General formula for determination of cross-section from measured SANS intensities

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A detailed derivation of the formula connecting measured SANS intensity with the smeared cross-section (raw-data treatment) is presented. The derivation is carried out considering also a possible high probability of the coherent small-angle scattering. The information content of the so-called transmission measurement is analyzed. The individual effects which contribute to the primary-beam attenuation as well as the different modes of the transmission measurement are described. Multiple scattering contribution to the excess of the forward scattering of the water calibration standard is discussed.

1. Symbol definitions

Scattering vector: \( \mathbf{Q} = \mathbf{k} - \mathbf{k}_i \) ... scattering vector (\( \mathbf{k}_i \), \( \mathbf{k} \) are the wavevectors of the incident and scattered neutron, resp.); \( \mathbf{Q} = |\mathbf{Q}| = 4\pi \sin \theta / \lambda_i \) ... magnitude of the scattering vector (20 full scattering angle, \( \lambda_i \) ... incident neutron wavelength); \( \mathbf{Q}_i \) ... scattering vector of the center of the pixel \( ij \) of position-sensitive detector (PSD) assuming elastic scattering (\( |\mathbf{k}| = |\mathbf{k}_i| \)).

Solid angle: \( d\Omega \) ... integration element; \( \Delta\Omega \) ... pixel \( ij \) as seen from the sample position; \( \Delta\Omega_{ij-H2O} \) ... pixel \( ij \) as seen from the water cell position (\( \Delta\Omega \) and \( \Delta\Omega_{ij-H2O} \) can differ due to the different sample-to-detector distances during sample and water measurement).

Thickness: \( d_i \) ... sample; \( d_{H2O} \) ... water.

True differential macroscopic cross-sections smeared by instrumental effects: \( [d\Sigma/d\Omega(Q)]^r_{ij} \) ... coherent small-angle scattering from sample (without substrate) assuming elastic scattering (in cm\(^{-1}\)Å\(^{-1}\)sr\(^{-1}\)); \( [d\Sigma/d\Omega(Q)]^i_{inc} \) ... incoherent scattering from sample; \( [d\Sigma/d\Omega(\lambda,\lambda,2\Omega)]^i_{inc} \) ... true cross-section of incoherent scattering from water - in cm\(^{-1}\)Å\(^{-1}\)sr\(^{-1}\) (\( \lambda \) ... neutron wavelength after leaving water).

Total scattering probabilities: \( p^r_{ij} \) ... SANS (coherent scattering) probability for sample; \( p^i_{ij} \) ... incoherent scattering probability for sample; \( p^i_{st} \) ... incoherent scattering probability for water (coherent scattering probability assumed to be equal to 0).

Efficiency: \( \eta_i \) ... mean; \( \eta_{ij} \) ... pixel \( ij \) of the PSD (\( \lambda \)-dependent).

Intensities (in neutrons/monitor count): \( I_{\text{inc}} \), \( I_{\text{st}} \) ... intensity of the primary beam in the sample, resp. water, position (can differ due to the different collimation and/or slits) without sample environment; \( I_{\text{gl}} \), \( I_{\text{st-D4}} \) ... cadmium background (detected intensity not coming directly from the beam used for the measurement) for sample, resp. water (can differ due to the different collimation and/or sample-to-detector distance); \( I_{\text{st}} \) ... measurement of substrate (or empty cell, empty slit, sample environment etc.) - usually called the sample background; \( I_{\text{s}} \) ... measurement of the empty cell for the water-calibration; \( I_{\text{H2O}} \) ... measurement of the empty cell for the calibration standard, too. The fact known for a long time (Nelkin, 1976) is that water embedded in a cell scatters the primary beam in the sample, resp. water (can differ due to the different collimation and/or sample environment, empty slit etc.); \( T_{\text{H2O}} \) ... empty cell (if water in a cell is measured like a sample in some attenuating environment, then \( T_{\text{H2O}} \) means transmission of empty cell times \( T_{\text{H2O}} \)); \( T_{\text{S}} \) ... sample; \( T_{\text{H2O}} \) ... water.

Transmissions due to absorption and large-angle coherent scattering (i.e. scattering not included in \([d\Sigma/d\Omega(Q)]^r_{ij}\))'s e.g. Bragg scattering; \( \gamma_{ij} \) ... sample; \( \gamma_{H2O} \) ... water.

