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Electron momentum distribution and Compton profiles of tin

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Abstract The Compton profile of Sn has been measured using a HPGe photon detector. The target atoms were exited by means of 59.54 keV gamma rays from Am-241 radioactive source of strength 300 mCi. Elemental foil of uniform aerial density and purity better than 99 9% was used as target The data was recorded and analyzed using a 4K multichannel analyzer The experimental data was corrected for instrumental resolution effects, sample absorption and energy dependence of the differential Compton cross-section. The Compton profiles measured in the present work for Sn constitute the first experimental report for 59.54 keV gamma rays scattered at 165° The results are compared with theoretical Hartree-Fock free-atom profiles

Keywords : Compton scattering; Compton profile; electron momentum density, impulse approximation

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1. Introduction

Studies on interaction of gamma radiation with matter and the associated processes are important because of the light they throw on many basic aspects of physics as well as immense practical applications in modern industry and technology. The gamma ray photons are absorbed or scattered in a single event when they pass through matter. There are 12 different processes by which gamma ray photons interact with matter [1,2]. The relative magnitude of these processes depends on the incident photon energy and the atomic number of the target atom. In the energy range 0.1 to 10 MeV of common interest, however, most of the interactions are due to one of the three processes: photoelectric effect, scattering by the atomic electrons and pair production.

The discovery of Compton scattering by Compton [3] is a milestone in the history of Modern Physics. Compton effect is one of the interactions between an incident radiation and electron in the target atom. Compton scattering is the predominant mode of interaction in the incident energy range from 0.1 to 1 MeV. In the Compton scattering, electron absorbs some of the momentum and the scattered photon has less energy than the incident photon. Photon scattering is most complete and satisfactory for photon energies much higher than the electron binding energies that the electrons can be considered as free. In this process, there is no phase relation between the radiations scattered by different electrons. Incoherent scattering of photons from electrons has become a well-established tool to measure wave functions [4] and it gives information about the phase of the valence band. It also provides a means to test quantum electrodynamics, the polarization of photons and the distribution of momentum of electrons within the atoms [5].

When radiation is Compton scattered, the wavelength of the emerging beam is increased depending upon the angle of scattering but independent of the material and also the emerging beam is Doppler-broadened. Ross was the first person to suggest that the momentum of the scattering electron might influence the structure of the modified line [6]. It was confirmed by Jauncey [7] and he transformed it into formal theory. Jauncey's analysis consists of two points. Firstly, he conceived of the interaction between the photon and the electron as taking place impulsively *i.e.* the interaction time is so short that the scattering is over, before the electron has had a chance to move in the potential well and change its potential energy. This approximation is known as the Impulse Approximation (IA) and is referred to as the starting point for the analysis of Compton

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profiles. The implication of this approximation is that the bound electron can be treated as free with the same momentum distribution. Secondly, Jauncey recognized that inelastic Compton scattering occurs only when the energy transfer to the electron is greater than its binding energy. If this is not satisfied, the photon interacts with the whole atom of mass M and the Compton shift is correspondingly reduced by m/M ~ 10^{-3}. Hence, the scattering is essentially elastic for incident photon energies in the X - ray region.

DuMond [8] formulated a description of the Doppler-broadening mechanism, which was independent of the atomic model. He showed that the effect of the electron's motion on the Compton scattering process could be described as a Doppler-broadening process like the Doppler-broadening of spectral lines produced by atoms in thermal motion. The Compton profile can be considered as the Doppler broadening of the Compton shifted line. The spectral analysis of the scattered radiation reveals the line shape. Within the framework of impulse approximation, the double differential Compton cross section is proportional to the Compton profile which is the projection of the electron momentum density along the direction of the scattering vector. The impulse approximation assumes that the reaction time involved in the Compton scattering is so small that the initial and final electrons see the same constant potential. This technique is particularly sensitive to the behaviour of the slowly moving outer electrons involved in bonding and hence it serves as a tool for testing the accuracy of the wave function. A comparison of the experimental and theoretical Compton profiles, provides an estimate of the reliability of the assumed electronic configuration and wave function. Such basic information is useful in the study of all the physical properties of a system.

Non-relativistic conservation equations for Compton effect are given by [9]

$$\text{Momentum}: \; hk^1 - hk = p - p^1, \tag{1}$$

$$\text{Energy}: \; hck^1 - hck = \left[(1/2m)\left(p^2 - p^{1^2}\right)\right]. \tag{2}$$

The scattering vector $s = k^1 - k$ and assuming that $|s| >> |k| - |k^1|$, the final electron momentum p^1 can be eliminated to give

$$\lambda^1 - \lambda = (2h/mc)\sin^2(\theta/2) - (2\lambda/mc)\sin(\theta/2)p_z, \tag{3}$$

where p_z is the electron momentum along the z-axis.

