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A new data treatment scheme for integrated intensities in neutron Compton scattering

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Abstract

A new data reduction scheme is presented for time-of-flight data collected in neutron Compton scattering experiments with the aim of obtaining the scattering intensities. The method proposed is a single number approach as it makes use of the count rates detected in the individual time-of-flight channels. The most convenient seems to be the variant of the method where time-of-flight channels are chosen corresponding to centers of recoil peaks of individual masses. With such a choice of time-of-flight channels, the method presented is more robust against unwanted background signals and noise than the method widely used in NCS studies based on fitting entire time-of-flight band shapes in the framework of the convolution approximation. Moreover, it should perform better than the model-free Dorner method as it does not require the numerical integration of the signal, which is also sensitive to baseline and noise. As an example of the performance of the new method, polyethylene data are treated and compared to results obtained previously using conventional data reduction and the model-free method proposed by Dorner. It is shown that all three data reduction schemes lead to the same results for the scattering intensities of protons in polyethylene, thus strengthening the conclusion about the anomalous scattering cross-section of protons in this substance. In the future the new data reduction scheme can be used to treat the data from other experiments where the conventional NCS data treatment and/or Dorner method fail due to noise and/or unwanted background signals present in the time-of-flight spectra.

1. Introduction

Neutron Compton scattering (NCS) is a unique tool for the investigation of ultra-fast dynamics in condensed matter [1]. It was the NCS method that led to the discovery [2] of the shortfall of the scattering intensity from protons, originally measured on the unique time-of-flight (TOF) spectrometer VESUVIO at the ISIS pulsed neutron source. Since then, this striking effect has been observed in liquids (water, benzene, etc) and solids (metal–hydrogen systems, organic polymers, etc) (see e.g. [2, 3, 5–8, 4]). Recently, this phenomenon has been confirmed with an independent method: electron Compton scattering from nuclei (ECS) [9].

Triggered by the observation of a striking anomaly of the scattering intensities from protons at high energy and momentum transfers was the recent upsurge of interest in the field of data treatment from the neutron Compton scattering (NCS) experiments [10–12, 14–18, 20]. The anomalous NCS intensities were measured with an experimental set-up where the neutron detectors are placed at fixed scattering angles and data are recorded as a function of the time of flight (TOF), usually with final neutron energy fixed by the resonance absorption energy of the analyzer foil (inverse geometry set-up) [10, 11]. The TOF data consist of a number of peaks centered at TOF values corresponding to recoil energies for neutrons scattered off individual masses present in the sample of interest. In the established NCS data reduction scheme, in order to compare the experimental values of scattering intensities with theoretical expectation, the entire profile of each recoil peak must be fitted in TOF by a theoretical

expression making use of the convolution approximation (CA) [10, 11].

Recently, another NCS data reduction scheme was introduced by Dorner [14] aiming at the determination of scattering intensities in a model free manner. This scheme does not require any assumption on the shape of momentum distribution of the target nuclei and the instrument resolution function. The Dorner scheme was successfully applied to the polyethylene (PE) TOF data recorded at the inverse geometry spectrometer VESUVIO at the ISIS spallation source at the Rutherford Appleton Laboratory [15, 16]. The anomaly of the scattering intensities of protons calculated using the Dorner scheme was found to be the same, to within the experimental error, as the anomaly calculated using the conventional CA data reduction. This result was also confirmed by Dorner in an independent study [17].

Here, we present for the first time a new NCS data reduction scheme. The scheme is based on the fact that, in the CA approximation, the count rate in each TOF channel is proportional to the scattering cross-section density, a single number. Thus, it is possible to calculate the scattering cross-section density based on the count rate recorded for each individual TOF channel. The prerequisite for the method is, however, that spectra recorded at sufficiently high scattering angles are selected for the analysis. This enables the separation of recoil peaks off different masses in a sample. Provided such an experimental situation is achieved, especially convenient is the calculation at time-of-flight channels corresponding to recoil peak centers. A recoil peak center for a given mass present in a sample is of special physical importance. It corresponds to a scattering event of a neutron off a nucleus having no component of nuclear momentum along the direction of neutron momentum transfer. Moreover, at this specific point in a TOF recoil peak the energy and momentum transfers from a neutron fulfill the dispersion relation exactly. Moreover, and most importantly for the numerical analysis, the ratio of the count rate recorded to the intensity of noise and/or background is highest at the recoil peak center.

