Fully Numerical Procedure for Anisotropic Small-Angle Neutron Scattering Modelling and Data Evaluation†

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Abstract

A numerical approach to the evaluation of small-angle neutron scattering (SANS) data is proposed. The procedure covers interparticle-interference and multiple-scattering effects. The influence of these effects as well as the resolution of a SANS instrument are discussed. As an example of the use of the procedure for SANS data modelling, two-dimensional scattering curves of cuboidal particles and ordered cubes are presented. Finally, a test of the fitting procedure is performed on measured data for a solution of polystyrene spheres in water.

1. Introduction

A number of procedures have been developed for the evaluation of isotropic small-angle scattering curves (see e.g. Glatter, 1982, 1991; Pedersen, 1994, and references therein), while only a few methods applicable for the treatment of 2D anisotropic data from pinhole systems exist (see, e.g., Hendricks, Schelten & Schmatz, 1974; Dauger, Fumeron, Guillot & Roth, 1979; Bellet, Royer, Bastie, Lajzerowicz & Legrand, 1992; Fratzl, Langmayr & Paris, 1993). Generally, in order to interpret anisotropic SANS measurements in detail, an appropriate model representing the microstructure of the studied material has to be chosen. The scattering curve corresponding to this model is then computed either analytically or numerically and compared with the experimental results. However, the evaluation of anisotropic SANS data is commonly confined to performing cuts through two-dimensional (2D) data measured with a position-sensitive detector (PSD). The drawback of this approach is that it does not use all of the experimental points from the PSD at once.

We propose a modelling and evaluation procedure based on numerical computation of 2D scattering curves. A numerical approach was chosen because derivation of analytical expressions, covering all the corrections mentioned below, is practically impossible in most cases for anisotropic scattering curves. The procedure is mainly applicable to the treatment of scattering from cuboidal precipitates in some single-crystal alloys. However, its modification for other anisotropically scattering samples can be carried out without much effort.

2. Theory

The usual output of a pinhole SANS experiment is the differential macroscopic SANS cross section smeared by multiple scattering, by the resolution function of the instrument and by the wavelength-distribution function. The following paragraphs describe, step by step, the theoretical background of the proposed numerical evaluation procedure, which extracts real-space information from the measured 2D cross section. The procedure is illustrated schematically in Fig. 1.

2.1. SANS cross section

The direction of a scattered neutron is characterized by the scattering vector \( \mathbf{Q} = (Q_x, Q_y, Q_z) = k - k_0 \), where \( k_0 \) denotes the cross section.

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and \( k \) are wavevectors of the incident and the scattered neutron, respectively. As the restriction for elastic scattering \( |k| = |k_0| = k_0 = 2\pi/\lambda \) (\( \lambda \) is the neutron wavelength) leads in the case of scattering at small angles to the condition \( Q_z = 0 \) (we assume that the incident beam passes along the \( z \) direction), the differential SANS cross section can be written in the form

\[
\frac{d\Sigma}{d\Omega}(Q_x, Q_y) = \frac{1}{V} \left| \sum_{k} \left[F_k F_k^*\right]_{Q_z=0}\right|
\]

where

\[
F(Q) = \int \int \int \Delta \rho(r) \exp(-iQr) \, dr
\]

(2)

is the amplitude. Here \( V \) represents the irradiated volume of the sample and \( \Delta \rho(r) = \rho(r) - \rho_0 \) is the scattering contrast [\( \rho(r) \) and \( \rho_0 \) are the scattering-length densities inside the particle and in the matrix, respectively].

Because of the limited resolution used in a SANS measurement [the full width at half-maximum (FWHM) of the resolution function is \( \Delta Q_x \) in the horizontal direction and \( \Delta Q_y \) in the vertical direction], we can assume that the scattering intensities from sufficiently distant places in the sample sum incoherently. The characteristic distance \( s \) at which this assumption is fulfilled is equal to or larger than the maximum of \( 2\pi/\Delta Q_x \) and of \( 2\pi/\Delta Q_y \). Using this approximation, we do not consider samples containing particles that are perfectly ordered on a scale larger than \( s \). Then the sample can be treated as consisting of cubic blocks with size \( s \) and (1) can be rewritten as

\[
\frac{d\Sigma}{d\Omega}(Q_x, Q_y) = \frac{1}{V} \sum_{m=1}^{G_0} F_m F_m^* Q_z = 0
\]

(3)

where

\[
F_m(Q) = \int \int \int \Delta \rho_m(r) \exp(-iQr) \, dr
\]

(4)

Here \( \nu \) represents the volume of one block, \( \nu = V/P_0 \), \( P_0 \) is the number of these blocks, and \( F_{FT} \) denotes the Fourier transform. It should be noted that the block can contain more than one particle and that the sizes of the particles inside one block are not necessarily equal. In this way, the approach automatically includes interparticle interference between the particles inside the block. The distance (or distances) between the particles can be assumed as another parameter (or parameters) of the model.