The second term of eq. (3) describes the broadening of the scattered radiation, which is proportional to the component of the electron's momentum parallel to the crystallographic scattering vector. This equation is the starting point of electron momentum distribution studies. At any point in the line profile corresponding to the component momenta p_z, the intensity will be proportional to the probability of observing that particular component momentum. The line shape - the Compton profile - can be evaluated as a function of that one component of momentum P_Z *viz*:

$$J(P_Z) = \int_{Px} \int_{Py} P_{(Px,Py,Pz)}\, dp_x\, dp_y\,, \tag{4}$$

where the probability distribution function $P_{(p)}$ is the momentum wave function. It is a one dimensional momentum distribution [10].

The primary cause of interest in the measurement of Compton profiles is the electron momentum distribution. Experimentally, Compton profiles measure the projection of electron momentum distribution on a line and hence provide considerable complimentary information on the basic aspects of physics and practical applications in industry and technology. The application of Compton profile measurements also cover several inter disciplinary areas like chemistry, materials science, physical metallurgy, polymer science and medical science.

In this paper, we report a systematic study of the Compton profile of Sn. In Section 2, we briefly describe the experimental arrangement. The results and discussion, and conclusion are given in Sections 3 and 4 respectively.

2. Experimental details

The gamma ray spectrometer used in this work has been described elsewhere [11]. In the present work, Compton profiles of a thin foil of element Sn (purity better than 99.9%) were measured using an IGC 15190 series HPGe photon detector supplied by M/s. Princeton Gamma-Tech, Inc, NJ. It has dimensions of 5.05 cm of active diameter and an active volume of 90 cc. The target atoms were excited using 59.54 keV gamma rays from 300 mCi Am-241 source. The optimum distance between the source and the scatterer was chosen to be 25 cm and that between the scatterer and detector, 20 cm. The gamma rays scattered at a mean angle 165^0, were detected by the detector having a resolution of 2 keV at 1332 keV and 780 eV at 122 keV. The linearity of the spectrometer was studied by using standard gamma ray sources and was found that it possesses very good linearity. The stability was also tested and it was observed that the shift in the peak channel was less than a channel over a period of 3 days. The data were collected and analyzed using a PC based 4K MCA. A separate measurement was made without the sample to obtain background contribution that was scaled to the measurement time of the foil and then subtracted point by point from the measured data. The signal to noise ratio was found to be 50:1. About 10000 counts were collected at the Compton peak. The spectrum recorded for 59.54 keV gamma rays scattered at 165^0 are presented in Figure 1. In order to reduce the absorption in the scatterer, very thin elemental foil of thickness 0.0913 gm/cm^2 and dimensions of 2.5 x 2.5 cm was employed as target scatterer and the criterion $\mu t < 1$ (μ is the linear attenuation coefficient and t is the target thickness) was satisfied [12]. The value of μt was equal to 0.5994. Hence, error due to Bremsstrahlung and multiple scattering are expected to be negligibly small. The double differential Compton cross section was measured from the scattered spectra. Compton profile was then derived from the measured cross sections since the double differential cross section and Compton profile $J(P_Z)$ are linearly related.

