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Experimental corrections in neutron diffraction of ambient water using H/D isotopic substitution

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Abstract. We report on the procedure to treat neutron diffraction data, in order to obtain the differential cross sections, a step that is essential in the analysis of structural information for liquids and amorphous materials. The treatment is applied to new measurements that have been made on the D4C diffractometer for eight different isotopic compositions of H₂O/D₂O mixtures at ambient temperature. The procedure is based on Monte Carlo simulations to perform multiple scattering, attenuation and detector efficiency corrections, applied iteratively. The normalization process allows the direct comparison of measured data from different samples, and requires the knowledge of the total cross-section at the incident neutron energy. The high contrast between the cross sections (coherent and incoherent) for heavy and light water allows to test the procedure under very different conditions of multiple scattering effects.

1. Introduction

The availability of improved neutron spectrometers, makes it possible to reach a high degree of refinement in the experimental data. However these improvements have not reached yet the customarily employed analysis techniques for diffraction, and outdated correction procedures borrowed from different techniques are still being employed, due to the lack of customary software specific for neutron diffraction.

It is accepted nowadays that the most reliable procedure to correct for multiple scattering and beam attenuation effects in neutron scattering experiments is achieved through Monte Carlo simulations. Since the great variety of neutron techniques pose very different experimental conditions, the numerical simulations must be devised for each specific situation. Prior to the present work, a correction tool had been previously developed and benchmarked for neutron diffraction in liquid and amorphous materials [1]. In the particular case of light and heavy water, different models were explored, and it was determined that in the case of deuterated samples, the multiple scattering signal showed a structure very different from the oversimplified calculations borrowed from X-rays techniques.

The structure of water has been a subject of intensive research during the last decades. The efforts aim at a better knowledge of the structural characteristics of liquid water in terms of the partial pair correlation functions and the orientational correlations between neighbouring molecules. The purpose of this work is to show the data processing procedure we apply to subtract the multiple scattering effects, attenuation of the neutron beam and detector efficiency to obtain $d\sigma(\theta)/d\Omega$ in an absolute scale in a series of light water/heavy water mixtures measured

at diffractometer D4C (ILL, Grenoble)[2], thus allowing the direct comparison of measured data from different samples. We show the theoretical foundations of the process, as well as the procedure of data normalizations to achieve differential cross sections expressed in a physically meaningful scale.

2. Theoretical background

In this section we will develop the mathematical expressions of the magnitudes calculated by the Monte Carlo program employed to process the data.

2.1. Overview

The magnitude measured in a neutron diffraction experiment is the macroscopic differential cross section, *i.e.* the angular distribution of the neutrons emerging from the sample. The goal of the experiment is to deduce the microscopic differential cross section, that is directly related with the structural and dynamical properties of the sample.

If the initial and final neutron wave vectors are \mathbf{k}_0 and \mathbf{k} respectively, the expression for the macroscopic cross section as a function of the scattering angle θ measured in diffraction experiments [3], is obtained after integration on the final energies, and results

$$\frac{1}{A(\hat{\mathbf{k}}_0)} \left(\frac{d\Sigma}{d\Omega} \right)_{\text{scatt}} = \frac{N\sigma_{\text{scatt}}}{4\pi A(\hat{\mathbf{k}}_0)} \int dE \frac{k}{k_0} \varepsilon(k) s(\mathbf{k}_0, \mathbf{k}) \quad , \quad (1)$$

where $\hat{\mathbf{k}}_0$ is the direction of the incident beam, $A(\hat{\mathbf{k}}_0)$ is the cross sectional area exposed at the incident beam, N is the number of atoms, σ_{scatt} the bound-atom scattering cross section of the sample, $\varepsilon(k)$ is the detector efficiency and $s(\mathbf{k}_0, \mathbf{k})$ is the effective scattering function defined by Sears [3]. This function can be decomposed in contributions according to the number of collisions. For systems consisting in a sample placed into a container, the function $s(\mathbf{k}_0, \mathbf{k})$ contains the information of the whole set, and it can be conveniently decomposed into a part due to singly scattered neutrons by the sample, another due to single scattering from the container, and a third due to multiply scattered neutrons with any combination of sample-can scattering events,

$$s(\mathbf{k}_0, \mathbf{k}) = s_1(\mathbf{k}_0, \mathbf{k}) + s_C(\mathbf{k}_0, \mathbf{k}) + s_M(\mathbf{k}_0, \mathbf{k}) \quad . \quad (2)$$

