

Effect of Re-correction in the Recoil Energy on K and L-shell X-ray Production Cross-Section by Proton Induced

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Abstract— Proton induced x-ray emission (PIXE) by proton beam is one of the very important technique to find out concentration of element present in the sample. Elemental analyses of low Z element by K-x-ray and heavy element ($28 < Z < 92$) is being done by L-shell x-ray for this, reliable values of K and L X-ray production cross-sections are important. The quantity of the element is directly related to K and L-shell x-ray production cross section. In present work K and L x-ray production cross section has been calculated to remove discrepancy between theory and available experimental data, by ECPSSR theory for target for Cr, Zn and Pb with correction of recoil energy of the proton in energy range 1.0-1.3 MeV. In ion-atom collision, although the recoil energy for low mass ions is not significant but we have seen a significant effect of recoil energy of proton in K and L shell x-ray production cross-section.

Keywords—PIXE, X-ray cross-section, ECPSSR theory, Characteristics X-ray, Recoil Energy, Ion-atom collision.

I. INTRODUCTION

Particle Induce X-ray Emission (PIXE) is an efficient and powerful analytical tool for major, minor, and traces elemental analysis in a variety of fields like biology, environment, medicine, archaeology and forensic science. This technique also used for analyzing the composition of rocks, metals, ceramics and other materials. PIXE is one the very favorable techniques because it is non-destructive and very fast. PIXE technique has several other advantages, such as requirement of analysis of very low concentration of trace elements i.e. quantity of the sample are in trace amount. In this technique ion beam is used to ionize the inner shell of target atoms of the sample and then vacancy is filled by upper-shell's electrons, which leads to emission of a characteristic x-rays. Energy and intensity of these x-rays are used for identification of the elements and for elemental composition in the sample [1]. The reliable knowledge of L x-ray production cross sections is important for these applications. Available literature shows discrepancy between theoretical and experimental x-ray production cross section [1, 3]. The process of x-ray production cross section can be affected due to presence of various other physical processes, such as, Auger process, Coster-Kronig transitions in which transitions do not produce i.e. non radiative transitions. They redistribute the primary vacancies between the different shells and between the different sub-shells of the same shell. As a result, these processes can change the intensity of the

characteristics x-rays. Hence, precise knowledge of the inner shell ionization cross section by proton impact is an important field of physics of ion-atom collision from theoretical as well as experimental point of view. The accurate knowledge of x-ray production cross-sections by ion impact is necessary 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 i.e. reference cross section. 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 great applications in various fields of research and determination of element in different samples. In PIXE technique low Z elements are analyzed by K-shell characteristics x-ray, while high Z elements are analyzed by L-shell characteristics x-ray. In order to get precise quantity of element, precise knowledge of x-ray production cross section is very important.

It has been observed that when theoretical K and 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 [3]. This unsolved problem motivated to carry out detailed study for proper understanding of the excitation mechanisms and atom-ion interaction processes. ECPSSR theory also fails to explain the direct ionization cross section for low velocity projectile in several studies [4-8]. ECPSSR calculations were carried out for Cr, Zn and Pb targets using low energy (proton) H^+ projectile.

This paper has been organized into six distinct sections- Introduction, Related works, ECPSSR theoretical model with re-correction in recoil energy of projectile, Results, discussion and conclusions. In introduction section briefly about x-ray cross section, 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 direct ionization-cross section. Results section provides variation of K and L sub shell x-ray production cross with re-correction in recoil energy of Projectile. In the discussion section, the results obtained is discussed and the conclusion section, major conclusions drawn from the results are provided.

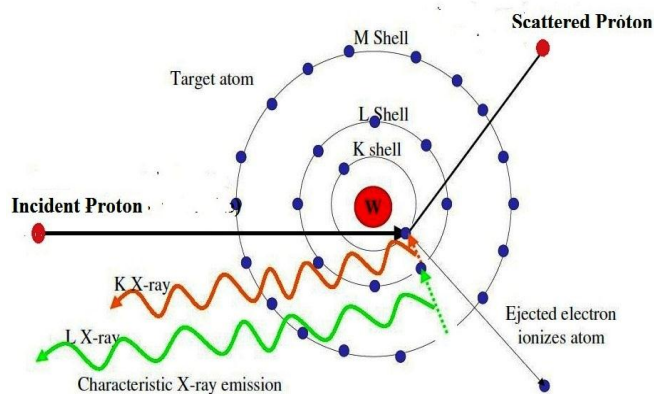


Figure 1. Characteristics X-ray emission

II. RELATED WORK

In order to remove deviation between theoretical and experimental K-shell and L-shell x-ray production cross-section we had carried out four works (i) Effect of re-correction in the recoil energy of Projectile for the X-ray Production cross-section by low Energy Proton[2] (ii) Effect of different data set of fluorescence yield on x-ray production cross section. Ref.[15].(iii) Investigation of screening effect on K-shell x-ray cross section for the target Cu, Ag and Cd using low energy proton.(iv) Investigation of Screening

