ФИЗИКО-МАТЕМАТИЧЕСКИЕ НАУКИ / PHYSICS AND MATHEMATICS

DATA ANALYSIS IN GAMMA-RAY COMPTON SPECTROSCOPY

S. A. Hamouda

University of Benghazi (Benghazi, Libya)
dr_s_hamouda@yahoo.ie

Compton scattering is a technique for determining the momentum distribution of electrons in condensed matter. Therefore, in the Compton scattering experiment all the available data about the electron's initial state is contained in the distribution of the inelastically scattered radiation, i.e. the Compton profile. However, before the data can be interpreted, a series of energy dependent corrections have to be applied. In this paper, general aspects of the Compton Scattering theory are introduced. Data analysis procedure for the γ-ray experiment is outlined and the sensitivity of these corrections on the quality of the final results is discussed.

Keywords: high energy gamma-ray spectroscopy, methods and technologies, material characterization, Compton data reduction procedure, materials properties, measuring methods and applications, detection techniques

АНАЛИЗ ДАННЫХ В КОМПТОНОВСКОЙ ГАММА-СПЕКТРОСКОПИИ

С. А. Хамуда

Университет Бенгази (г. Бенгази, Ливия)
dr_s_hamouda@yahoo.ie

Введение. Комптоновское рассеяние является методом оценки распределения электронов по импульсам в конденсированных средах. В статье рассматриваются общие аспекты теории комптоновского рассеяния.
Материалы и методы. Для изучения комптоновского рассеяния были применены данные, полученные с помощью нового комптоновского гамма-спектрометра высокой энергии. Статья описывает влияние поправок в зависимости от мощности энергии в ходе эксперимента с использованием вольфрама на источнике 137Cs.
Результаты исследования. В ходе эксперимента по изучению рассеяния по Комптону все имеющиеся данные о начальном состоянии электрона были получены из распределения неупругого рассеянного излучения, т. е. профиля Комптона.
Обсуждение и заключение. В статье обсуждается необходимость внесения корректировки для точного понимания конечных результатов; доказывается необходимость подобного уточнения в ходе интерпретации данных эксперимента в зависимости от мощности энергии.

Introduction

When monochromatic photons are Compton scattered (inelastically scattered) in a fixed direction, the observed energy spectrum of the scattered photons is Doppler-broadened due to the motion of the target electrons. This broadened line shape, referred to as the Compton profile, $\mathbf{J(p_z)}$, can be analyzed to yield detailed information about the electron momentum distribution, $\mathbf{n(p)}$, in the sample under study. Within the impulse approximation [1], the Compton profile, $J(p_z)$, is defined as the projection of the ground state electron momentum density distribution, n(p), along the scattering vector (chosen as the p_z axis) and is given by;

$$J(p_z) = \iint n(p_x, p_y, p_z)\, dp_x\, dp_y . \quad (1)$$

Therefore, in the Compton scattering experiment all the available information about the electron's initial state is contained in the distribution of the inelastically scattered radiation, i.e. the Compton profile. A detailed review of this topic can be found in [2–3].

Over the range of energies below 1MeV, the Compton cross-section is proportional to the atomic number Z whereas the photoelectric cross-section is approximately proportional to Z^4/ω_1^3 where ω_1 is the incident photon energy. This implies that the ratio of Compton to photoelectric cross section is approximately proportional to ω_1^3/Z^3. For 662 keV gamma ray radiation, the Compton cross section is greater than the photoelectric cross section up to about Z = 90 [4]. As a result, the higher energy of the gamma ray makes Compton profile measurements to be performed on a wide range of high Z-materials and their alloys which are completely impractical at the present x-ray energies.

However, before the data can be interpreted, a series of energy dependent corrections have to be applied [5]. In this paper an outline of the data corrections is presented and the sensitivity of these corrections on the quality of the final results is discussed.

An outline of data process

The order of data corrections is illustrated schematically in Fig. 1.