In this paper we apply the new data reduction scheme to calculate the scattering cross-section densities in polyethylene (PE). The values of scattering cross-section densities are calculated from known experimental count rates at centers of hydrogen (H) and carbon (C) recoil peaks. This calculation is performed for each detector in the forward scattering direction, where good H and C peak separation is achieved (thus for scattering angles greater than 50°). The values obtained are compared to the result of previous study on PE, making use of the conventional CA method and the model free Dorner method. It is shown that, within experimental errors, all three methods yield the same results. The presented new data treatment scheme yields a result that strengthens the experimental conclusion on NCS data obtained on PE, namely, that the scattering cross-section off protons shows a striking anomaly. Moreover, it opens a new possibility of obtaining scattering cross-section densities in NCS measurements in cases where the conventional CA method fails due to the presence of strong background signals or noise in TOF spectra.

2. NCS scattering in impulse approximation

In all NCS experiments the accessible quantity is the double differential cross-section $\mathrm{d}^2\sigma/[\mathrm{d}\Omega\,\mathrm{d}E_1]$. Following van Hove's scattering formalism [21, 22], the double differential cross-section is related to the dynamic structure factor $S(\mathbf{q}, \omega)$, with $\mathbf{q}$ and ω being the transferred momentum and energy, respectively. If $S(\omega, \mathbf{q})$ is assumed to depend only on the magnitude of the momentum transfer $q = |\mathbf{q}|$ one can write for one type of scattering atom

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E_1} = Nb^2\sqrt{\frac{E_1}{E_0}}S(q,\omega). \tag{1}$$

Here b is the bound scattering length, $\mathrm{d}\Omega$ is the solid angle and $\mathrm{d}E_1$ the range of final energies into which the neutron is scattered, N is the particle number density, and E_0 and E_1 are the initial and final neutron energies, respectively.

The double differential cross-section $\mathrm{d}^2\sigma/[\mathrm{d}\Omega\,\mathrm{d}E_1]$ is calculated per unit incident flux into a solid angle $\mathrm{d}\Omega$ and an energy interval $\mathrm{d}E_1$ [22]. The incident neutron spectrum varies with incident neutron energy, E_0, and has a distribution $I(E_0)\,\mathrm{d}E_0$ [12]. For the fixed final energy E_1 and constant scattering angle θ the count rate $C(\theta = \text{const}, E_0)$ in an NCS experiment can be written as [12]

$$C(\theta = \text{const}, E_0) = ANb^2\sqrt{\frac{E_1}{E_0}}I(E_0)S(\theta = \text{const}, \omega) \tag{2}$$

where the proportionality constant A contains the instrumental parameters that are independent of the scattering mass M and the scattering angle θ.

In the NCS regime the energy and momentum transfers from the neutron to the scattering nuclei are so high that the scattering process can be treated within the impulse approximation (IA) limit [19, 23–27]. In the IA limit, i.e. infinite q, $S(q, \omega)$ reduces to a single peak centered at the recoil energy $\omega_\mathrm{r} = q^2/2M$ of the corresponding nucleus of mass M, i.e.,

$$S(q,\omega) = \int \delta[\omega - \omega_\mathrm{r} - (\mathbf{q}/M)\cdot\mathbf{p}]n(\mathbf{p})\,\mathrm{d}\mathbf{p}, \tag{3}$$

where $\mathbf{p}$ is the momentum of the scattering atom and $n(\mathbf{p})$ is the momentum distribution function [19].

It was first emphasized by West [28] that, in the simultaneous limit $q \to \infty$ and $\omega \to \infty$, $qS(q, \omega)$ does not depend on q and ω separately, but on the scaling variable y,

$$S(q,\omega) = \frac{M}{q}J(y), \tag{4}$$

where y is the momentum $\mathbf{p}$ of the nucleus projected onto the scattering vector $\mathbf{q}$ [19, 23], i.e.,

$$y = \mathbf{p}\cdot\hat{\mathbf{q}} = (M/q)(\omega - \omega_\mathrm{r}) = (M/q)(\omega - q^2/2M) \tag{5}$$

where $\hat{\mathbf{q}}$ is the unit vector in the direction of the momentum transfer. $J(y)$ is the so-called Compton profile [23, 19] representing the momentum distribution of the scattering

nucleus along y. For an isotropic system, in which $n(\mathbf{p})$ depends only on the magnitude of $\mathbf{p}$, $p = |\mathbf{p}|$, $J(y)$ can be written [19]

$$J(y) = 2\pi \int_{|y|}^{\infty} n(\mathbf{p})\, p\, \mathrm{d}p. \tag{6}$$

Thus, equation (2) can be rewritten in the following form:

$$C(\theta = \text{const}, E_0) = ANb^2 \sqrt{\frac{E_1}{E_0}} I(E_0) \frac{M}{q} J(y). \tag{7}$$