The Monte Carlo code samples the density of neutrons in the steady state regime. To this end Copley's scheme [4, 5] provides an efficient method, that consists in generating neutron histories biased in such way that the neutron never leaves the sample nor is absorbed. To compensate this bias, a weight (that is initially 1) is computed for the history, that decreases at every path traversed and at every scattering step as described in Ref. [1]. Neutron histories are originated in a random point of the sample surface that faces the incoming beam. The distance traveled by the neutron between two scattering steps is determined by the mean free paths of the materials that the neutron has to traverse at the current flight direction and energy E , to emerge from the sample. After the scattering event, new energies and directions of flight are randomly sampled from the joint probability distribution

$$P(E_0, E, \theta) = \frac{1}{\sigma_{\text{scatt}}(E_0)} \frac{d^2\sigma}{d\Omega dE} \quad , \quad (3)$$

where $\sigma_{\text{scatt}}(E_0)$ is the total scattering cross section at energy E_0 (before the scattering interaction) and $d^2\sigma/d\Omega dE$ is the double differential cross section. For molecular systems a suitable model for these magnitudes is provided by Granada's Synthetic Model [6]. Although this is an incoherent model, it proved to be sufficient in the calculation of multiple scattering events, even when coherent scattering dominates.

The scored magnitudes at each step are the contributions of the history to the detectors. The most useful estimators to evaluate the corrections needed in a diffraction experiment are enumerated in the following paragraphs.

2.1.1. Singly scattered neutrons The basic information that provides a diffraction experiment is contained the *angular distribution of neutrons after the first scattering*. In the Monte Carlo procedure this value is calculated by sampling the first collision point from the probability distribution

$$P(x) = \frac{\Sigma_{\text{tot}}(\mathbf{k}_0) \exp[-\Sigma_{\text{tot}}(\mathbf{k}_0)x]}{w_1} \quad , \quad (4)$$

with

$$w_1 = 1 - \exp[-\Sigma_{\text{tot}}(\mathbf{k}_0)d(\mathbf{r}_0, -\hat{\mathbf{k}}_0)] \quad , \quad (5)$$

where $d(\mathbf{r}_0, -\hat{\mathbf{k}}_0)$ is the total thickness of the sample measured from the point of incidence \mathbf{r}_0 in the direction $\hat{\mathbf{k}}_0$, and $\Sigma_{\text{tot}}(\mathbf{k}_0)$ is the macroscopic total cross section. The term w_1 is a bias in the probability so the neutron does not leave the sample.

w_1 is the probability that the neutron incident at \mathbf{r}_0 will interact within the sample, and is the weight of the history at the first step. When a container is present, the factor $\exp[-\Sigma_{\text{tot}}(\mathbf{k}_0)d(\mathbf{r}_0, -\hat{\mathbf{k}}_0)]$ (called *attenuation factor*) must also include the path traversed in the container and its cross section.

The sought distribution is calculated by scoring over a large number of histories the estimator

$$\chi_1(\mathbf{r}, \mathbf{k}_0, \mathbf{k}) = w_1 \frac{\Sigma_{\text{scatt}}(\mathbf{k}_0)}{\Sigma_{\text{tot}}(\mathbf{k}_0)} P(\mathbf{k}_0, \mathbf{k}) \quad , \quad (6)$$

which is the probability that the incoming neutron is scattered, times the probability distribution in \mathbf{k} of the scattered neutrons. $P(\mathbf{k}_0, \mathbf{k})$ is the same function introduced in Eq. (3). As described in Ref. [1], this probability can be evaluated making resource the experimental data and implementing an iterative correction scheme as described below.

In the sampling process the estimator (6) must be weighed by the density of first collisions [7]

$$\tilde{\Psi}_1(\mathbf{r}, \mathbf{k}_0) = \frac{1}{A(\hat{\mathbf{k}}_0)} \frac{\exp[-\Sigma_{\text{tot}}(\mathbf{k}_0)L(\mathbf{r}, -\hat{\mathbf{k}}_0)]}{w_1} \quad , \quad (7)$$

where the tilde over Ψ indicates that the function has been modified (dividing by w_1) to compensate the bias and $L(\mathbf{r}, -\hat{\mathbf{k}}_0)$ is the distance from point \mathbf{r} (inside the sample), to the sample surface in the direction $\hat{\mathbf{k}}_0$. The estimator (6) weighed over the collision density (7) in the Monte Carlo process, is the integral over the sample volume (see Ref. [3])

$$z_1(\mathbf{k}_0, \mathbf{k}) = \int d^3r \tilde{\Psi}_1(\mathbf{r}, \mathbf{k}_0) \chi_1(\mathbf{r}, \mathbf{k}_0, \mathbf{k}) = \frac{\Sigma_{\text{scatt}}(\mathbf{k}_0)}{\Sigma_{\text{tot}}(\mathbf{k}_0)} (1 - t(E_0)) P(\mathbf{k}_0, \mathbf{k}) \quad , \quad (8)$$

where $t(E_0)$ is the total fraction of transmitted neutrons. Equation (8) expresses that the intensity of singly scattered neutrons is equal to the ratio of the scattering and the total cross sections, times the fraction of neutrons interacting in the sample ($1 - t(E_0)$), and it is distributed according to the microscopic double differential cross section. The integration of Eq. (8) over final energies is the magnitude of interest in diffraction experiments