When enough counts have been accumulated in the Compton profile, the obtained primary data are the measured spectrum, M (ω). When these corrections shown in Fig. 1, are applied to the measured spectrum, they can be either additive, multiplicative or convolutive. The measured Compton energy spectrum can be described in terms of these corrections as,

$$M(\omega) = R(\omega) * E(\omega)\, G(\omega) * S(\omega) * {} \\ * A(\omega)\, [\, D(\omega) + B(\omega)], \quad (1)$$

where ***** represents a convolution and these corrections are defined in Fig. 1. The Compton profile is then extracted from the measured Compton data, M(ω) by rearrangement of Eq. 1, and can be expressed as,

$$J(p_z) = N\, C^{-1}(\omega)\, A^{-1}(\omega)\, E^{-1}(\omega)\, S^{-1}(\omega) \\ * G^{-1}(\omega) * R^{-1}(\omega)[\, M(\omega) - B(\omega)], \quad (2)$$

where $^{-1}$ represents a deconvolution and N is the normalization constant characterized by the sample (i. e. number of

electrons for normalization) and all other corrections are defined in Fig. 1. The order of corrections illustrated schematically in Fig. 1, has been adopted for the analysis of Compton data obtained from the new high energy gamma-ray Compton spectrometer. The following sections describe the effect of the energy dependent corrections on measurement made on tungsten sample using the 137-Cs source spectrometer employed in the present study.

Background Subtraction $M(\omega)-B(\omega)$

Deconvolution of resolution function $R(\omega)$

Deconvolution of geometrical broadening function $G(\omega)$

Deconvolution of source broadening function $S(\omega)$

Detector efficiency correction $E(\omega)$

Sample absorption correction $A(\omega)$

Ribberfors cross section correction $C(\omega)$

Initial normalization N

Multiple scattering correction $J_{multiple}(p_z)$

Final normalization N
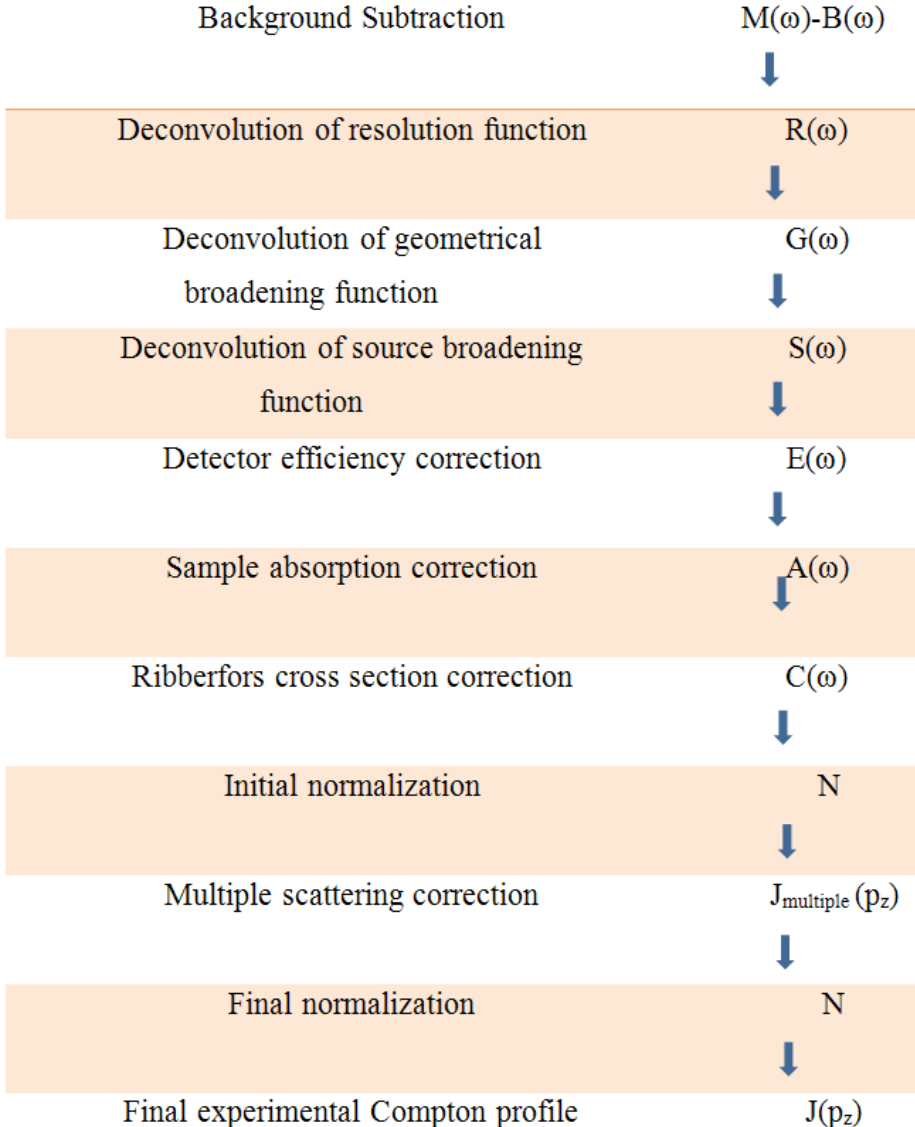
Final experimental Compton profile $J(p_z)$