The most common assumption in the NCS studies is that the momentum distribution $J(y)$ has a normalized Gaussian form [10, 27, 11, 29, 24]:

$$J(y) = \frac{1}{\sqrt{2\pi\sigma_p^2}} \exp\left(\frac{-y^2}{2\sigma_p^2}\right) \tag{8}$$

with standard deviation σ_p.

The spectra are however recorded and plotted as a function of time-of-flight instead of E_0 with $C(t) = C(E_0)\mathrm{d}E_0/\mathrm{d}t$. The Jacobian $\mathrm{d}E_0/\mathrm{d}t$ is given by the following expression [10]:

$$\frac{\mathrm{d}E_0}{\mathrm{d}t} = \frac{2}{L_0}\sqrt{\frac{2}{m}} E_0^{3/2}. \tag{9}$$

Using the Jacobian $\mathrm{d}E_0/\mathrm{d}t$ one writes [10] for the count rate $C(\theta = \text{const}, t)$ in a time-of-flight channel t

$$C(\theta = \text{const}, t) = \frac{E_0(t) I[E_0(t)]}{q(t)} A' M I_M J_M[y_M(t)] \tag{10}$$

where A' is another mass independent experimental constant.

If atoms of different masses M are present in the sample, it follows for the count rate in the time-of-flight channel t that ([10], equation (2.22))

$$C(\theta = \text{const}, t) = A' \frac{E_0(t) I[E_0(t)]}{q(t)} \sum_M I_M M J_M(y_M(t)) \tag{11}$$

where both the experimental constant A' and the factor $\frac{E_0(t) I[E_0(t)]}{q(t)}$ are mass independent and can be written in front of the sum over M.

Integrated peak intensities I_M for a mass M of the scatterer are proportional to the total bound scattering cross-section density $I_M = AN_M\sigma_M$, where $\sigma_M = 4\pi b_M^2$ is the total bound scattering cross-section [30]. Hence, the measured value of $[I_H/I_X]_{\text{exp}}$ can be compared to the value of $[I_H/I_X]_{\text{theor}} = (N_{\text{H}}\sigma_{\text{H}})/(N_X\sigma_X)$ calculated taking the tabulated [30] value of σ_M and N_M, for a mass M, known from chemical formula and/or sample preparation. The ratio $R = \frac{[I_H/I_X]_{\text{exp}}}{[I_H/I_X]_{\text{theor}}}$ is smaller than unity in our experiments on hydrogen containing materials [2, 3, 5–8], thus indicating the anomalous neutron Compton scattering from protons.

3. Materials and methods

3.1. The VESUVIO spectrometer at the ISIS spallation source and the convolution approximation

The VESUVIO spectrometer is an inverted geometry time-of-flight instrument [10]. Incident neutrons travel a distance L_0 from the pulsed source to the sample. After scattering at an angle θ, neutrons of final energy E_1 travel a distance L_1 to the detector position (figure 1). The sample is exposed to a polychromatic neutron beam. The energy E_1 of the neutron after the scattering process is analyzed by taking two spectra, one with a thin foil of a neutron absorbing material between the sample and the detector and one without such a foil. In most NCS experiments a thin gold foil, absorbing neutrons with final energy $E_1 = 4.9$ eV, is used. This was also the case for the NCS measurement on the polyethylene sample reported here. The spectrum to be analyzed is obtained by taking the difference of these two spectra. This standard technique is referred to as single difference (SD) [10].