$$z_1(\mathbf{k}_0, \theta) = \frac{\Sigma_{\text{scatt}}(\mathbf{k}_0)}{\Sigma_{\text{tot}}(\mathbf{k}_0)} (1 - t(E_0)) \frac{1}{\sigma_{\text{scatt}}(E_0)} \frac{d\sigma}{d\Omega}(E_0, \theta) \quad , \quad (9)$$

i.e. the intensity of the *angular distribution of neutrons after the first scattering*. This equation shows that the sought magnitude ($d\sigma/d\Omega$) is proportional to $z_1(\mathbf{k}_0, \theta)$, and shows the proportionality constant. This magnitude is not directly accessible from the experiment due to the presence of multiple scattering, and even when we can subtract this component (by calculation) the single scattering component is still affected by attenuation and detector efficiency, as will be shown in the next section. When all the corrections have been performed, the resulting component is expressed by Eq. (9), which is the expression that must be employed to compare the diffractograms from different samples.

2.1.2. Detected singly scattered neutrons The mentioned contribution of the singly scattered neutrons (at position \mathbf{r}) to the detectors (placed in the direction \mathbf{k}) is scored by the estimator

$$\chi'_1(\mathbf{r}, \mathbf{k}_0, \mathbf{k}) = w_1 \frac{\Sigma_{\text{scatt}}(\mathbf{k}_0)}{\Sigma_{\text{tot}}(\mathbf{k}_0)} P(\mathbf{k}_0, \mathbf{k}) e^{-\Sigma_{\text{tot}}(\mathbf{k})L(\mathbf{r}, \hat{\mathbf{k}})} \varepsilon(k) \quad , \quad (10)$$

where $e^{-\Sigma_{\text{tot}}(\mathbf{k})L(\mathbf{r}, \hat{\mathbf{k}})}$ is the attenuation factor from \mathbf{r} to the detector position and $\varepsilon(k)$ is the detector efficiency.

When a container is present, the attenuation factor must also include the path traversed in the container and its cross section. In the Monte Carlo code this estimator is scored over the neutron histories as in Eq. (8). The result converges to the integral over the sample volume of the estimator (10) weighed over the collision density (7), resulting

$$\tilde{z}_1(\mathbf{k}_0, \mathbf{k}) = \frac{V}{A(\hat{\mathbf{k}}_0)} \Sigma_{\text{scatt}}(\mathbf{k}_0) P(\mathbf{k}_0, \mathbf{k}) \varepsilon(k) H_1(\mathbf{k}_0, \mathbf{k}) \quad , \quad (11)$$

where $H_1(\mathbf{k}_0, \mathbf{k})$ is the primary attenuation factor described by Sears [3]. This expression is directly related with the single scattering component of Eq. (1) through

$$\tilde{z}_1(\mathbf{k}_0, \mathbf{k}) = \frac{N\sigma_s}{4\pi A(\hat{\mathbf{k}}_0)} \frac{k}{k_0} \varepsilon(k) s_1(\mathbf{k}_0, \mathbf{k}) \quad . \quad (12)$$

As in Sect. 2.1.1 the integration of (11) over energies gives the specific result for diffraction

$$\tilde{z}_1(\mathbf{k}_0, \theta) = \frac{V}{A(\hat{\mathbf{k}}_0)} \Sigma_{\text{scatt}}(\mathbf{k}_0) \int dE \frac{1}{\sigma_{\text{scatt}}(E)} \sigma(E_0, E, \theta) \varepsilon(E) H_1(E_0, E, \theta) \quad . \quad (13)$$

2.1.3. Container singly scattered neutrons Similar expressions as (11) and (13) hold for the singly scattered neutrons in the container. The transmission factors must include the traversed paths in different media and their cross sections. The calculated component $\tilde{z}_C(\mathbf{k}_0, \theta)$ is related with an expression similar as (12) to obtain the corresponding component in Eq. (1).

2.1.4. Multiply scattered neutrons The estimator for the detected multiply scattered neutrons, scored in the Monte Carlo procedure is evaluated by the recurrence relation

$$\chi'_n(\mathbf{r}, \mathbf{k}_{n-1}, \mathbf{k}) = w_n \frac{\Sigma_{\text{scatt}}(\mathbf{k}_{n-1})}{\Sigma_{\text{tot}}(\mathbf{k}_{n-1})} P(\mathbf{k}_{n-1}, \mathbf{k}) e^{-\Sigma_{\text{tot}}(\mathbf{k})L(\mathbf{r}, \hat{\mathbf{k}})} \varepsilon(k) \quad , \quad (14)$$

where the weight at the n -th step is determined from the weight at step $n - 1$ as

$$w_n = w_{n-1} \left\{ 1 - \exp[-\Sigma_{\text{tot}}(\mathbf{k}_{n-1})L(\mathbf{r}_{n-1}, -\hat{\mathbf{k}}_{n-1})] \right\} \frac{\Sigma_{\text{scatt}}(\mathbf{k}_{n-1})}{\Sigma_{\text{tot}}(\mathbf{k}_{n-1})} \quad . \quad (15)$$

Similarly as in Eq. (4) the path length from the $(n - 1)$ -th to the n -th step is sampled from a biased probability so the neutron never leaves the sample, changing $d(\mathbf{r}_0, -\hat{\mathbf{k}}_0)$ by $L(\mathbf{r}_{n-1}, -\hat{\mathbf{k}}_n)$, *i.e.* the distance from position \mathbf{r}_{n-1} to the sample surface in the direction of \mathbf{k}_n .