F i g. 1. Flow chart of the data reduction procedure used to extract the Compton profile $J(p_z)$ from the measured energy spectrum, $M(\omega)$

Р и с. 1. Блок-схема процедуры сжатия данных, используемых для извлечения Комптоновского профиля $J(p_z)$ из измеренного энергетического спектра, $M(\omega)$

The Background Subtraction

The background is defined as the signal obtained with the source opened and no sample in position. The main sources of the background are: (1) the natural radioactivity such as cosmic rays; (2) stray radiation from the source; (3) scattering from the sample chamber, sample holder, air in the scattering chamber, and detector collimator. Therefore, it is necessary to measure the background spectrum and then subtract this from the Compton scattering data before the remaining data processing procedures can be used.

Fortunately, in gamma-ray experiments the background can be measured independently compared with x-ray experiments. Since the background can be measured in an independent experiment an appropriate energy calibration of the spectra is required. It is important to emphasize the point that the experimental condition (i. e. geometry, collimation, shielding arrangement) in which the Compton data are obtained should not differ from the experimental condition in which the background is measured. But unfortunately it does because the sample itself masks off part of the scattering volume of the scattering chamber. In the background measurement only the sample is removed, and everything else must remain the same. This will allow for the background measurement to be consistent and minimize the systematic error. Because the 137-Cs source has a long half-life (30 years), the background contribution is considered to be time-independent. Since the background spectrum is subtracted from the Compton data on point-by-point basis, the background measurement should have good statistics so that time scaling is properly performed.

Detector Response Function Correction

The detector response function is defined as a measure of the amount of broadening of a monoenergetic radiation line in the Compton peak range. Its main features are a Gaussian peak and an extended tail on the low energy side of the line. The low energy tail originates from partial absorption processes such as imperfect charge collection within the germanium crystal. The existence of the low energy tail in the detector response function influences the shape of the true symmetric Compton profile in such a way that the measured Compton peak is the convolution of the detector response function and the true symmetric Compton profile [6]. When the resolution function is convoluted with the true symmetric Compton profile it produces a progressive asymmetric broadening on the low energy side of the profile, leaving the high energy side of the profile largely unaffected. Therefore, the extraction of the true symmetric Compton profile from the measured data requires the removal of the low energy tail (i.e. deconvolution) from the measured data.

In the present studies, the detector resolution function was measured using a 123-Hg 297,1 keV point source. The point source is placed at the sample position in order to mimic the experimental geometrical condition. The measured resolution function is shown in Fig. 2. Since the Compton energy is located at 288 keV the error involved in the resolution function measurement is about 1%. This error is eliminated by shifting the energy of the resolution function peak to the Compton energy with the corresponding FWHM at Compton energy. On the other hand, the height of the tail shown in Fig. 2, and its detailed shape measured with 123-Hg source at 297,1 keV is not expected to differ had the measurement been made at Compton energy (288 keV). This is because the detector efficiency remains almost the same in the energy range between the two energy points (i. e. 10,17 % at 279,1 keV and 10 % at 288 keV). Therefore, the measured resolution function is considered reliable and is used in the present studies for data analysis.