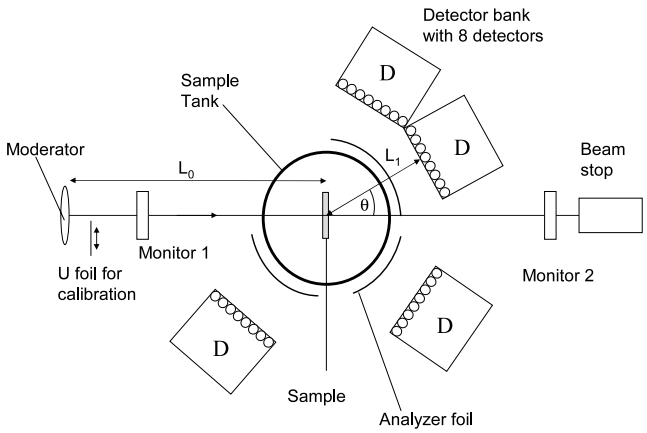

Figure 1. A schematic representation of the VESUVIO spectrometer at ISIS.

In the real experimental situation the measured count rate $C(\theta = \text{const}, t)$ for every time of flight t is an average over the possible values of all geometrical parameters characterizing the paths of the neutrons L_0, L_1, and the scattering angle θ as well as the final neutron energy E_1, weighed by their probability of occurrence. To account for this, a resolution function is introduced [10]. The usually applied NCS data reduction scheme accounting for the effects of the resolution of a TOF spectrometer is based on the so-called 'convolution approximation' CA. In the framework of CA it is assumed that a TOF spectrum is described by a convolution of the total mass dependent resolution function of the instrument $R(y_M)$ and the neutron Compton profile of the scatterer $J(y_M)$ [10]. Usually the momentum distribution $J(y_M)$ is assumed to have the Gaussian shape described by equation (8) and the resolution function $R(y_M)$ is assumed to be described by the Voigt function in the case of gold foil used as the final energy analyzer [10]. The convolution is performed in the y space for each mass M and then the sum over contributions from different masses is performed to account for the total count rate recorded in a time-of-flight NCS spectrum ([10], equation (2.24)):

$$C(\theta = \text{const}, t) = A' \frac{E_0(t) I[E_0(t)]}{q(t)} \times \sum_M I_M M J_M[y_M(t)] \otimes R_M[y_M(t)]. \tag{12}$$

3.2. A new data treatment scheme for NCS scattering intensities

As pointed out above (see section 1) a new NCS data treatment scheme is possible, within the framework of the CA, as far as scattering intensities are concerned. In order to derive an alternative expression for the scattering cross-section density the following remarks are in order. Firstly, it is worth noting that in an inverse geometry instrument such as VESUVIO, each time-of-flight value t corresponds, through kinematic relations [10], to a unique value of momentum transfer $q(t)$, initial neutron energy $E_0(t)$, energy transfer $\omega(t)$, and thus consequently to a unique value of the West scaling variable $y(t)$. Thus, the NCS signal intensity $C_M(\theta = \text{const}, t)$ collected for an individual scatterer mass M in a time-of-flight bin t can be written in the following form using equation (12):

$$C_M(\theta = \text{const}, t) = A' \frac{E_0(t) I(E_0(t))}{q(t)} \times I_M M J_M[y_M(t)] \otimes R_M[y_M(t)] \tag{13}$$

where J_M is the neutron Compton profile for mass M given by equation (8).

Secondly, in order for a count rate $C(t)$ recorded in a TOF channel t to be fully described by equation (13) and not by the sum of contributions from different recoil masses (given by equation (12)) the experimental situation must be achieved where a separation of neighboring recoil peaks from different scatterer masses is possible. Thus, a TOF spectrum must be selected recorded in a detector placed at sufficiently high scattering angle θ. In this respect, the above prerequisite for the application of the method is similar to the condition needed for the model-free Dorner method [14, 17, 15, 16].

In the new method proposed, in order to compare the experimental value of the scattering cross-section density for a given mass M with the theoretical expectation, two further steps must be performed. First, the left-hand side of equation (13) must be divided by all time of flight dependent terms and the mass to yield the product of I_M and A':

$$A' I_M = \frac{C_M(\theta = \text{const}, t)}{\frac{E_0(t) I(E_0(t))}{q(t)} I_M M J_M[y_M(t)] \otimes R_M[y_M(t)]}. \tag{14}$$