2. Introduction

SANS technique is widely used for a determination of a morphology of particles in many fields of physics, chemistry and biology. Frequently, very similar formulas connecting intensities measured at pin-hole experiment with smeared cross-sections are employed for all kinds of samples (Lindner, 1995; Ghosh, 1989; Keiderling, 1998). However, these formulas mainly originated from chemical and biological investigations where the SANS technique was initially used several decades ago. In these fields, a relatively low coherent scattering probability is usually expected and only the contributions to background need to be discussed here (Horkay, Hecht, Mallam, Geissler & Rennie, 1991). However, the opposite situation frequently occurs in materials science, requesting corresponding refinement of the formula used for raw data treatment. Strongly correlated with the formula is the question how to measure the transmissions and what is the meaning of such a measurement. In many papers and textbooks, the term "sample transmission" is not explained in detail (see e.g. Wignall & Bates, 1987; Jacot, 1976; Jacot & Zacc, 1981; Williams, 1994; Lindner, 1995), in others (Ghosh, 1989; Kostorz, 1979; Knoll, Schmidt & Ibel, 1985) it is defined precisely from the point of view of high coherent scattering probabilities and some papers deal only with the case where the dominant attenuation effect is due to the incoherent scattering (May, Ibel & Haas 1982; May, 1992). This paper intends to contribute to the clarification of this question.

Another topic connected with the raw-data treatment formula is the absolute calibration by means of water which is employed in many laboratories (Jacot, 1976; May, 1992; Keiderling, 1998). Using water for this purpose has several advantages (high incoherent scattering cross-section, negligible coherent scattering and absorption, automatic correction for different solid angles covered by different pixels and for the different efficiency of pixels of the PSD). However, there are several drawbacks complicating its use as a calibration standard, too. The fact known for a long time (Nelkin, 1960; Bayster, 1968) is that water embedded in a cell scatters relatively more neutrons in the forward direction. This excess is often ascribed to the quasielastic incoherent structure factor (May, Ibel & Haas, 1982; Jacot & Zacc, 1981). The last part of the paper gives an explanation of another contribution to the excess, which dominates the other effects for 6 Å neutrons. The theoretical considerations - based on multiple scattering effect - are confirmed by a measurement and by a Monte Carlo simulation.

3. Definition of basic terms

The following sections show rigorously how the true differential-macroscopic-SANS cross-section (Schelten & Schmatz, 1980) corresponds to the intensities measured by the 2D PSD during the SANS experiment employing quasi-monochromatic beam. The formulas are derived on the basis "measured effect = sum of all possible contributions with proper attenuation factors".
The attenuation of the primary beam intensity in the sample environment (empty cell, substrate, cryostat windows etc.) - if present - is taken into account by an attenuation factor $T_{EB}$ in what follows. Then, the neutron from the primary beam attenuated in this way can undergo several different processes when passing through the sample. The individual processes and corresponding intensities are the following: (i) neutrons absorbed and coherently scattered to large angles (e.g. Bragg diffraction), overall intensity $(1-t_S)I_{S-ij}$, (ii) neutrons incoherently scattered by the sample, $t_S(1-p_c)I_{S-ij}$, (iii) neutrons coherently scattered by the sample to small angles, $I_{coh-S-ij}$, and (iv) neutrons not interacting with the sample at all, $I_{inc-S-ij}$. The total true incoherent scattering probability $p_{inc}$ used here is integrally connected with the true coherent cross-section and the total true coherent scattering probability $p_c$ is integrally connected with the true coherent cross-section:

$$p_{inc} = d_i \int \frac{d \Sigma}{d \Omega}(Q) \overline{d \Omega} \quad p_c = d_i \int \frac{d \Sigma}{d \Omega}(Q) \overline{d \Omega} \quad (1)$$

The probability $p_{inc}$ includes at least once coherently scattered neutrons without regard to how many times they were further coherently scattered. It should be noted that the function which can be extracted from a SANS experiment is not directly the ideal (apparent) cross-section but only the true cross-section smeared by instrumental effects. Apparent and true cross-sections are approximately equal only for small scattering probabilities. For understanding the connection between true and apparent cross-section see the paper of Schellen & Schmatz (1980). Together with a smearing effect, the true coherent cross-section already includes the attenuation of the primary beam due to small-angle scattering events and therefore $p_{inc} \leq 1$. The same is valid for the incoherent cross-section and $p_c$; however, the true incoherent cross-section is not so simply connected with the apparent incoherent cross-section (which is constant) as in the case of coherent small-angle scattering.