The contribution of the n -th scattered neutrons is obtained after sampling the estimator (14) with the modified density of n -collisions. The resulting expression similarly as in Eq. (8), is

$$\tilde{z}_n(\mathbf{k}_0, \mathbf{k}) = \int d^3r \tilde{\Psi}_n(\mathbf{r}, \mathbf{k}_{n-1}) \chi'_n(\mathbf{r}, \mathbf{k}_{n-1}, \mathbf{k}) \quad , \quad (16)$$

where $\tilde{\Psi}_n$ results from the recursive relation

$$\tilde{\Psi}_n(\mathbf{r}, \mathbf{k}_{n-1}) = \int d^3k' P(\mathbf{k}', \mathbf{k}_{n-1}) \int_0^{L(\mathbf{r}, \hat{\mathbf{k}}_{n-1})} ds \exp[-\Sigma_{\text{tot}}(\mathbf{k}_{n-1})s] \tilde{\Psi}_{n-1}(\mathbf{r} - s\hat{\mathbf{k}}_{n-1}, \mathbf{k}') \quad . \quad (17)$$

As in Eq. (12) the multiple scattering component is related with Eq. (1) through

$$\tilde{z}_n(\mathbf{k}_0, \mathbf{k}) = \frac{N\sigma_{\text{scatt}}}{4\pi A(\hat{\mathbf{k}}_0)} \frac{k}{k_0} \varepsilon(k) s_n(\mathbf{k}_0, \mathbf{k}) \quad (18)$$

and its corresponding magnitude for diffraction is

$$\tilde{z}_n(\mathbf{k}_0, \theta) = \frac{N\sigma_{\text{scatt}}}{4\pi A(\hat{\mathbf{k}}_0)} \int dE \frac{k}{k_0} \varepsilon(E) s_n(E_0, E, \theta) \quad . \quad (19)$$

The total contribution of multiple scattering is

$$\tilde{z}_M(\mathbf{k}_0, \theta) = \sum_{n=1}^{\infty} \tilde{z}_n(\mathbf{k}_0, \theta) \quad . \quad (20)$$

In practice the sum is truncated by the Russian roulette method, when the neutron weight drops below significant values [7].

2.2. Correction Method

The Monte Carlo code calculates the measured macroscopic cross section as well as its components as shown in the former sections. The total magnitude calculated by Monte Carlo is

$$\frac{1}{A(\hat{\mathbf{k}}_0)} \left(\frac{d\Sigma}{d\Omega} \right)_{\text{scatt}} = \tilde{z}_1(\mathbf{k}_0, \theta) + \tilde{z}_C(\mathbf{k}_0, \theta) + \tilde{z}_M(\mathbf{k}_0, \theta) \quad , \quad (21)$$

which is a description of the measured diffractogram and provides the means to separate \tilde{z}_1 from the rest of the contributions that must be evaluated. The sought magnitude z_1 (Eq. (9)), is also calculated in the Monte Carlo procedure.

The proposed procedure to process the experimental data is performed through correction factors following an iterative procedure. We define the multiple scattering factor at the iteration i as

$$f_{\text{MS}}^{(i)}(\mathbf{k}_0, \theta) = \frac{\tilde{z}_1^{(i)}(\mathbf{k}_0, \theta)}{\tilde{z}_1^{(i)}(\mathbf{k}_0, \theta) + \tilde{z}_C^{(i)}(\mathbf{k}_0, \theta) + \tilde{z}_M^{(i)}(\mathbf{k}_0, \theta)} \quad , \quad (22)$$

and the attenuation factor

$$\mathcal{A}^{(i)}(\mathbf{k}_0, \theta) = \frac{\tilde{z}_1^{(i)}(\mathbf{k}_0, \theta)}{z_1^{(i)}(\mathbf{k}_0, \theta)} \quad . \quad (23)$$