Although the condition \( Q_z = 0 \) can reduce the three-dimensional (3D) Fourier transform in (4) to the 2D task, we decided to perform the numerical 3D transform. The reason for this is that in the future we intend to include modelled particles (or sets of particles inside the block) which are differently oriented in space in the evaluation procedure. Computation of the cross section of particles (or sets of particles) having different orientations is then reduced to calculation of different planar sections through the computed 3D array \([F_k F_k^*]\). This is discussed further in §3.

Owing to the enormous developments in computer hardware and software, the cross section can, in many cases, be computed numerically from the \( \Delta \rho(r) \) model using (3) and (4). However, the number of terms on the right side of (3) should be reduced in order to attain acceptable computing time.

### 2.2. Size distribution

The summation in (3) is performed for all the blocks. In reality, we can group the blocks so that each group contains blocks of the same or nearly the same configuration (i.e. sizes and shapes of the particles, distances between the particles, their mutual orientations, etc.). Then the number of summations can be reduced as follows:

\[
\frac{d\Sigma}{d\Omega}(Q_x, Q_y) = \frac{1}{V} \sum_{m=1}^{G_0} D_m F_m F_m^* Q_z = 0
\]

(5)

where \( G_0 \) is the number of groups and \( D_m \) denotes the number of blocks in the group \( m \). Even this decrease in the number of terms on the right side does not necessarily lead to acceptable computing time. The sum over different configurations 'sizes of particles - distances between them' has to be reduced in order to perform the time-consuming 3D Fourier transform as few times as possible. Therefore, some other assumptions have to be made. The first one is that one block contains only particles having the same size. This condition corresponds to the local monodisperse approximation introduced by Pedersen (1994). The second assumption concerns the distances between particles. As the procedure is supposed to be used mainly for the evaluation of scattering from precipitates in single-crystal alloys, the distance between particles, \( l_m \), is assumed to be proportional to their size (Pedersen, 1994). We suppose only one characteristic distance between particles in one group (particles are positioned on the nodes of a cubic or square grid), but that the different groups contain particles with different characteristic distances. In this way, the positions of interparticle-interference maxima change from group to group and the sum in (5) can result in broad interference maxima.

We are usually interested in the volume distribution of the particles between different groups, \( u_m = U_m V_{\rho_0} \) (\( \sum u_m = 1 \)), where \( U_m \) is the overall volume of the particles in the group \( m \) and \( V_{\rho_0} = \sum U_m \) is the overall volume of the particles in the sample. For this purpose, \( D_m \) can be rewritten as
\[ D_m = N_m(1/J_m) = (U_m/V_{pm})(1/J_m) = (V_{pm}/U_m)(1/J_m) \]

where \( N_m \) is the overall number of particles in the group \( m \), \( V_{pm} \) is the volume of one particle in the group \( m \) and \( J_m \) is the number of particles in one block in the group \( m \). Therefore

\[ d\Sigma/d\Omega(Q_x, Q_y) = \frac{1}{V} \sum_{m=1}^{G_0} F_m F_m^* \]

\[ = c_p \sum_{m=1}^{G_0} (1/J_m)(1/V_{pm})(F_m F_m^*)_{Q_0=0} \]

where \( c_p = V_{pm}/V \) is the overall volume fraction of the particles in the sample. The term \( 1/J_m \) in (7) renormalizes the scattering from the whole block (which can contain several particles) to the scattering from one particle only. If interparticle interference need not be taken into account, \( F_m \) can be simply computed for one particle only (\( J_m = 1 \) for each \( m \)).

By repeating the numerical computation of \( F_m \) for different particle sizes (and corresponding distances between particles, if applicable), we can arrive at the cross-section size distribution of the particles. With some assumptions, other populations of particles inside the sample (which differ, e.g., in shape or in scattering contrast) could be included in the procedure.