Because once coherently scattered neutron can be further scattered incoherently and vice versa, a part of the scattered neutrons cannot be clearly ascribed to the coherent or to the incoherent scattering. Therefore, a special type of separation is applied in (1) - and consequently in other formulas in the paper - which is the most advantageous from the point of view of the data evaluation. The most important part which provides information on the morphology of particles is pure (although multiple) coherent scattering. The neutrons which are scattered only coherently (maybe several times) are thus considered by the coherent true cross-section. The neutrons which are at least once scattered incoherently (the number of preceding or consequent coherent events do not play a role here) are described by the incoherent true cross-section; these neutrons give nearly constant scattering in the small-angle region.

4. Raw-data treatment formula

4.1. Measurement of small-angle scattering from the sample

The similar counting - as that which was done in the previous section for the overall intensities - can be carried out for the PSD pixel by pixel. This detection of course does not contain the neutrons absorbed in the sample; on the other hand, a term containing background not detectable. On the other side, the fourth term in (2) contains attenuation due to incoherent scattering events. It has to be pointed out that the second and the third term in (2) do not contain attenuation equal to the total removal transmission. These (coherently and incoherently) scattered neutrons are not lost as those absorbed, but they leave the sample and therefore are detectable. The fourth term in (2) contains the total removal transmission because it concerns the part of the primary beam not interacting with the sample.

It follows from (2) that the coherent cross-section can be determined from the measurement using the following formula:

$$\frac{d \Sigma}{d \Omega}(Q_{inc}) = \frac{I_{coh-S-ij}}{T_{in}T_{n}} - \frac{T_{in}}{t_{coh}}\int d_i \left[ \frac{d \Sigma}{d \Omega}(Q_{inc}) \right] \overline{d \Omega} = \frac{1}{(1-p_c)} \int d_i \left[ \frac{d \Sigma}{d \Omega}(Q_{coh}) \right] \overline{d \Omega} \quad (3)$$

In certain cases, the quantity $I_{coh-S-ij}$ can be directly determined from a measurement without the beam-stop (a well-defined attenuator can be used for this purpose) if the relative efficiency $\eta/\bar{\eta}$ is known.

4.2. Measurement of water for absolute calibration

However, the $I_{coh-S-ij}$ value is frequently unknown and some kind of indirect determination has to be used. If absolute calibration of the measured data is required, one way to find this quantity is to take advantage of the incoherent scattering from the pure water. The general formula (2) can be used to obtain an approximation of the intensity measurement of water in a cell; only a simple symbol exchange is applied and the negligible coherent scattering is not considered here:

$$I_{H2O} = I_{coh-H2O} + I_{inc-H2O} + I_{inc-H2O} \int d_i \left[ \frac{d \Sigma}{d \Omega}(Q_{inc}) \right] \overline{d \Omega} \quad (4)$$

where

$$I_{H2O} = d_i \int d_0 \left[I_{coh-H2O} + I_{inc-H2O} \int d_i \left[ \frac{d \Sigma}{d \Omega}(Q_{inc}) \right] \overline{d \Omega} \right]$$

is the intensity of incoherent scattering from water (the $\lambda$-dependence of PSD efficiency is taken into account). $P_{H2O}$ in the formula is the total probability that neutron is at least once incoherently scattered:

$$P_{H2O} = d_i \int d_0 \left[ \frac{d \Sigma}{d \Omega}(\lambda,2\theta) \right] \overline{d \Omega} \quad (5)$$