In the first step the uncorrected experimental data function $\mathcal{E}^{(0)}(\mathbf{k}_0, \theta)$ is employed to calculate the estimators given in Eqs. (6), (10) and (14) in the Monte Carlo code, and \tilde{z}_1 , \tilde{z}_C , and \tilde{z}_M are obtained as outputs. After the convergence of the Monte Carlo runs, the factors (22) and (23) are defined and applied to $\mathcal{E}^{(0)}(\mathbf{k}_0, \theta)$, thus defining $\mathcal{E}^{(1)}(\mathbf{k}_0, \theta) = \mathcal{E}^{(0)}(\mathbf{k}_0, \theta) f_{\text{MS}}^{(1)} / \mathcal{A}^{(1)}$. The corrected data are employed as input of the next Monte Carlo run, thus defining an iterative process. In general the corrected spectrum at run i -th is defined as

$$\mathcal{E}^{(i+1)}(\mathbf{k}_0, \theta) = \frac{f_{\text{MS}}^{(i)}(\mathbf{k}_0, \theta) \mathcal{E}^{(0)}(\mathbf{k}_0, \theta)}{\mathcal{A}^{(i)}(\mathbf{k}_0, \theta)} \quad . \quad (24)$$

The iterative process converges typically after 8 runs. We thus obtain the experimental angular distribution of singly scattered neutrons, $\mathcal{E}_1(\mathbf{k}_0, \theta)$. Its expression is proportional to $z_1(\mathbf{k}_0, \theta)$ (Eq. (9)), with a proportionality constant that links the experimental data with the theory

$$\mathcal{E}_1(\mathbf{k}_0, \theta) = K z_1(\mathbf{k}_0, \theta) \quad . \quad (25)$$

Integrating over all directions of solid angle in Eq. (25) (or equivalently from 0 to $2k_0$ in Q), from Eq. (9) we get the value of K

$$K = \frac{\Sigma_{\text{tot}}(\mathbf{k}_0)}{\Sigma_{\text{scatt}}(\mathbf{k}_0)} \frac{1}{1 - t(E_0)} \frac{2\pi}{k_0^2} \int_0^{2k_0} dQ \mathcal{E}_1(\mathbf{k}_0, Q) Q \quad . \quad (26)$$

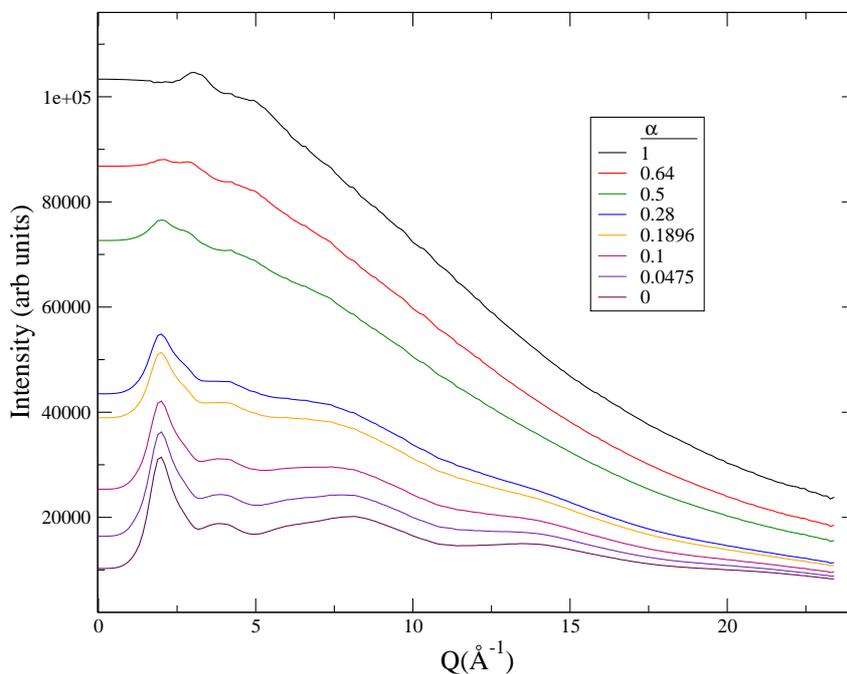


Figure 1. Experimental results of diffraction on the eight samples, classified according their light water concentration (α).

3. Experimental procedure

The samples employed in the present work were the water mixtures. Eight different isotopic mixtures ($\text{H}_{2\alpha}\text{O}_\alpha / \text{D}_{2(1-\alpha)}\text{O}_{(1-\alpha)}$, α being the concentration of light water) were used in this