However, it is important to point out that the correction on the low energy side of the measured Compton line is very sensitive to the exact form of the resolution function. The deconvolution correction was found to be very sensitive to the height of the low energy tail with respect to the peak height. The tail height of the resolution function shown in Fig. 2, extends from 0,3 % to about 1 % of the peak height. The increase of the tail height at the low energy side of the line simply reflects the efficiency curve of the detector.
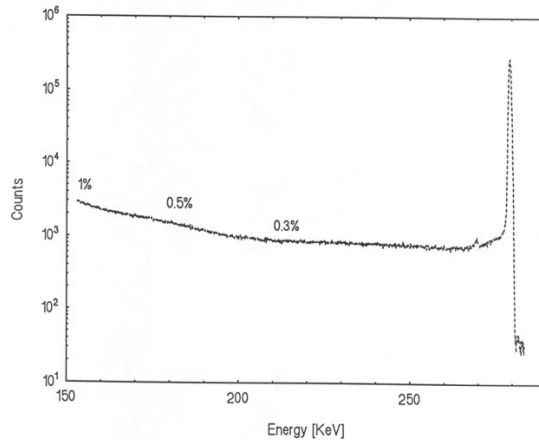

F i g. 2. The detector resolution function measured with the 123-Hg line.
The tail/peak ratio (%) is shown

Р и с. 2. Функция разрешения детектора, измеренная с линией 123-Hg.
Показано отношение хвост/пик (%)

As can be seen from Fig. 2, the tail height to peak height ratio of the measurement was 0,3 %. The task now is what tail height should be selected that can reduce the asymmetry of the measured Compton profile to a minimum. This can be done by using different tail heights and looking for the minimum asymmetry produced by the deconvolution correction procedure. This empirical approach is based on the fact that after all corrections have been made the profile must be centrosymmetric. Fig. 3, shows the results of the Compton profiles for a tungsten sample as a function of the tail height (in % of the peak height). The asymmetry of the Compton profile is referred to the difference (%) between the high energy side and the low energy side of the Compton profile.

As can be seen from Fig. 3, that the minimum asymmetry was obtained (i. e. 1 % asymmetry) when the tail height was 0,3 % of the peak height which reflects the true ratio of the measurement. When the tail height increases above 0,3 % of the peak height the asymmetry of the Compton profile becomes worse. If the height of the tail is higher than a certain limit (i. e. > 0,3 % of the peak height) the deconvolution (removal of the tail) correction becomes large. When the Compton profile is normalized the high energy side of the Compton profile is lifted up, thus increases the asymmetry of the resulted Compton profile. This can be seen in Fig. 3, which shows that the deconvolution correction is in fact very sensitive to the height of the resolution function tail.
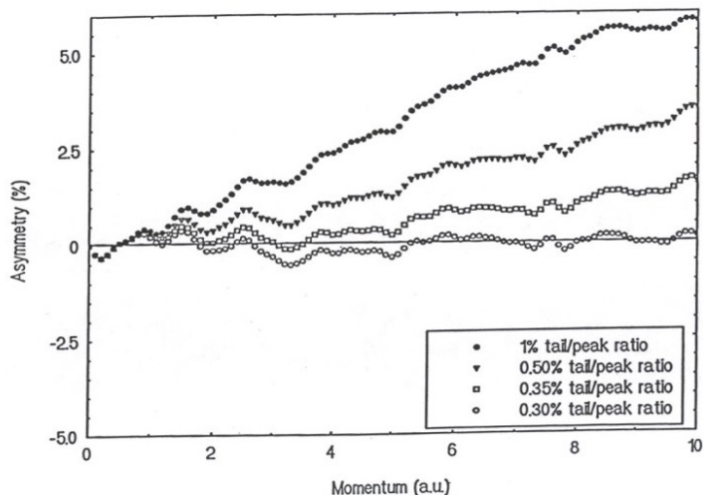
Физико-математические науки

F i g. 3. The asymmetry of the Compton profiles (%) produced as a function
of the tail/peak ratio of the resolution function

Р и с. 3. Асимметрия комптоновского профиля (%) в зависимости
от отношения хвост/пик функции разрешения

Geometrical Broadening Function Correction

The geometrical broadening results from the beam divergence due to finite collimation. The uncertainty of the scattering angle, due to beam divergence, results in an energy dispersion which broadens the experimental profile. Therefore, in order to minimize the asymmetry as well as improving the accuracy of the experimental profile, the effects produced by the geometrical broadening must be removed from the measured profile [7].