To determine precisely $I_{H2O}/\eta$ from Eq. (4), one has to know

$$\int 0 \left[ \eta_0 / \eta_0 (\lambda, \theta) \right] d(\Sigma / d \Omega) dl$$

in the measured range of $2\theta$ and also the total removal transmission. While $\tau_{H2O}$ can be relatively simply measured, the determination of above mentioned integral is a more difficult problem. If the water in a cell scattered elastically and isotropically into the full solid angle, its value would be simply determined from Eq. (5) to be equal to the constant $(1 - \tau_{H2O}/4\pi d_{H2O})$ for every scattering angle. In reality, this value is only the average cross-section and the scattering from water in the cell is not isotropic in the whole $4\pi$ range (see section 7). The intensity increase or decrease with respect to the variance can be described by
factor $K(\lambda,2\theta)$ and thus
\[ \int_{0}^{\pi/2} \frac{\eta_0(\lambda)}{\eta_0(\lambda)} d\Omega \left(\frac{\lambda}{\lambda_0} - 2\theta\right) d\lambda = K(\lambda,2\theta) \frac{1 - \tau_{\text{H}2\text{O}}/\tau_{\text{H}2\text{O}}}{4\pi \tau_{\text{H}2\text{O}}} . \] (6)

Nevertheless, within a certain angular range around the normal to the planeparallel water layer, the scattered intensity from water can be assumed to be constant ($K(\lambda,2\theta) \equiv K(\lambda) = \text{const.}$ for $28^\circ \leq 15^\circ$). It follows from (4) and (6) that the searched value can be written as
\[ I_{\text{pH}2\text{O}} = \frac{\tau_{\text{H}2\text{O}}}{1 - \tau_{\text{H}2\text{O}}/\tau_{\text{H}2\text{O}}} \frac{1}{4\pi} \] (7)

4.3. Final formula

If the ratio $r = I_{\text{pH}2\text{O}}/I_{\text{pH}2\text{O}}$ is known ($r$ is equal to 1 in the case when the same slit size and collimation for the sample and the water measurements are used), the formula for the cross-section of the sample when using water calibration can be derived from (3) and (7):
\[ \frac{d\Sigma}{d\Omega}(Q_i)\tau = \frac{\left[ I_{\text{H}2\text{O}} - I_{\text{H}2\text{O}} - I_{\text{EC}} - I_{\text{H}2\text{O}} \right]}{I_{\text{EC}} \tau_{\text{H}2\text{O}}} \times K \frac{\tau_{\text{H}2\text{O}}}{4\pi t_{\text{H}2\text{O}} d_{\text{H}2\text{O}}} \frac{d\Omega}{d\Omega} \tau = \frac{1}{1 - (1-p_c)} \frac{d\Sigma}{d\Omega}(Q_i)\tau \] (8)

where the incoherent scattering term on the right side can be assumed to be a constant within approximately $15^\circ$ around the forward scattering. It is usually not subtracted during raw-data treatment but fitted as a constant term in the further data analysis. The formula can be simply rewritten to another form, useful for a measurement of particles in aqueous solutions where the attenuation due to the incoherent scattering is dominant. Then, the total removal transmission of the sample can be determined by measurement and the first numerator in (8) can be written in the form:
\[ \frac{\left[ I_{\text{H}2\text{O}} - I_{\text{H}2\text{O}} - I_{\text{EC}} - I_{\text{H}2\text{O}} \right]}{I_{\text{EC}} \tau_{\text{H}2\text{O}}} \times K \frac{\tau_{\text{H}2\text{O}}}{4\pi t_{\text{H}2\text{O}} d_{\text{H}2\text{O}}} \frac{d\Omega}{d\Omega} \tau = \frac{1}{1 - (1-p_c)} \frac{d\Sigma}{d\Omega}(Q_i)\tau \] (9)

The formulas appear to be similar to the formulas written in some raw-data evaluation manuals and textbooks (Ghosh, 1989; Williams, 1994; Lindner, 1995; Keiderling, 1998) but they differ in several significant points (these are discussed in the following sections):

i) the precise definition of transmissions,

ii) the presence of the term $(1-p_c)$,

iii) the factor $K_c$ (similar factor - but explained by a different way - appears in some former formulas – see e.g. Jacrot, 1976).

5. Transmission measurement

The easy way for the determination of several factors appearing in the final formulas is to use the so-called transmission measurement. This measurement is performed by collecting the signal with and without sample by the 2D PSD and by analyzing the integral of such measurements over the PSD or over a part of it.