Effect on L- sub shell X-ray Production Cross-Sections by Low Energy Proton for PIXE Application[15]. These work motivate to us for proper investigation of recoil energy correction effect on K and L sub-shell x-ray production cross section. In ion atom collision, although the recoil energy for low mass ions is not significant, but their effect has been investigated on K shell and L- shell x-ray cross section. Our interest in L- shell x-ray cross-section due to involvement of multiple ionization effect.

III. ECPSSR THEORETICAL MODEL

The details of the calculation of direct ionization by ECPSSR (Energy loss, Coulomb deflection perturb stationary state with relativistic effect) theoretical model are described elsewhere [5-11]. Which is modified form of the Plane wave -Born approximation (PWBA) theory and it includes the effect of projectile energy loss (E), Coulomb deflection of the projectile (C), polarization effects of the target electron and relativistic effects (R). To convert Ionization cross-section into x-ray production cross section it is multiplied by emission rate and fluorescence yield. In the present calculation we adopt simple inelastic collision in which after collision energy of projectile (Proton) reduced by μE , where $[\mu = m_p / (m_p + M_T)]$, m_p , M_T and E is represent mass of Proton, mass of chosen target and the energy of Proton respectively. Hence modified energy of projectile become $E' = E - \mu E$. In present calculations K-shell emission rate taken from ref [12] and K-shell fluorescence yield from [10], L-shell emission rate from J.H. Scofield [13] and fluorescence yield from Campbell [9] has been taken. ECPSSR calculation is carried out by ERCS08 FORTRAN program. ERCS08 is a windows based program for calculating the atomic Ionization cross sections (Direct+ Electron capture). It is written in FORTRAN using double precision, ERCS08 that makes it easy to quickly prepare the input file, run the program, and give the output. The program has the feature with selective options inclusion or exclusion of individual contributions to the ionization cross sections from physical effects such as perturbation of electron's stationary state (polarization effect and binding capture of e from higher atomic shell) projectile energy loss, Coulomb deflection of the projectile as well as relativistic nature of the target's electron.

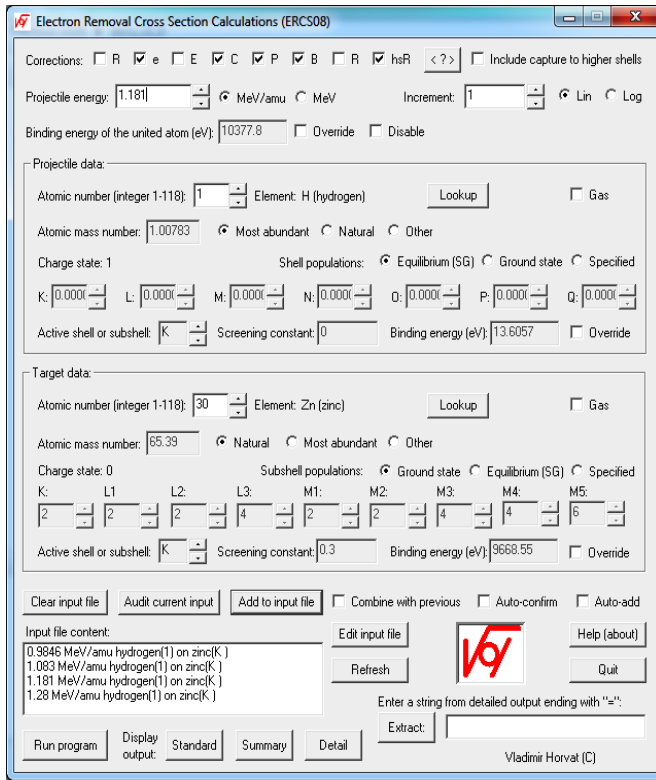


Figure 2. Application of ERCS08 program for present calculations.