Since the geometrical broadening can not be measured in an independent experiment, it is calculated by Monte Carlo simulation of the ray path. In this calculation only one slit collimator for both source and detector was considered. Fig. 4. shows the shape of the geometri-cal resolution function obtained from the simulation for 100 000 photons. The simulated angular intensity distribution curve is approximated by a polynomial of an 8th order in order to remove the random statistical fluctuations from the calculated intensity distribution.

As can be seen from Fig. 4, the geometrical resolution function is a Gaussian with FWHM = 0,5 a.u. (1 a.u. Of momentum is 2.0×10^{-24} kg m s^{-1}). The objective of data correction discussed in this section is to deconvolute the geometrical resolution function from the experimental profile. In the data analysis, the geometrical resolution function is convoluted with the detector resolution function (discussed in section 4) and then deconvoluted from the experimental data by means of the fast Fourier transform method.
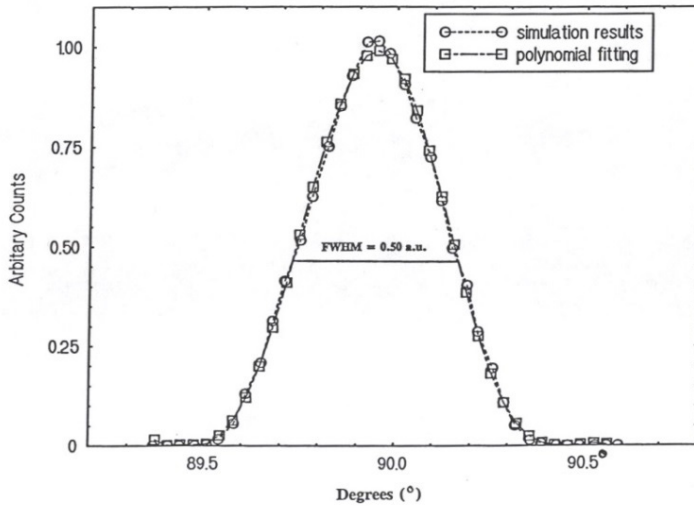
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F i g. 4. The calculated geometrical resolution function
for the 137-Cs spectrometer

Р и с. 4. Расчетная геометрическая функция разрешения
для спектрометра 137Cs

Source Broadening Function Correction

The source broadening arises from the fact that the incident mono-energetic photon radiation can be degraded by inelastic scattering within the source and emerge with a wide range of lower energies, thus contributing to Compton profile asymmetry [7]. Therefore, in order to minimize the Compton profile asymmetry, the spectral distribution of the inelastic scattering within the source has to calculated and removed from the experimental profile. In the present studies, the source broadening function of the 137-Cs disc source (of 6 mm diameter and 4 mm thick) was calculated by Mote Carlo simulation developed by [8]. To remove the effects produced by the inelastic scattering within the source, an additional deconvolution correction is required. When this correction is applied, the deconvoluted profile is then convoluted with a Gaussian of FWHM equal to the experimental resolution. The overall effect of all the deconvolution corrections discussed in the present data analysis procedure is to remove the low energy asymmetry and smooth the experimental data. Accordingly, the theoretical profile must also be convoluted with a Gaussian of FWHM equal to the experimental resolution before comparing it with experimental profile.

Detector Efficiency Correction

The need to apply a detector efficiency correction to Compton data when using high gamma-ray energy (> 60 keV) is well established [9]. In the low gamma-ray energy range (i. e. < 60 keV) a detector efficiency correction is unnecessary because the efficiency of a solid state detector is 100 %. However, at higher gamma-ray energies (> 60 keV) the efficiency curve of a solid state detector falls rapidly, decreasing from 100 % at 60 keV to 31 % at 160 keV to 10 % at 288 keV (Compton energy). This is shown in Fig. 5. Therefore, the efficiency correction formulated in this section is only applicable to Compton data measured with the 662 keV 137-Cs spectrometer.