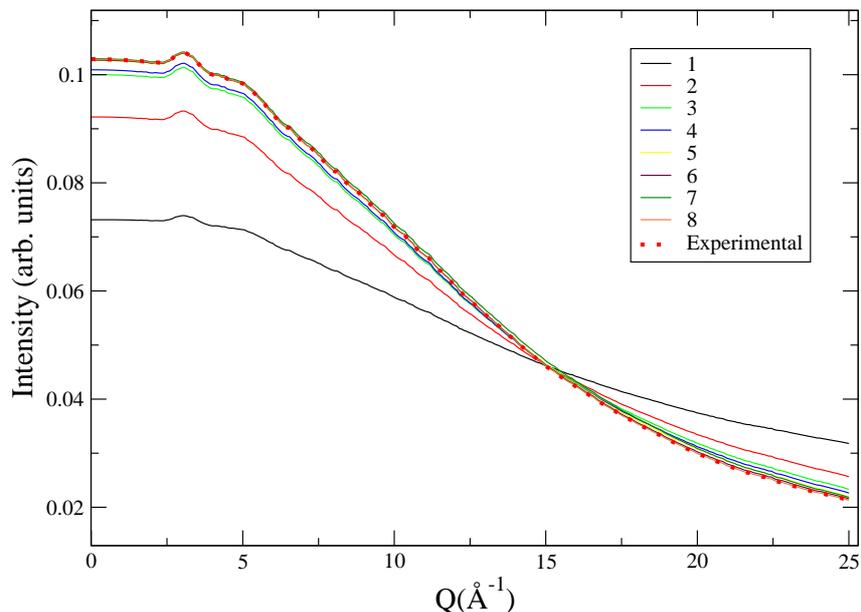


Figure 2. Convergence of the iterative method as a function of the iteration number, for the case of light water. The dotted line represents the experimental data. Starting from iteration 8 no significant changes are observed.

experiment and were prepared by careful weighing inside a moisture-controlled glove box. The mixtures were prepared with $\alpha = 1, 0.64, 0.5, 0.28, 0.19, 0.1, 0.05$ and 0. The sample holder was a thin-walled cylindric vanadium can, 6 mm inner diameter and 60 mm height, situated at the centre of an evacuated bell jar.

The diffraction experiments were carried out at room temperature, $(25 \pm 2)^\circ\text{C}$, at the diffractometer D4C [2]. The incident neutron beam wavelength was $\lambda_0 = 0.5 \text{ \AA}$ (energy 0.324 eV). The beam size was chosen to bath the central part of the sample. Its width was chosen to cover exactly the width of the sample. The scattered intensity was recorded moving the multidetectors over the available angular range, which effectively covered a Q -range from 0.05 to 24 \AA^{-1} . Similar measurements were made for the empty cell, background and a standard vanadium rod of 6 mm diameter. The detector efficiency profile was determined from measurements using a vanadium sample.

4. Data treatment

In Fig. 1 we show the experimental results for all the samples as a function of the elastic Q_e value defined as $Q_e = 4\pi/\lambda_0 \sin(\theta/2)$. In the results, the background (measured by removing the sample from its position), was subtracted from the experimental data.

The experimental results serve as starting point for the above described iterative correction method. In Fig. 2 we show the behavior of the iterative process described in Sect. 2.2, in the case of the light water sample ($\alpha = 1$). The criterion of convergence is that the total scattering as calculated by Monte Carlo, should reproduce the experimentally observed spectra. A good convergence to the experimental data is achieved starting from the eighth iteration, and no significant changes are observed in the subsequent iterations.

Figure 3 displays the contribution of single, multiple and container scattering (barely visible) to the total observed spectra as calculated from the last Monte Carlo iteration, for each sample. We also show the calculated distributions of neutrons after the first scattering (Eq. (8)).