Then, in order to get rid of the experimental constant A', the same operation must be repeated for another scatterer mass X. The resultant expression for mass M is divided by an analogous expression for mass X to yield the experimentally determined ratio of the cross-section densities R_{exp}:

$$R_{\text{exp}} = \frac{C_M(\theta = \text{const}, t_M)}{C_X(\theta = \text{const}, t_X)} \times \frac{X \frac{E_0(t_X) I(E_0(t_X))}{q(t_X)} J_X[y(t_X)] \otimes R_X[y_X(t_X)]}{M \frac{E_0(t_M) I(E_0(t_M))}{q(t_M)} J_M[y(t_M)] \otimes R_M[y_M(t_M)]} \tag{15}$$

where the time of flight bins t_M and t_X can be chosen differently for masses M and X. Most conveniently, the values of t_M and t_X corresponding to the recoil peak maxima for masses M and X, respectively, can be chosen. As already pointed out in section 1, the choice of the TOF value corresponding to the center of a recoil peak has a special physical significance. Namely, the count rate $C(t)$ at this TOF channel t corresponds to a scattering event on a nucleus having no component p of its momentum distribution $n(p)$ along the direction of the neutron momentum transfer $\hat{q}$, i.e. $p \cdot \hat{q} = 0$. Moreover, the TOF value t at this point corresponds to energy transfer from neutron $\omega(t)$ and the momentum transfer $q(t)$ fulfilling the dispersion relation $\omega(t) = q(t)^2/2M$, where M is the mass of the nucleus the neutron is scattered off. This fact is very important in the light of recent discussion on the relevance of the Jacobian of the transformation from a constant θ scan, as usually recorded on VESUVIO, to a fictitious constant q scan [12, 17, 18]. It was argued namely that the Jacobian is numerically exact only for the center of a recoil peak. Thus, by choosing this point in the data reduction proposed here, one ensures that for the count rate recorded at this point for a constant θ scan there is always an exact transformation to a count rate recorded in a fictitious constant q scan (for more details on this issue see section 4). Moreover, the choice of the recoil peak center maximizes the ratio of signal to noise and/or other unwanted background signals. Such choice of the time bins for two peaks will be referred to as the center-of-peak method in further discussion.

The overall procedure in the center-of-peak method is thus the following. First, the conventional CA fit is performed for all masses present in the sample as described in the literature [10]. The widths σ_p of nuclear momentum distributions $J_M(y_M)$, given by equation (8), are calculated from the fit. These widths are then fixed in the expressions for the count rates $C_M(t_M)$ for individual masses in the convolution approximation, given by equation (12), calculated for particular time-of-flight values t corresponding to centers of recoil peaks. Then, the recorded count rates for the time-of-flight bins corresponding to peak centers are divided by theoretical expressions for count rates and the experimental ratio R_{exp} is calculated from equation (15). Finally, R_{exp} is divided by the theoretical expectation $R_{\text{theor}} = [I_H/I_X]_{\text{theor}} = (N_{\text{H}}\sigma_{\text{H}})/(N_X\sigma_X)$ and the factor $R = R_{\text{exp}}/R_{\text{theor}}$ is calculated accounting for the possible reduction of scattering cross-section densities.

3.3. Dorner method

The NCS data reduction method proposed by Dorner to calculate the scattering cross-section densities in a model-free way is described already quite extensively in the literature [14, 17, 15, 16]. Thus, here only an outline will be given. The whole data reduction scheme can be summarized in the following steps.

(1) The TOF spectrum consisting of count rates $C(\theta = \text{const}, t)$, collected for different TOF values t for a given fixed scattering angle θ, is normalized to a constant flux of the incoming neutrons by point-wise division by the factor $E_0(t)I[E_0(t)]$. As the result, the quantity $C_{\text{norm}}(\theta = \text{const}, t)$ is obtained.
(2) The individual values of the TOF in $C_{\text{norm}}(\theta = \text{const}, t)$ are replaced by the corresponding values of the energy transfer $\omega(t)$ without the use of any Jacobian.

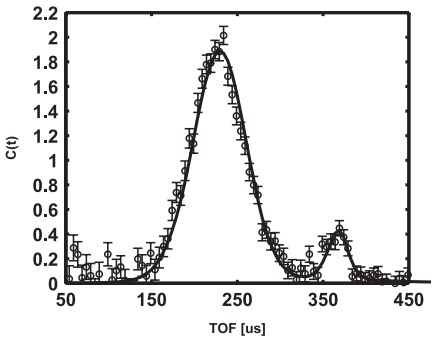

Figure 2. The TOF spectrum recorded for PE in detector no 55, scattering angle $\theta = 55°$. Two recoil peaks are visible: a broad peak at low values of time of flight for protons, and a narrow peak due to scattering off carbon nuclei at longer scattering times. The thick solid line represents a CA fit to the experimental data.