The main result of the rapid variation in the detector efficiency for the Cs-

spectrometer is to produce an asymmetrical Compton profile. In order to restore the symmetry of Compton profile, it is necessary to determine accurate efficiency curve of the solid state detector in the region of interest. This is because efficiency corrections to the measured data are large, and a consequently small error in the efficiency curve will be amplified when the data is normalized.

The detector efficiency correction procedure is as follows; (i) energy calibration for the multi-channel analyzer (MCA). (ii) determining the detector efficiency function, $E(\omega)$. (iii) dividing the data (point-by-point) by the detector efficiency function. In the familiar way the detector efficiency is calculated using the expression,

$$E(\omega) = 1 - \exp\left[- (\mu)\, t \right], \qquad (3)$$

where (μ) is the energy dependent photoelectric attenuation coefficient of the detector crystal and t is the effective detector crystal thickness. In the present case the detector crystal was germanium (Ge) with an effective thickness of 7 mm. In order to test whether the calculated detector efficiency function given by Eq. 3, is a proper function and can be used for detector efficiency correction, it is necessary to carry out actual detector efficiency measurement and then to compare the measured efficiency with the efficiency calculated using Eq. 3. In the present study the detector efficiency was determined experimentally by comparing the measured intensities of the 8 most noticeable gamma-lines of the 133-Ba point source, with the known relative intensities of the gamma-emission taken from [10]. The 133-Ba point source was placed at the sample position as to mimic the actual experimental situation.
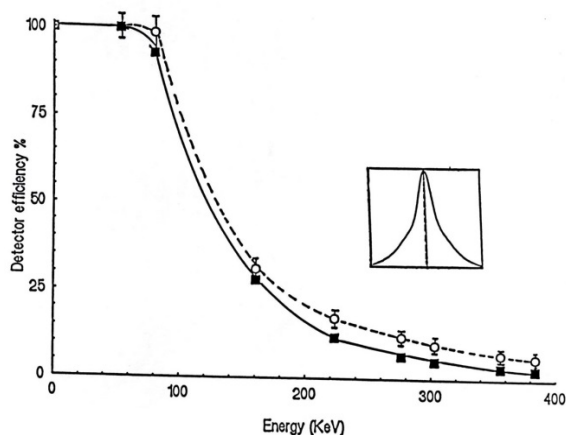

F i g. 5. The measured detector efficiency from the emission lines of 133-Ba (dashed line, open circles) and the calculated efficiency using eq. 3 (solid line, filled squares).The schematic Compton profile shown in the figure indicates the profile peak position for the 137-Cs spectrometer

Р и с. 5. Измеренная эффективность детектора от линий излучения 133-Ba (пунктирная линия, полые кружочки) и расчетная эффективность с использованием формулы 3 (сплошная линия, сплошные квадраты). Схематический профиль Комптон, показанный на рисунке, указывает на пик положения профиля для спектрометра 137-Cs

The experimentally determined detector efficiency and the calculated efficiency using Eq. 3, are shown in Fig. 5. As can be seen from the figure, the efficiency curve determined experimentally gave higher efficiency values than that predicted by Eq. 3. This implies that the behavior of the efficiency curve of the solid state detector may not be as simple as that described by Eq. 3, which depends only on the photoelectric absorption coefficients and the crystal thickness. A calculation of efficiency is difficult because of the complicated way in which the photon interaction processes contribute to the total photopeak. At high γ-ray energy Compton scattering within the crystal may also contribute to the photopeak and therefore Compton absorption coefficients may need to be included in Eq. 3.