2.3. Orientation distribution

Generally, the particles can be tilted with respect to their mean orientation. Up to now, we could model an orientation distribution of particles around the primary neutron beam, \( o_n \), only (\( o_n \) corresponds to the relative number of particles with the particular orientation \( \psi_n \)). The presence of this orientation distribution changes the cross section to

\[ d\Sigma/d\Omega(Q_x, Q_y) = \sum_{n=1}^{O_0} \{d\Sigma/d\Omega(Q_x, Q_y) \}^{\psi_n}(\varphi + \psi_n), Q_x, Q_y \]

where \( O_0 \) is the number of different particle orientations and \( (Q_x, \varphi) \) are the radial coordinates corresponding to the Cartesian coordinates \( (Q_x, Q_y) \) of the modelled \( d\Sigma/d\Omega(Q_x, Q_y) \).

2.4. Multiple scattering corrections

Another feature that can influence the measured SANS curve is multiple scattering [some authors, e.g. Berk & Hardman-Rhyne (1985), use the term 'incoherent multiple scattering']. Its smearing effect depends on the sample thickness \( d \) and on the morphology of the particles which determine the total scattering probability. Owing to multiple scattering, the measured (true) cross section \( [d\Sigma/d\Omega(Q_x, Q_y)]_T \) differs considerably from the cross section \( [d\Sigma/d\Omega(Q_x, Q_y)]_i \) (Schelten & Schmatz, 1980) for strongly scattering samples. By including a possible influence of multiple SANS in the evaluation procedure, we would not be restricted to weakly scattering samples only. The problem of transformation of \( [d\Sigma/d\Omega(Q_x, Q_y)]_i \) into \( [d\Sigma/d\Omega(Q_x, Q_y)]_T \) was solved by Schelten & Schmatz (1980): we use the results of their analysis here. They arrived at a relation connecting \( [d\Sigma/d\Omega(Q_x, Q_y)]_i \) with \( [d\Sigma/d\Omega(Q_x, Q_y)]_T \) in the form

\[ h(r_s, r_r) = \exp[-s(0, 0)/k_0^2]k_0^2[\exp[s(r_s, r_r)/k_0^2] - 1] \]

where

\[ h(r_s, r_r) = dF_{FT}([d\Sigma/d\Omega(Q_x, Q_y)]_T)(r_s, r_r) \]

\[ s(r_s, r_r) = dF_{FT}([d\Sigma/d\Omega(Q_x, Q_y)]_i)(r_s, r_r) \]

\( (F_{FT} \) denotes the 2D inverse Fourier transform). We simply compute the \( s(r_s, r_r) \) function from (10), put it into (9) and compute the \( h(r_s, r_r) \) function. Then the Fourier transform is applied on \( h(r_s, r_r) \) which results in

\[ [d\Sigma/d\Omega(Q_x, Q_y)]_T \] [see (10)].

2.5. Wavelength-distribution smearing

In neutron scattering experiments we are usually considerably limited by the low intensities of the available sources. In order to obtain a high flux at the sample position, we are commonly forced to use a relatively wide wavelength distribution and a relatively poor collimation of the incident beam in pinhole SANS experiments. This implies a non-negligible influence of instrumental and \( \lambda \)-distribution smearing on the measured curve (Pedersen, Posselt & Mortensen, 1990). As \( |\Delta \lambda/\lambda| \) is approximately equal to \( |\Delta Q_x/Q_x| \) for common settings (\( \Delta \lambda \) is the FWHM of the \( \lambda \) distribution and \( \Delta Q_x \) is the corresponding FWHM of the radial component of \( Q \)), we can simulate the influence of the \( \lambda \) distribution by smearing in the radial direction of \( Q \). Then we arrive at the cross section smeared by the wavelength spread

\[ [d\Sigma/d\Omega(Q_x, Q_y)]_\lambda = \sum_{n=1}^{L_0} w_n[d\Sigma/d\Omega((Q_x + \Delta Q_x) \times \sin \varphi, (Q_y + \Delta Q_y) \cos \varphi)]_T \]

where \( w_n = \sum w_n = 1 \) is the distribution approximated in \( L_0 \) discrete points \( \Delta \lambda = \lambda_0 \) (\( \lambda_0 \) is the mean wavelength) and \( \Delta Q_x = -Q_x(\Delta \lambda_0/\lambda_0) \) is the change of the scattering vector corresponding to the change of \( \lambda \).