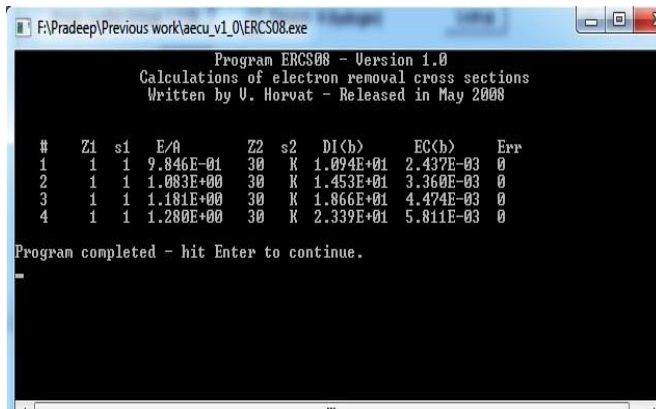


Figure 3. Output results after run of ERCS08 program.

IV. RESULTS

Table: K-shell X-ray Cross-section at different energy for Cr+H⁺.

Energy (MeV)	ECPSSR Theory	ECPSSR (Corrected)	Experimental data (Ref.[2])
1.0	28.71	27.32	24.2
1.1	36.54	34.84	31.5
1.2	45.12	43.12	37.4

Energy (MeV)	ECPSSR Theory	ECPSSR (Corrected)	Experimental data (Ref.[2])
1.0	28.71	27.32	24.2
1.3	54.36	52.03	47

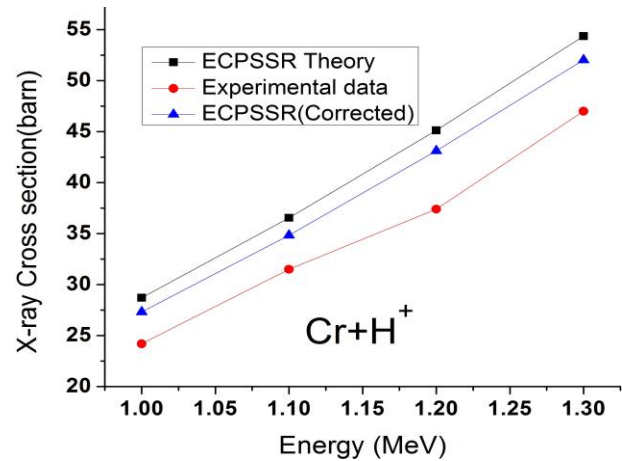


Figure 4. Variation of K-shell x-ray production cross section with corrected and uncorrected projectile energy, Chromium as a target and proton as projectile.

Table: K-shell X-ray Cross-section at different energy for Zn+H⁺.

Energy (MeV)	ECPSSR Theory	ECPSSR (Corrected)	Experimental data (Ref.[2])
1.0	5.43	5.18	4.7
1.1	7.20	6.88	6.3
1.2	9.25	8.84	8.3
1.3	11.57	11.08	10.1

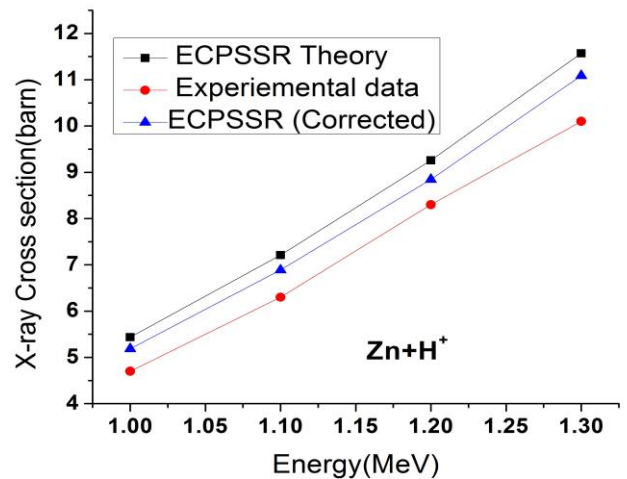


Figure 5. Variation of K-shell x-ray production cross section with corrected and uncorrected energy. Zinc as a target and proton as projectile.

Table: L-shell X-ray Cross-section at different energy for Pb+H⁺.