However, in order to find an efficiency function which can describe to a very good approximation the determined effi-

ciency curve, one must look for an empirical analytical function of the photon energy. The empirical analytic function that is found to describe the behavior of the experimental efficiency curve over a limited energy range centered around the Compton profile and is used for data analysis is of the form,

$$E(\omega) = a \ \exp(-b\omega), \qquad (4)$$

where ω is the photon energy, a and b are the fitted parameters determined from the straight line that fits the measured efficiency points best (see Fig. 6). Since the Compton energy is located at 288 keV, the fitted parameters a and b were chosen in such a way that the analytical efficiency function given by Eq. 4, describes very well the experimental efficiency in the energy range from (223 keV – 356 keV).
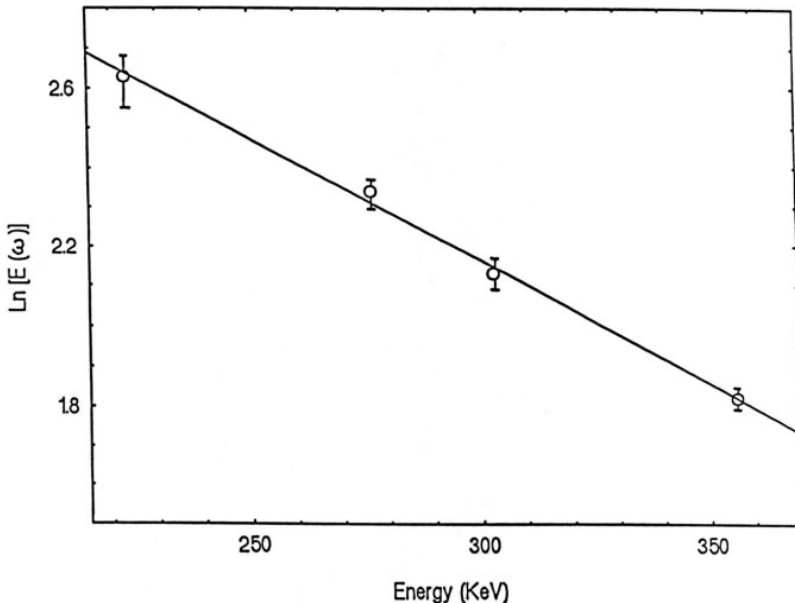

F i g. 6. The detector efficiency function used for the 137-Cs experiment. The parameters a and b are determined from the curve shown and are applied in Eq. 4, which is used for efficiency correction

Р и с. 6. Функция эффективности детектора используется для эксперимента с 137-Cs. Параметры **a** и **b** определяются из кривой, показанной и применяются в уравнении (4), которое используется для коррекции эффективности

Multiple Scattering Correction

One of the main energy dependent corrections is that the experimentally observed Compton profile consists of unavoidably a significant amount (10–20 %) of multiply scattered events occurred in a specimen. Fig. 7 (a), shows the refection geometry for a single scattering events and Fig. 7 (b) shows the double scattering events. The presence of multiple scattering events within the same energy range as the single scattering events is the main difficulties in interpreting the Compton spectra.

The multiple scattering events and their wide energy distribution tends to enhance the high momentum component of the observed Compton profile. However, experimental methods to minimize multiple scattering are impracticable [11–14]. The complexity of multiple scattering together with the variation in experimental conditions i.e. scattering angle, collimation, energy, sample thicknesses, and sample density make analytical solutions almost impossible. Currently corrections for multiple scattering in Compton profiles use Monte Carlo techniques originally developed by [15]. The correction for multiple scattering in the sample is performed by subtracting the simulated spectra of the multiply scattered photons from the experimental profile.
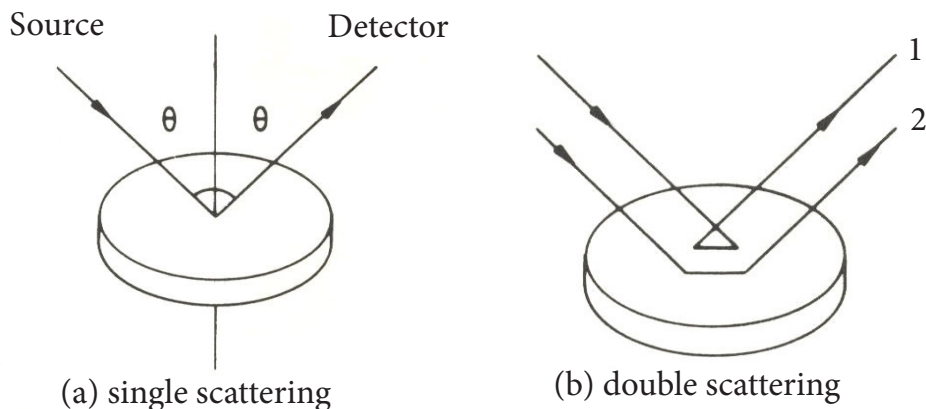

