shells by light ions is considered. For heavy ions, the complexity arises due to multiple ionizations, energy loss of projectile, Coulomb deflection, relativistic effects of target

electrons etc. and proper estimate of x-ray cross section becomes very difficult. Measurement of x-ray Cross-sections by impact of a proton is a useful technique for elemental composition analysis and it is also provide knowledge about various physical processes such as fundamental research involving projectile charge change and energy loss, recoil ion production, vacancy rearrangement in target's atomic shell. It has been observed that when theoretical L -shell x-ray production cross-section from low energy H^+ ions with atoms are compared with the experimental cross section significant discrepancy observed particularly in low energy region [2]. This unsolved problem motivated to carry out detailed study for proper understanding of the excitation mechanisms and atom -ion interaction processes. Theoretical model ECPSSR also fail to explain the direct ionization cross section for low velocity projectile in several study [4-8]. In ECPSSR based theoretical investigation the need of more accurate value of the binding energy of the active target electron (U_{2s}) was suggested Ref.[10]. It is important to mention here that U_{2s} is mainly depend on the screening constant (s_{2s}) for the concerning electron in the sub shell. The screening constant is calculated from the Slater's rule. Therefore it is interesting to investigate the effect of screening constant's value on the x-ray production cross section. In this work, Pb was chosen for the investigation and ECPSSR calculations were carried out for Pb target using low energy (proton) H^+ projectile. Further interest to investigate these x-ray production cross section was that the ECPSSR under predicts the cross section for Pb has been selected to see the effect of screening values.

This paper has been organized into six distinct sections-

Int. J. Sci. Res. in Physics and Applied Sciences

Introduction, related works, ECPSSR theoretical model, results, discussion and conclusions. In introduction section briefly about PIXE and importance of x-ray cross section has been discussed, in related work section we have some brief literature review related to our present work. ECPSSR Theoretical model section contains the application of ERCS08 program and theoretical calculation of x-ray cross-section using x-ray ionization-cross section. Results section provides variation of x-ray production cross section with enegy at different value of screenig constant.In the discussion section, the results obtained is discussed and the conclusion section, major conclusions drawn from the results are provided.

II. RELATED WORK

In order to remove deviation between theoretical and experimental K-shell x-ray production cross-section we had carried out two works (i) Effect of different data set of fluorescence yield on x-ray production cross section. Ref.[14].(ii) Investigation of screening effect on K-shell xray cross section for the target Cu, Ag and Cd using low energy proton and result was presented at Proceedings of the DAE Symposium on Nuclear Physics India(2015), Ref.[3].From these work we motivate to investigate variation of screening constant on L sub-shell x-ray production cross section also suggested in literature[10,15].

III. ECPSSR THEORETICAL MODEL

The details of the ECPSSR (Energy loss, Coulomb deflection perturb stationary state with relativistic effect) model are described elsewhere [4-10] which is modified form of the PWBA theory and it includes the effect of projectile energy loss (E), Coulomb deflection of the projectile trajectory (C), polarization effects of the target electron and relativistic (R) effects. Ionization cross section multiplied by emission rate and fluorescence yield gives theoretical x-ray cross section. In the present calculation for L-shell emission rate from J.H. Scofield Ref.[12] and fluorescence yield from Campbell [8] has been taken. ECPSSR calculation is carried out by ECRS08 FORTRAN program. ERCS08 is a windows based program for computing the atomic Ionization cross sections. It is written in FORTRAN, ERCS08 that makes it easy to quickly prepare the input file, run the program, as well as view and analyze the output. The calculations are based on the ECPSSR theory for direct ionization and non-radiative electron capture. The program has the feature with selective inclusion or exclusion of individual contributions to the cross sections from effects such as perturbation of electron's stationary state (polarization and binding) projectile energy loss, Coulomb deflection of the projectile, as well as relativistic nature of the target electron wave function.

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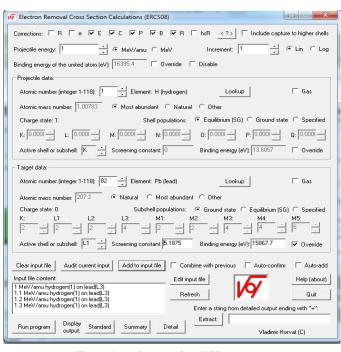


Figure 1. Application of ERCS08 program

IV. RESULTS

Table: Cross-section at different screening value.

Energy (MeV)	Calculated x-ray cross - section (barn) by ECPSSR Theory			Experimental Data
	S=4.15	S=3.1125	S=5.1875	(Ref.[2])
1.0	3.9902	4.1109	3.9459	3.92
1.1	5.2823	5.4340	4.952	5.36
1.2	6.7523	6.9406	6.4872	6.6
1.3	8.4283	8.6234	8.3414	7.6

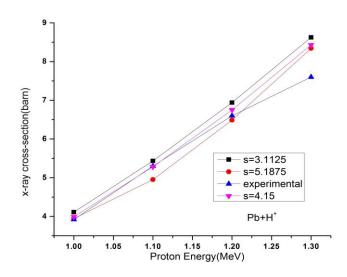


Figure 2. (variation x-ray production cross section with enegy at different value of screenig constant)

V. DISCUSSION

ECPSSR calculations for L-shell x-ray production were carried out for H⁺ projectile at low energy range, 1.0-1.3 MeV, for which experimental data is available [2]. The value of screening constant was s=4.15 as per Slater's rule for Lshell electron. In this work the value of screening constant was varied in steps up to the 25% (up and down) from the suggested value in order to see its effect on the x-ray production cross section. Results for Pb target are shown in figure 1 and compared with the available experimental data [2]. The agreement between experimental and theoretical data seems to improve very little when once consider s= 5.1578 and it deviates further for lower value i.e. s = 3.1125compare to the standard value (s=4.15). The screening constant value calculated using the Slater's rule for L-shell electron for the standard value s=4.15. Further calculation show almost no change in the x-ray production cross section with the variation of screening value as shown in figure 2, from these calculations we see almost no effect in L-shell xray production cross section due to the change in screening constant. Hence modification of screening value ruled out and need precise experimental measurement or theoretical improvement with consideration of some other physical processes involve in ECPSSR theory.

VI. CONCLUSION AND FUTURE SCOPE

The Effect of screening constant on L-shell x-ray production cross-section has been investigated using ECPSSR theoretical model. Screening study shows the similar result as we obtained results on K-shell x-ray cross-section [3]. Theoretical calculations suggests that already existing theoretical (ECPSSR) models may not require much refinement in screening value of L-sub shell to reliably predict the experiments. Consequently study of L sub-shell x-ray cross-section for PIXE application remains as open problem. In order to remove discrepancy of experimental and theoretical x-ray production cross-section, now we plan to study the effect of other basic physical processes involve in ion-atom collisions as our future work.

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