2.6. Collimation and detector resolution-function smearing

The resolution function of a SANS instrument used in our procedure includes smearing due to both the collimation and the PSD resolution. Although the resolution function should generally be 3D (Harris, Lebech &
Pedersen, 1995), we suppose that its width in the direction perpendicular to the Ewald sphere (z direction) approaches a \( \delta \) function and, therefore, the planar section \( Q_z = 0 \), instead of a convolution, is a sufficient approximation to obtain the 2D cross section. Harris, Lebech \\& Pedersen (1995) calculated, for a usual SANS setting, that the width of the resolution function in the \( z \) direction is at least one order of magnitude smaller than in the other two perpendicular directions. Therefore, we consider the resolution function \( R_{xy} \) to be 2D. The resulting smeared cross section \([d \Sigma / d \Omega(Q_x, Q_y)]_M\) is then described by the 2D convolution of \([d \Sigma / d \Omega(Q_x, Q_y)]_\lambda\), with \( R_{xy}(Q_x, Q_y)\).

\[
[d \Sigma / d \Omega(Q_x, Q_y)]_M = R_{xy}(Q_x, Q_y) \\
\otimes [d \Sigma / d \Omega(Q_x, Q_y)]_\lambda \tag{12}
\]

where the symbol \( \otimes \) denotes the convolution and the integral from \( R_{xy}(Q_x, Q_y) \) over \( Q_x \) and \( Q_y \) is equal to 1.

3. Program

On this theoretical basis, a VAX Fortran program was written for modelling and, optionally, for least-squares fitting of the measured SANS data to the chosen model.

3.1. Characteristics of the program

In the program, one population of particles having the same shape and scattering contrast is modelled. The model of the particle (or the model of a set of particles in one block) is created as a binary map in \( N_{\text{FFT}} \times N_{\text{FFT}} \times N_{\text{FFT}} \) points. The volume distribution \( u_v \) and the orientation distribution \( o_o \) are represented by histograms of Gaussian shape \((G_0 \, \text{and} \, O_0, \text{respectively, are the numbers of points in which these distributions are approximated). This model is applicable to systems which can be characterized by one mean size \( a_0 \) and one mean orientation \( \psi_0 \) of the particles. Cuboidal precipitates in some single-crystal alloys can display such morphology. The use of more complicated functions for the description of the volume and orientation distributions would increase the number of free parameters of the model. However, the other representations of the distributions as well as more populations of particles can be incorporated into the program.

The program employs the fast Fourier transform (Press, Flannery, Teukolsky \\& Vetterling, 1986) for computing the cross section from the particle model, for the multiple-SANS smearing, as well as for convolution with the resolution function. The necessary size of the 3D real-space array (in points), in which the model is computed, depends on two conditions. The first one, which determines the size of the real-space array (in \( \AA \)), is identical to the size \( s \) defined in §2.1. The second condition is connected with the maximum measured (or requested when modelling) \( Q_x \) or \( Q_y \) (which can be referred to as \( Q_{\text{max}} \)). It determines the minimum size (in \( \AA^{-1} \)) of the reciprocal space array, \( 2Q_{\text{comp}} = 2^{1/2}Q_{\text{max}} \). The factor \( 2^{1/2} \) arises from the fact that the computed-data array should fully cover the measured-data array even when rotated by 45°. Another reason for extending the array by this factor is further smearing by the \( \lambda \) distribution (see §2.5). Owing to the use of the fast Fourier transform, the size of one pixel in the real space \( \Delta r \) (in \( \AA \)) is connected with the size of the reciprocal space array by the formula \( \Delta r = 2\pi/2Q_{\text{comp}} \). Combination of these two conditions leads to the real-space array size in points of the binary map \((\approx s/\Delta r)\). Because fast Fourier transform can be performed only in arrays having edge sizes, \( N_{\text{FFT}} \), equal to the power of two, the array is further extended to a power of two larger than \( s/\Delta r \). This can be done either in real (extension of \( s \)) or reciprocal (extension of \( 2Q_{\text{comp}} \)) space, or partially in both spaces. The typical magnitude of \( N_{\text{FFT}} \) is 64 or 128.