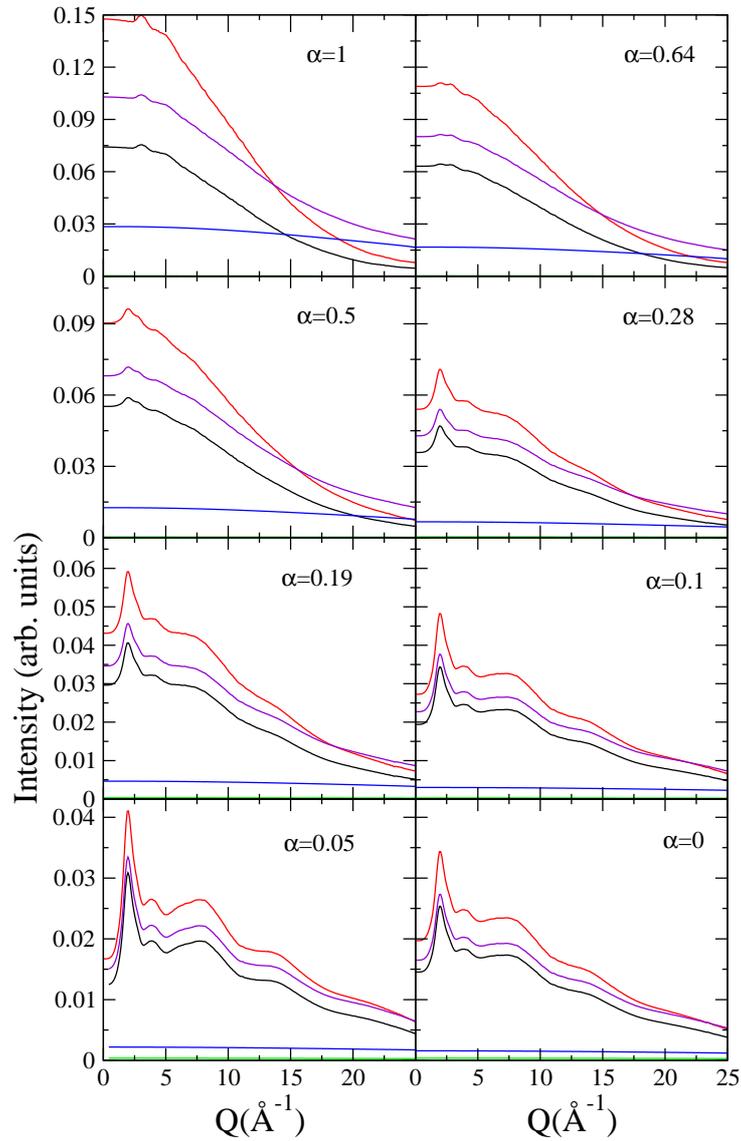


Figure 3. Detail for the contribution of the detected single scattering (black) \tilde{z}_1 , multiple scattering (blue) \tilde{z}_M , scattering from container (green) \tilde{z}_C and the total (violet) \tilde{z}_{tot} , from the Monte Carlo simulations for each sample. In red, the sought distribution of neutrons after the first scattering z_1 (Eq. (9)).

The results shown in Fig. 3 provide the necessary functions to apply the correction procedure described in Sect. 2.2, obtaining the functions $\mathcal{E}_1(\mathbf{k}_0, \theta)$ for each sample.

To obtain the functions $d\sigma/d\Omega$, we firstly need the total cross sections $\sigma(E_0)$, at the incident neutron energy, which were calculated by means of Granada's Synthetic Model [6]. The cross sections are shown in Fig. 4. We observe that the values of $\sigma(E_0)$ differ from the free atom limit, due to the chemical bonding effects. Thus, the values can not be obtained directly from tables. Instead, either a model or a measurement are necessary to determine them.

It is also necessary to know the ratio $\Sigma_{tot}(\mathbf{k}_0)/\Sigma_{scatt}(\mathbf{k}_0)$, that can be calculated from Fig. 4 and the absorption cross sections, from tables [8]. With all the collected information now we can calculate the values of K from Eq. (26). To calculate the integral of $\mathcal{E}_1(\mathbf{k}_0, \theta)$ we have to

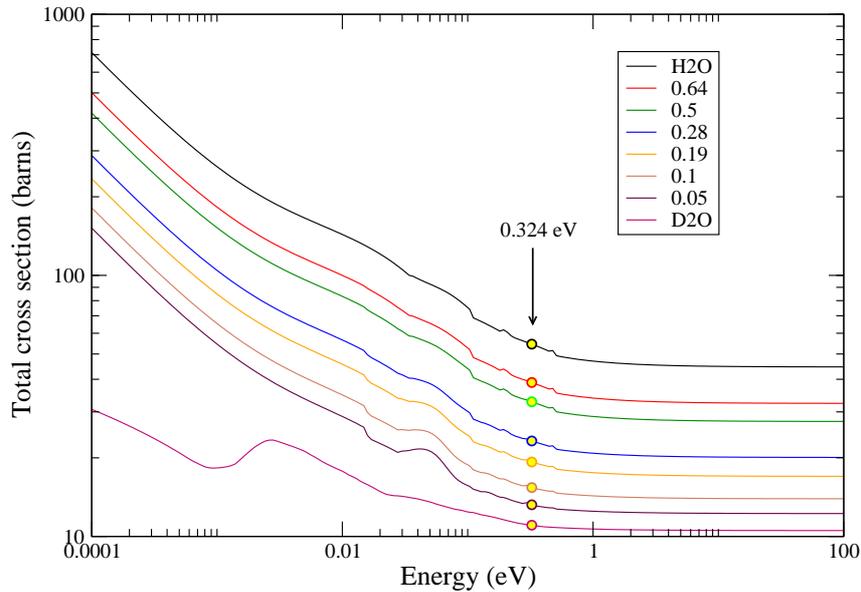


Figure 4. Total cross sections as a function of neutron energy for the different water mixtures (values of α indicated). The total cross sections at the incident energy (0.324 eV) are shown.