Because of the lack of coherently scattered neutrons, the measured quantity is nearly equal to $\tau_{\text{H}2\text{O}}$ for water transmission measurement. The (unwanted) part of incoherently scattered neutrons is also detected during this measurement. The influence of these neutrons on the error of determined $\tau_{\text{H}2\text{O}}$ can be roughly estimated by calculating the ratio of the solid angle covered by the PSD $\alpha$ and the full solid angle. The angle $\alpha$ is connected with the scattering angle $2\theta_{\text{MAX}}$ corresponding to the edge of the PSD (or to the border of a selected central area on it). The ratio $\alpha/4\pi$ is equal to 0.16% for 4m sample-to-detector distance (SDD) and 0.018% for SDD=12m (calculations performed for the 64x64 cm$^2$ detector). It can be deduced, that the error due to this contamination is lower than the statistical error for usual measuring times already at SDD=4m. The pure transmission due to absorption cannot be easily measured. Thus, $\tau_{\text{H}2\text{O}}$ has to be extrapolated from the known tabulated values; $\alpha=1$ for 1 mm thick pure water layer can be usually assumed.

To make the explanation of the sample transmission measurement easier, inset in Fig. 1 displays the transmission for a porous sample as a function of $\alpha$ (this and the other measurements used in the paper were performed at BENSf at HMI Berlin on facility V4 - Keiderling & Wiedenmann, 1995). Here, the absorption and incoherent scattering are rather small ($T_{\text{H}2\text{O}} = 0.92$) and nearly the whole total removal transmission can be attributed to the coherent scattering events. It has to be noted that $\tau_{\text{H}2\text{O}}$ cannot be determined precisely: neutrons scattered within the primary beam spot on the PSD cannot be removed and they are always detected together with the part of the primary beam not interacting with the sample. This contamination causes that - even for the smallest $\alpha$ - only the upper limit of the total removal transmission $\tau_{\text{H}2\text{O}} > \tau_{\text{H}2\text{O}}$ can be determined ($\tau_{\text{H}2\text{O}} = 0.04$ in the inset). In fact, $\tau_{\text{H}2\text{O}}=0$ for the demonstrated sample and the difference can be even larger for other types of samples. Therefore, $p_c$ cannot be found from the transmission measurement exactly: only its lower limit $1 - (1-p_c) \leq p_c$ can be determined. This estimate can be used in Eq. (8); an alternative approach is to calculate $p_c$ directly from the model which is used for the data evaluation (see Strunz et al., 2000).

On the other hand, $T_{\text{H}2\text{O}}$ can be relatively simply determined from the transmission measurement. It takes advantage of the fact, that small-angle scattered neutrons are mainly concentrated within relatively small angles around the primary beam while incoherently scattered ones are spread over the full solid angle. When increasing the solid angle $\alpha$ (see Fig. 1), the state when the measured transmission does not change substantially with changing $\alpha$ should be usually reached (this is not valid only when the scattering curve determined by $[d\Sigma d\Omega(Q_i)\tau]$ is too broad to be detected with an usual SANS setting and this case is not discussed here in detail). The plateau indicates the situation when nearly all neutrons coherently scattered to small angles can be detected by the PSD while incoherently scattered ones do not yet contaminate the measured intensity substantially and thus determines transmission $T_{\text{H}2\text{O}}$. The influence of the contamination by incoherent scattering is approximately given by the value $(p_c/4\pi)$ for $p_c$. It can be non-negligible when the coherent scattering probability is small (of the order of 1% or smaller). In this case, only $\tau_{\text{H}2\text{O}}$ can be determined which, nevertheless, nearly equal to $\tau_{\text{H}2\text{O}}$ and also to $\tau_{\text{H}2\text{O}}$. Then, the Eq. (9) can be used for the raw data treatment which can be further simplified when assuming $p_c=0$. In all other cases, the Eq. (8) or (3) should be employed with a corresponding modeling or estimation of the $p_c$ value.

* Figure 1
The basic scheme of the transmission measurement. Inset: measured transmission for a porous plasma-sprayed alumina layer.
6. (1-\(p_{\text{cS}}\)) factor

The main difference in the new formulas (8), (9) with respect to the former ones is that those omit the difference between transmissions \(T_{\text{S}}\) and \(\tau_{\text{c}}\), probably assuming the negligible coherent scattering probability. However, the factor \((1-p_{\text{cS}})\) - which arises when this neglecting is not done - can have a significant effect on the result.