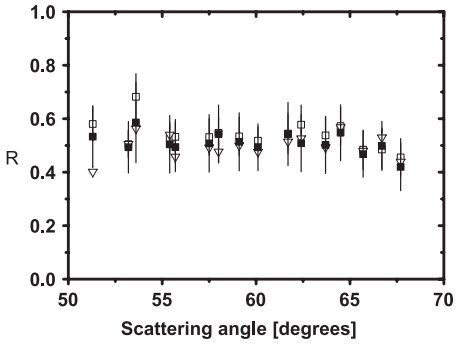

Figure 3. Scattering intensities of protons expressed in the units of scattering intensities of carbon nuclei plotted as a function of scattering angle θ. Three different NCS data reduction schemes are compared: full squares—new 'center-of-peak' method, open squares—conventional CA method, and open triangles—model-free Dorner method.

(3) Transformation from $C_{\mathrm{norm}}(\theta = \mathrm{const}, \omega)$ into $C_{\mathrm{norm}}(q = \mathrm{const}, \omega)$. At this point it is crucial to have well separated peaks corresponding to the scattering from different masses M. Each of them is multiplied point-wise by the corresponding mass dependent Jacobian for the transformation from a constant θ scan into a fictitious constant q scan using a Jacobian J by Waller and Froman ([13, 12]):

$$J = 1 - \frac{m}{M}\left(1 - \frac{k_1}{k_0}\cos(\theta)\right). \tag{16}$$

(4) The signals $C_{\mathrm{norm},M}(q = \mathrm{const}, \omega)$ are numerically integrated over the respective ω range to obtain the scattering intensities from different masses M.

4. Results and discussion

Low density polyethylene foil (0.15 mm thick) was chosen for the comparison of the conventional NCS and the model-free data reduction schemes with a newly proposed center-of-peak NCS data reduction scheme described above.

The typical TOF spectrum collected for PE is shown in figure 2.

In the TOF spectrum shown in figure 2 two recoil peaks are visible: a broad peak at low values of time of flight for protons, and a narrow peak due to scattering off carbon nuclei at longer scattering times. Clearly, a separation of two recoil peaks is achieved experimentally for this (and higher) forward scattering angle θ. This was the prerequisite for the application of the Dorner method to the PE data in order to calculate the scattering cross-section densities for H and C and to compare them with the result of the conventionally applied CA data reduction. This task has been achieved for NCS spectra recorded for PE measured by two forward detector banks at the VESUVIO spectrometer [16]. The range of the scattering angles θ for the chosen detectors varied between 51.3° and 67.7°. In this angular range the TOF spectra consisted of two separated scattering peaks: one broad, intense peak centered at around 200 μs due to scattering on protons, and a weaker carbon peak centered at around 370 μs [16]. The results of both data reduction schemes were shown to be the same within the experimental error for the scattering angle range chosen [16]. Here the results of the procedure performed by us on the PE sample [16] are compared, for the same scattering angle range, with the results of the new center-of-peak data reduction scheme described above.

As the initial step for the new data reduction method proposed, the widths of nuclear momentum distribution obtained in the previous study [16] were used to calculate the theoretical curves describing the count rates at centers of H and C recoil peaks, respectively. Then, the ratios of count rates recorded at H and C peak centers to the theoretical expressions, given by equation (13), were calculated for H and C peaks, respectively, and the experimental ratios of scattering cross-section densities $R_{\mathrm{exp}} = [I_{\mathrm{H}}/I_{\mathrm{C}}]_{\mathrm{exp}}$ were obtained. Finally the experimentally obtained ratios R_{exp} were compared with theoretical values R_{theor} and plotted versus scattering angles θ for the same range of θ as previously done for the PE sample in the case of the analysis using the CA and Dorner methods [16]. A comparison of the results obtained for PE for the ratio $R = R_{\mathrm{exp}}/R_{\mathrm{theor}}$ using three methods is shown in figure 3.

One can see clearly in figure 3 that the results obtained for PE using the newly proposed center-of-peak method agree within the experimental error with the results of the data reduction using the conventional CA formalism and the model-free data reduction using the method proposed by Dorner.