Energy (MeV)	ECPSSR Theory	ECPSSR (Corrected)	Experimental data (Ref.[2])
1.0	4.08	4.02	3.9
1.1	5.40	5.32	5.3
1.2	6.90	6.80	6.6
1.3	8.57	8.46	7.6

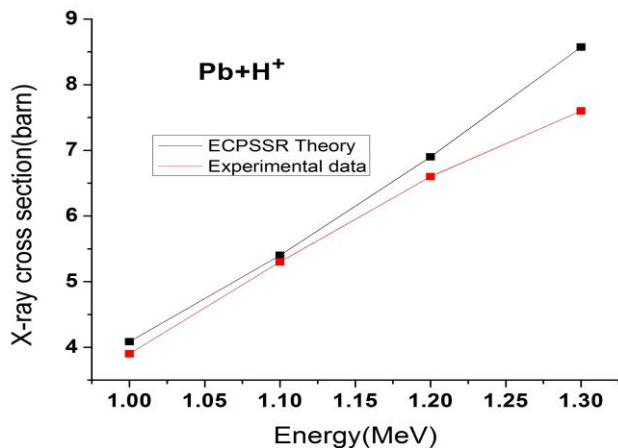


Figure 6. Variation of L-shell x-ray production cross section with corrected and uncorrected energy of projectile. Lead as a target and proton as projectile.

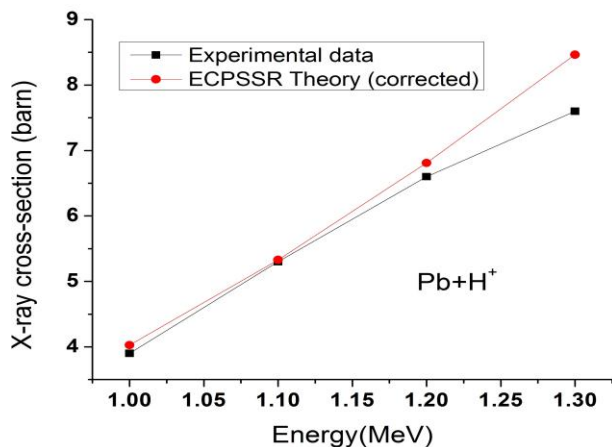


Figure 7. Variation of L-shell x-ray production cross section with corrected and uncorrected energy of projectile. Lead as a target and proton as projectile.

The X-ray production cross section have been calculated for K, L-shell using H⁺ ion as a projectile, incident on Cr, Zn and Pb for various energies where experimental data available [3]. Theoretical Calculations were performed without considering recoil energy and with a re-correction for the recoil energy. Results of both the calculations are

shown in plot (figure 4-7) and also compared with the experimental data [3]. In these calculations emission rates and fluorescence yields for particular shells are taken from Campbell [9] and Krause [10].

Since theoretical model has energy loss effect but if we consider our proposed energy loss correction in the projectile then the discrepancy between experiment and theoretical x-ray cross section for K shell seems to be reduced from 12% to 5% in Cr and Zn target, while in L-shell x-ray for Pb target it is only significant change, due to the re-correction of recoil energy (figure 4-5.). This demonstrates theoretical result need proper correction to remove discrepancy with experimental data. For have a clear picture, a systematic investigation is being done to check the effect on various targets and projectiles combinations, which will be our future works.

V. Discussion

Theoretical mode (ECPSSR) calculations for K and L-shell x-ray production were carried out for H⁺ projectile at low energy range, 1.0-1.3 MeV with different targets Cr, Zn and Pb, for which experimental data is available [3]. The recoil energy correction of projectile Proton has been done in order to see its effect on the x-ray production cross section. Results for Cr, Zn (K-shell x-ray) and Pb (L-shell x-ray) target are shown in figure 4-7- and compared with the available experimental data [3]. The discrepancy between experimental and theoretical (ECPSSR) data seems to improve very little up to 5% for K-shell x-ray and a significant change in L-shell x-ray production cross section. The re-corrected recoil energy of the projectile proton calculated using the simple inelastic collision concept. L-shell x-ray cross section calculation show almost very little significant change in the L-x-ray production cross section with the correction of recoil energy value as shown in figure 6-7. Hence modification of recoil energy value lead some significant change in both K and L-shell x-ray production cross section.

VI. CONCLUSION AND FUTURE SCOPE

The Effect of recoil energy correction on K and L-shell x-ray production cross-section has been investigated using theoretical model (ECPSSR). Recoil energy correction shows the significant change in result as we obtained results on K-shell x-ray cross-section for Cu atom [2]. Theoretical calculations using ECPSSR theory suggests that already existing theoretical models may require some refinement in projectile energy loss value for K and L-sub shell x-ray cross section to reliably predict the experimental data. Consequently proper study of K, L and M sub-shell x-ray cross-section is important to understand basic physical phenomena and for PIXE application. It remains as open problem for research work. In order to understand

discrepancy between experimental and theoretical x-ray production cross-section, we plan to study of other basic physical processes involve in ion-atom interactions, as our future work.

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