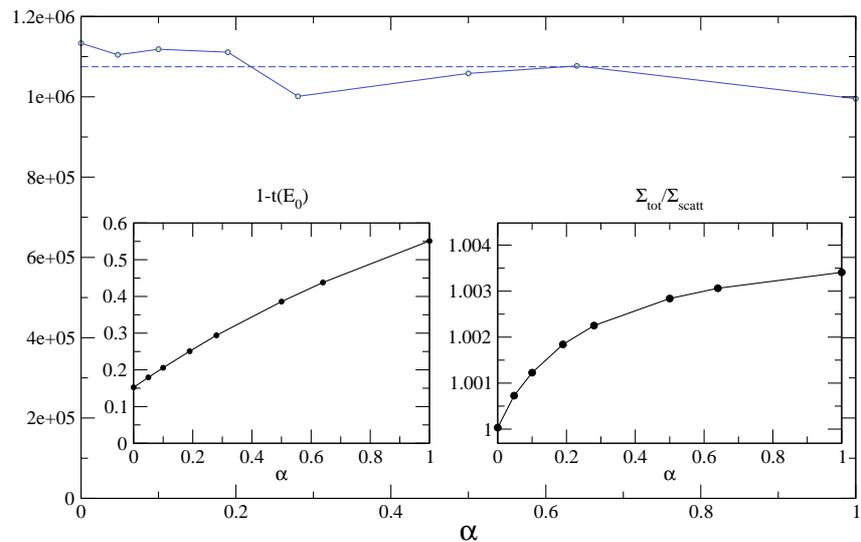


Figure 5. The normalization constant K defined in Eq. (26) for the different water mixtures. Left inset: $1 - t(E_0)$ (scattering power of the samples as a function of α). Right inset: the ratio $\Sigma_{\text{tot}}(\mathbf{k}_0)/\Sigma_{\text{scatt}}(\mathbf{k}_0)$ at the incident neutron energy.

extrapolate the experimental data to $\theta = 180^\circ$ (the experimental data not going beyond 140°), and the transmission coefficient can be calculated as shown in Ref. [1].

Figure 5 shows the resulting K factors for all samples, with a mean value of 1.074×10^6 and a spread of about 7%. A difference between the samples of lower and higher hydrogen contents is also observed. With the values of K obtained in this process we can calculate $z_1(\mathbf{k}_0, \theta)$ from Eq. (9), and from them $d\sigma/d\Omega$ employing $\sigma_{\text{scatt}}(E_0)$ shown in Fig. 4. In Fig. 6 we show the final results of $d\sigma/d\Omega$ as a function of Q .

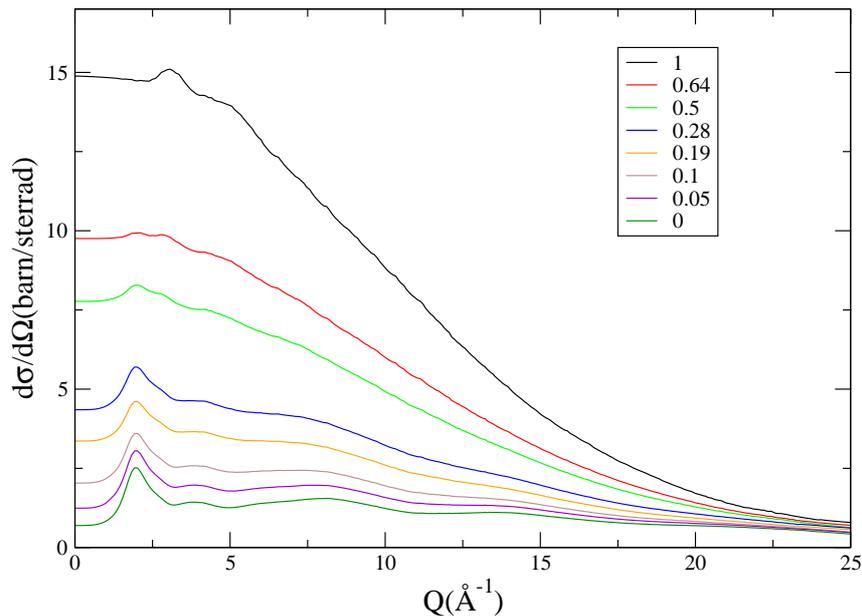


Figure 6. The differential cross sections of the water mixtures analyzed in this paper.

5. Summary and conclusions

In this paper we showed the procedure to obtain the link between the arbitrary experimental scale in neutron diffraction experiments (number of recorded counts per monitor counts) with the corresponding cross sections. The process involves multiple scattering, attenuation and detector efficiency corrections, that are calculated by a Monte Carlo method. We have developed the mathematical expressions of the magnitudes calculated by Monte Carlo and their experimental counterparts.

It is worth to comment about the coefficient K , the constant linking the scattering power of the samples with the number of registered counts. This coefficient should be an instrumental constant independent of the sample. However, we observe a decreasing trend with the higher Hydrogen-containing samples, *i. e.* the samples with the higher scattering power. A similar effect was observed in Ref. [1]. The causes there analyzed were a possible improper description of the detector bank efficiency, and the presence of a sample-dependent background, that increases with the higher Hydrogen-containing samples. Regarding the detector efficiency, it was exhaustively checked during the process of calibration of D4C [2]. However, the sample-dependent background is a subject that remains to be treated, both from the numerical and the experimental points of view, and is not only a problem in diffraction experiments but a general issue in neutron scattering experiments.

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