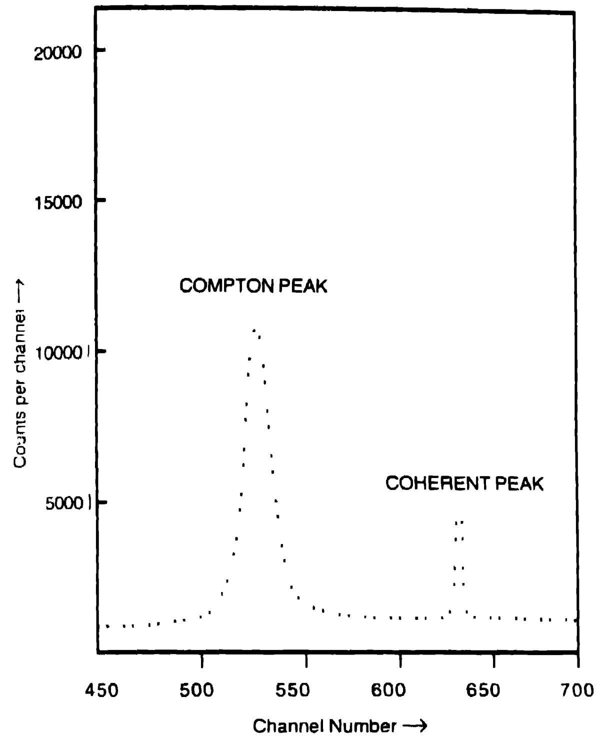

Figure 1. The spectrum recorded for 59.54 keV gamma rays scattered at 165°

The uncertainty in setting the target foil angle was about 2%, which contributes a negligible error in the measured Compton profile. The statistical error due to count rate were reduced and kept within 2% by counting the data for a long time. The counts under the peak were determined accurately after subtracting the background counts and applying Gaussian fitting. The error due to the uncertainty in evaluating the solid angles was less than 1%. The estimated error in the determination of photopeak efficiency of the detector using the standard weak sources was about 2%. The errors associated in evaluating the source strength was estimated to be about 3%. All the errors were compounded according to the well-known rules of propagation of errors and the resultant error was quoted on the measured Compton profiles. The raw data were corrected for background, absorption in the sample, instrumental resolution and differential scattering cross section [13,14]. The binding energy of K shell in Sn is greater than the recoil energy and hence, these 1*s* electrons do not contribute to the Compton profile in the present measurements. The present data was thus normalized to 19.86 electrons being the area of the corresponding free atom profile in the momentum region 0 to 7 a.u., excluding the contribution of 1*s* electrons. The Compton profile of Sn obtained with 59.54 keV gamma rays through a mean angle of 165° in the present work constitute the first measurement.

3. Results and discussion

The Compton profile of Sn was measured with the aid of experimental set-up described in Section 2. The measured Compton profiles of Sn are compared in Table 1 and Figure 2 with theoretical values calculated from the relativistic Hartree-Fock wave functions [15]. For $P_Z = 0$ a.u., the measured value is smaller (~ 19%) than the Hartree-Fock values. This deviation is due to the fact that the contribution of inner-core electrons is smaller in this region. Also, it indicates the neglect of electron correlation beyond the HF parallel spin exchange. A proper inclusion of electron correlation produces an isotropic correction, which reduces the difference between experiment and theory [16]. However, between 0.6 and 5.0 a.u., the present results are slightly broader than the theory. This broadening may be due to electron-electron correlation, which pushes a part of the occupied states below the Fermi momentum to momentum values above the Fermi momentum. At higher P_Z values ($P_Z > 4$ a.u.), the present data agree well with the Hartree-Fock free atom values. In this momentum transfer region, the contribution of valence electron is very small and hence, most of the contribution may be due to the inner-core electrons. These

Table 1. Comparison of Compton profiles of Sn with theory.

P_Z a.u	$J(P_Z)_{Expt}$ Present work	$J(P_Z)_{Theo[15]}$ HF
0.0	7.899 ± 0.236	9.40
0.1	7.845 ± 0.235	9.28
0.2	7.623 ± 0.228	8.92
0.3	7.330 ± 0.219	8.35
0.4	7.065 ± 0.211	7.68
0.5	6.871 ± 0.206	7.02
0.6	6.658 ± 0.199	6.46
0.7	6.367 ± 0.191	6.02
0.8	5.940 ± 0.178	5.70
0.9	5.634 ± 0.169	——
1.0	5.320 ± 0.159	5.28
1.2	5.075 ± 0.152	4.97
1.4	4.782 ± 0.143	4.66
1.6	4.432 ± 0.132	4.32
1.8	4.097 ± 0.122	3.97
2.0	3.684 ± 0.110	3.62
3.0	2.313 ± 0.069	2.23
4.0	1.627 ± 0.048	1.56
5.0	1.296 ± 0.038	1.24
6.0	0.989 ± 0.029	1.02
7.0	0.829 ± 0.024	0.833

inner-core electrons are reasonably described by the free-atom values.

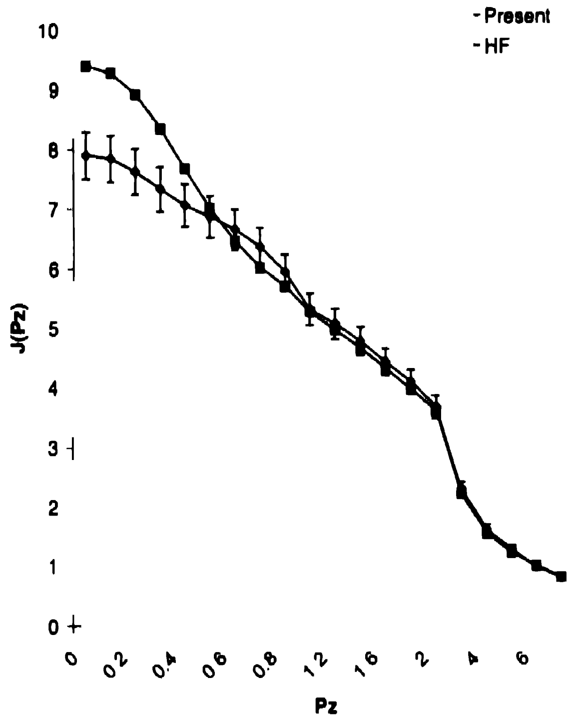

Figure 2. Comparison of the present results of Sn with theoretical values based on Hartree-Fock wave functions

4. Conclusion

In this paper we have reported experimental data on Compton profile of element Sn. The results are in relatively good agreement with Hartree-Fock Compton profile data particularly in the high momentum transfer region. In order to throw more light on the electron momentum distribution of high Z elements, improvement in the calculations and more extensive and systematic measurements particularly with high-energy gamma ray photons are needed.

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