When \(p_{\text{cS}}\) is not negligible but the value of \(\tau_{\text{c}}\) can be well estimated, the use of Eq. (9) leads to the absolute-scale shift by a factor \((1-p_{\text{cS}})\). This factor is sample dependent, but (because it otherwise does not appear in the old formulas - e.g. Jacrot & Zaccai, 1981; Lindner, 1995) it has to form - together with the parameter \(K'_{\text{S}}\), the so-called Jacrot factor \(\tau = 1/(K'_{\text{S}} (1-p_{\text{cS}}))\).

Neglecting of the term \((1-p_{\text{cS}})\) has, however, more serious consequences in the case of strong coherent scattering, i.e. in the case of measurement of \(T_{\text{S}}\) and the use of Eq. (8). When the intensity measured without sample \(I_{\text{S,meas}}\) is negligible for every pixel with respect to \(I_{\text{S,meas}}^{\text{SANS}}\) the influence of the \((1-p_{\text{cS}})\) term on the resulting curve is obviously very small. This condition is mostly not fulfilled for the double-crystal arrangement (Kulda & Mikula, 1983; Strunz, Šaroun, Mikula, Lukáš & Eichhorn, 1997). But it is not fulfilled as well for the pin-hole facility for certain experiments (e.g. measurement without the beam stop, strongly scattering sample mounted on some strongly scattering substrate, sample measured in an environment containing windows).

Fig. 2 demonstrates how the improper \((1-p_{\text{cS}})\) value can influence the curve resulting from sample-background subtraction procedure. The example is taken from an investigation of plasma-sprayed materials. During the experiment, plasma-sprayed layer was measured together with its substrate, Ni-based superalloy. This type of experiment is technologically important because such plasma-sprayed coating is used as a thermal barrier protecting Ni-based superalloy components of turbines. An investigation of the porosity in such coating by SANS without removing the substrate can provide more realistic characterization of pores in the layer near the metal-coating interface. However, the scattering has to be compared with the reference curve measured without the coating but with the substrate of the same properties as the original one. It implies a broadening of the instrumental curve due to the scattering on the substrate and an increase of the sample background. Because \(p_{\text{cS}}=1\) for the used plasma-sprayed sample, the proper shape of the smeared scattering curve of the layer alone is identical with the one which was measured (black points in the figure). A significant deviation of the curve after the improper \((p_{\text{cS}}=0)\) sample-background subtraction from the right one is observed in the broad Q-range (see Fig. 2).

7. Scattering from water

Up to this section, only the shape of the scattering curve has been discussed. But important information on the sample microstructure is also carried by the absolute value of the scattering cross-section. Frequently, the scattering from 1 mm water layer is used for the calibration of SANS data to the absolute scale.

The use of water as a primary standard is complicated by the well known fact that the scattering from water is neither elastic nor isotropic. Three effects are usually reported to contribute to the factor \(K'_{\text{S}}\): anisotropy of the single-scattering cross-section (the term anisotropy means here 20 dependence of the scattered intensity), \(\alpha\)-dependence of detector efficiency and multiple scattering (see e.g. May, Ibel & Haas 1982; Jacrot, 1976; Wignall & Bates, 1987; Ghosh & Rennie, 1990). The first effect is well described already by early models of scattering on water (Nelkin, 1960) and confirmed by measurements (Reinsch, 1961; Beyster, 1968). The results of Beyster (1968) clearly show that the single-scattering anisotropy plays important role for thermal and higher neutron energies - it tends to be isotropic for cold neutrons. The anisotropy of single-scattering cross-section was included in the simulations performed by Copley (1980) by employing model of Egelsstaff & Schofield (1962). Formula reported in this paper describes, however, only diffusive motion without Debye-Waller factor for bounded motion, which is mostly responsible for the anisotropy. In fact, Copley’s results include both the effects of anisotropy and multiple scattering and it is therefore not clear, which effect is dominant.

To the authors’ opinion supported by the results of Beyster (1968), the main contribution to the anisotropy of the scattering from water embedded in a flat cell positioned perpendicularly to the beam may come from multiple scattering for cold neutrons. This interpretation of the anisotropy was also suggested by Boyer & King (1988), who found very good agreement of simulations and measurements on protonated toluene while considering only multiple scattering effect. Actually, the anisotropy of the scattering from water can be explained even when taking into account only the geometry of the cell and a relatively small free path of neutron in water. While the neutrons which are scattered first time to the direction corresponding to the normal to the cell can more probably leave the water without any other interaction, the neutrons scattered in the perpendicular direction most probably do not leave the cell and they are re-scattered (maybe several times) until their direction allows them to leave the cell. It causes that the scattering within the broad surrounding of the normal to the cell (corresponding to the direction of the forward- and backward-scattering for the usual geometry) is higher than in other directions. The situation is demonstrated in Fig. 3 where an arbitrary orientation of the 1 mm cell with respect to the primary beam is used in order to demonstrate the dependence of the scattered intensity on the angular deviation from the normal.