F i g. 7. Reflection and sample orientations showing (a) single scattering events and (b) double scattering events. Paths I and 2 refer to the most probable double scattering events within a thin sample

Р и с. 7. Отражение и ориентация образца, показывающие **(a)** события однократного рассеяния и **(b)** события двойного рассеяния. Контуры I и 2 относятся к наиболее вероятным событиям двойного рассеяния в тонком образце

The angular distribution of the multiple scattering depends on the scattering angle. At a scattering angle θ the angular distribution of the multiple scattering extends from θ to (360-θ). The shape of the multiple scattering distribution and magnitude depend on material thickness and the incident photon energy. Fig. 8, shows the multiple scattering distribution produced by tungsten sample of 1mm thickness scattered at 90^0 with an incident gamma-ray energy of 662 keV [13]. The spectral distribution of the multiply scattered photons shown in Fig. 8, was determined by a Monte Carlo simulation and contained 2×10^4 photons from an input of 38 million photons. Since the photoelectric absorption in tungsten is high at lower energies, photons with energy range around 288 keV are able to escape absorption in the sample (see the inset Fig. 8).
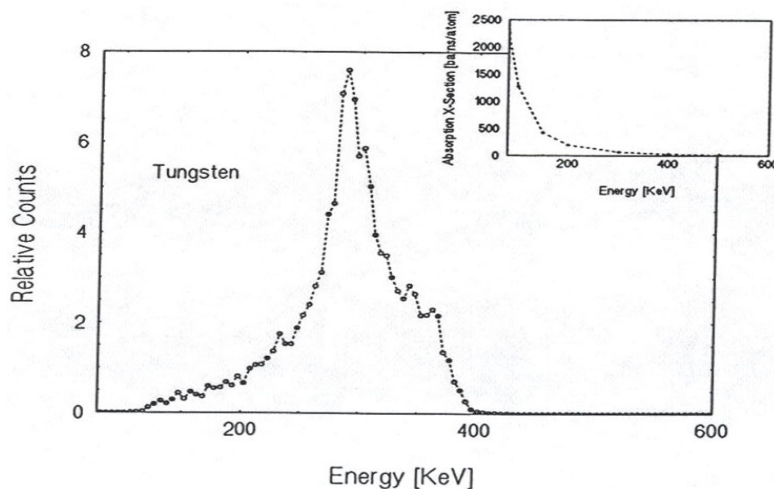
F i g. 8. The multiple scattering distribution from tungsten at 90^0 scattering angle
with 662 KeV incident photon

Р и с. 8. Распределение многократного рассеяния вольфрама под углом 90^0
с рассеянием падающего фотона энергией 662 KeV

Summary

Gamma-ray Compton spectroscopy is a technique for determining the momentum distribution of electrons in condensed matter. Therefore, in the Compton scattering experiment all the available information about the electron's initial state is contained in the distribution of the inelastically scattered radiation, i.e. the Compton profile. However, before the data can be interpreted, a series of energy dependent corrections have to be applied. These corrections can be either additive, multiplicative or convolutive. In this paper, only an outline of the data corrections is presented and the effect of these corrections on the final Compton lineshape are discussed in detail. If undetected error is introduced in these corrections it will make the interpretation of the final results very difficult.

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About the author:

Samir A. Hamouda, professor of Department of Physics of Faculty of Science, University of Benghazi (Benghazi, Libya), Ph.D. (Physics), **ORCID: http://orcid.org/0000-0002-9958-0257**, dr_s_hamouda@yahoo.ie

Об авторе:

Самир А. Хамуда, профессор кафедры физики факультета науки Университета Бенгази (г. Бенгази, Ливия), кандидат физических наук, **ORCID: http://orcid.org/0000-0002-9958-0257**, dr_s_hamouda@yahoo.ie