For the general assessment of the applicability of the new method for the NCS data reduction a few important remarks seem to be in order.

Firstly, as mentioned already in section 3.2, two recoil peaks under consideration must be sufficiently separated from one another in order for the method to work properly. However, the following remark is here in order. In principle, in the NCS data reduction method proposed here the total peak separation is not required as the scattering cross-section densities are deduced from count rates that can be chosen for TOF channels arbitrarily far apart from one another (e.g. lying on opposite tails of two recoil peaks, or at their respective peak centers as in the present study). In the Dorner method, however, the

peak separation must be complete in order to ensure the proper numerical integration of recoil peaks. This feature seems to be a clear advantage of the center-of-peak method over the Dorner scheme, as it enables the new method to be applied over a wider range of scattering angles.

Secondly, the following specific point of the Dorner method must be pointed out. Intrinsically, the accuracy of the Dorner method relies on the accuracy of the Waller and Froman Jacobian used to transform the TOF spectra from a constant θ to a constant q scan [17]. This Jacobian, however, was originally derived under the assumption that scattering peaks are infinitesimally narrow and concentrated in the region of energy transfer ω around the peak center, where the dispersion relation $\omega = \frac{q^2}{2M}$ is strictly fulfilled. However, for scattering peaks off protons, the width of the scattering peak increases with increasing value of momentum transfer q as the scattering angle θ increases. This leads to broader proton recoil peaks at higher values of θ, for which the Jacobian by Waller and Froman does not fully account. This in turn leads to slight problems with the convergence of the integrals of the scattering function in the ω domain at q = constant for the spectra transformed from very high scattering angles θ. This fact has already been mentioned by Dorner [17]. Also, this problem with the applicability of the Jacobian in its original Waller and Froman form for very high scattering angles has its consequences when a single number correction approach with the Jacobian calculated only at the peak center is applied, as pointed out by Cowley and Mayers [18]. The proposed new NCS data reduction scheme is free of this problem from the following reason. As pointed out by Mayers [10], the NCS data analysis based on the y scaling in the framework of the CA does not need any Waller and Froman Jacobian, as the y scaling itself naturally accounts for the fact that the instrument trajectory is along a constant θ line on the q–ω plane. The method proposed by us uses the y scaling and thus should be free of the problem with the Jacobian at very high scattering angles.

Moreover, an additional advantage of the center-of-peak method seems to manifest itself at very high scattering angles (say, higher than 75°). Namely, for so high scattering angles the tail of the proton recoil peak is shifted towards very low TOF values [18] ($t \sim 30\ \mu$s). At such short values of the time of flight, corresponding to very large initial neutron energies E_0 and thus also very large energy transfers ω, the band shape of the proton TOF peak tends to be distorted by unwanted noise and background signals present. Moreover, the overall count rate of the proton peak decreases considerably at short scattering times due to the $\frac{E_0 I(E_0)}{q}$ term decreasing asymptotically towards zero as E_0 increases at short times. The center-of-peak method would have the advantage here that it would operate at TOF values t where the count rate for the proton recoil peak $C(t)$ is still relatively high and the peak shape is not distorted by background signals and/or noise. Obviously, the center-of-peak analysis for any nucleus having mass heavier than the mass of a proton would be free of artifacts described above.

To sum up, the new method of the determination of integrated peak intensities proposed here seems to overcome some difficulties associated with recoil peak fitting using band shape analysis based on the convolution approximation. Moreover, it is free of the problem associated with the accuracy of the Jacobian used in the Dorner method. However, as already pointed out in section 3.2, the price for this is that widths of nuclear momentum distribution previously determined (at least from NCS spectra recorded in some detectors) from the full band shape analysis in the framework of CA must be used as an input to the method. This makes the new method proposed model dependent.

5. Conclusions

A new method of NCS data treatment for the determination of integrated peak intensities was proposed. The method is based on the comparison of NCS data collected at the center of each recoil peak present in a TOF spectrum with the theoretical expression for the count rate at the peak center making use of the convolution approximation. The results of the analysis of the PE sample agree within experimental error with the results of analysis previously applied [16]. The result obtained for the PE sample supports existing strong evidence for the striking anomaly of the scattering cross-section of protons observed in polyethylene. The new method presented can be used for other samples, especially in the case of low signal to noise ratio and/or unwanted background signal when the conventional method based on fitting entire peak profiles fails.

Acknowledgment

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