![Figure 3](image-url)

**Figure 3** Scheme of the scattering in water filled in the cell (the thickness substantially lower than the other dimensions). The radius of the drawn circle is equal to the mean free path of the neutron in water (e.g. approx. 1 mm for 6 Å). The neutrons scattered nearly perpendicularly to the normal are almost always again scattered. The black arrows of different thickness around the cell demonstrate the intensity which can be detected in different directions. The angle \(\beta\) determines the deviation of a scattered neutron from the normal to the cell.
The influence of multiple scattering on the anisotropy can be either simulated by Monte Carlo method or measured. A measurement, where the water in the cell was rotated around its vertical axis, was carried out. The aim of this experiment was to prove that the decrease of the scattered intensity is not connected to the direction of the primary beam but rather to the direction of the normal to the cell. The scheme of the experiment is identical to that displayed in Fig. 3. The whole measured curve (see Fig. 4) is composed of four individual measurements carried out with a relatively large round cell (18.5 mm diameter) and with a small slit in front of the cell (diameter 3.95 mm) under the rotation angles of the cell of 0°, 20°, 40° and 60°. In Fig. 4, the vertical axis displays the anisotropy factor $K(\alpha, \beta)$ (see (6)). The curve shows evidently the expected tendency, i.e. decrease of the scattered intensity with the increasing deviation from the normal to the cell without respect to the primary beam direction. Thus the anisotropy in the scattering from water is mostly not connected to the forward direction but to the geometry of the cell for the used wavelength 6 Å.

The solid line in Fig. 4 corresponds to the curve simulated by Monte Carlo method where only the multiple scattering effect was modeled. It was assumed, that each scattering event is fully elastic and isotropic. As can be seen, even this simplified approach corresponds very well to the measured data. If the scaling factor equal to 0.96 is used, the simulated data match exactly the measured ones. This means, that while nearly all the measured factor $K_0$ can be ascribed to the multiple scattering, combination of all the other important effects (different PSD response to the inelastically scattered neutrons, the quasielastic structure factor) decrease the scattered intensity in the measured angular range by about 4%. It should be noted, that also the uncertainty in the determination of the attenuation factor of the used attenuator (=2%) can play a role here.

8. Conclusions

In view of Eq. (1), the formulas (3), (8) and (9) are the integral equations for the determination of the coherent cross-section which can be solved simply only for two limiting cases: $p_\alpha=0$ or $p_\alpha=1$. Therefore, the SANS experimenter should pay attention to the facts mentioned in this paper not only before starting to extract the real-space information from the cross-section but already before raw-data treatment in order to avoid an absolute-scale shift or even a substantial change in the scattering curve shape. Particularly, it should be clear what can be concluded from the transmission measurement and the overall small-angle scattering probability should be at least approximately known. Otherwise, the obtained cross-section can be incorrect in a part of the measured Q-range. The deviation becomes definitely significant, when a special sample environment is used or when the measurement without the beam-stop is carried out.

A special care should be taken about which mode of transmission measurement to employ for a particular type of sample. When coherently scattered neutrons cannot be neglected with respect to the other attenuation factors during the transmission measurement, they have to be detected all (it means to use a sufficiently wide solid angle) and $T_0$ can then be calculated. The second mode of the transmission measurement (i.e. PSD as far as possible from the sample position and sum over a small number of pixels in the center only) is then used for estimation of $p_\alpha$.

Our considerations, measurements as well as simulations suggest the conclusion that the dominant effect causing anisotropy of 6 Å neutrons scattering from water in the cell is not the anisotropy of the single-scattering cross-section but the multiple scattering. The factor $K_0$ necessary for the calibration of the primary beam and thus for the precise SANS-data evaluation can be well determined by the Monte Carlo simulation for the used wavelength. However, the dependence of the PSD efficiency on $K_0$ can become more important for larger $\lambda$.

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