When fitting the model to the measured 2D data, the \([d \Sigma / d \Omega(Q_x, Q_y)]_M\) array calculated in \( N_{\text{FFT}} \times N_{\text{FFT}} \) discrete points is recomputed to the measured-data array by a linear interpolation from three nearest points. The shift \((Q_{xo}, Q_{yo})\) of the computed array relative to the center of the measured array can be refined.

3.2. Calculation time

The computing time necessary for the evaluation of one curve depends mainly on the number of points in which the size distribution is calculated. For example, if the data-array size of \( 128 \times 128 \times 128 \) points is used and the size distribution is computed for \( G_0 = 5 \), the calculation of the scattering curve model is finished after 15 min (for a \( 64 \times 64 \times 64 \) array, the time is reduced eightfold). When the measured data are fitted to the model, the data modelling procedure has to be repeated many times and the typical evaluation time is then 1–4 h. Nevertheless, this time depends strongly on the number of fitted parameters. This information is valid for an Alpha 3000 workstation.

Generally, the computing time should not significantly exceed the measurement time of the SANS experiment. When comparing the above-mentioned calculation times with the time necessary for carrying out a typical SANS measurement (20 min to 4 h per curve), the time of evaluation is acceptable.

We also tested the computing time which would be necessary for a numerical calculation of the 2D cross section of particles oriented differently in space (we supposed \( N_{\text{ori}} \) different orientations). We compared an approach which would use a definition of the particle orientation in real space followed by a 2D Fourier transform with our approach, which employs a 3D Fourier transform. In our approach the calculation of the model as well as the 3D Fourier transform needs to be performed once and only the planar section of the 3D
array needs to be performed $N_{ori}$ times, while using the 2D Fourier transform the binary map of the model has to be computed $N_{ori}$ times. The results of the test clearly revealed that the latter approach is more efficient for $N_{ori} < 20$, whereas our procedure is significantly faster for higher numbers of points.

3.3. Resolution function

The resolution function $R_{xy}(Q_x, Q_y)$ of a SANS instrument can be found by several methods. We use direct determination by SANS (Pedersen, 1993), which takes advantage of the fact that $R_{xy}(Q_x, Q_y)$ relates to the shape of the incident-beam profile on the PSD. Such a measurement cannot usually be performed without attenuation of the neutron beam and an appropriate attenuator has to be selected cautiously in order not to change the beam divergence substantially. The normalized beam profile can then be used directly to approximate $R_{xy}(Q_x, Q_y)$. However, a Gaussian function is commonly a satisfactory approximation of the beam profile (Harris, Lebech & Pedersen, 1995). Therefore, a 2D Gaussian with FWHM $\Delta Q_x$ and FWHM $\Delta Q_y$ is used for this purpose in the program. $\Delta Q_x$ and $\Delta Q_y$ can be found from the beam-profile measurement by applying our evaluation procedure with the ‘empty’ sample [i.e. $\rho(r) = \rho_0 = \text{constant}$].

The $\lambda$ distribution $w_{\lambda}$ is also approximated by a Gaussian function in the program (Pedersen, 1993). Nevertheless, functions describing other shapes could replace the Gaussian if necessary for more precise evaluation.

![Fig. 2](image-a.png)

Fig. 2. The influence of the resolution function width on the SANS curve shape: (a) $\Delta Q_x = 0.00150$ and $\Delta Q_y = 0.00236$ Å$^{-1}$; (b) $\Delta Q_x = 0.00305$ and $\Delta Q_y = 0.00473$ Å$^{-1}$. The particles were of cubic shape ($a_0 = 2000$ Å). Here, as well as in Figs. 3–6, displayed contour lines correspond to the equidistant levels of the macroscopic differential cross section $d \Sigma / d Q$ (cm$^{-1}$ sr$^{-1}$) in the logarithmic scale, the $Q$ ranges on both the horizontal and the vertical axes are in Å$^{-1}$, one edge of the cubic particle is parallel to the incident-beam direction and the second one to the PSD edge.

![Fig. 3](image-b.png)

Fig. 3. The influence of multiple SANS on the shape of the scattering curve (cubic particles, $a_0 = 2000$ Å, $c_p = 0.005$, $\Delta \rho = 3.66 \times 10^{10}$ cm$^{-2}$, $\Delta Q_x = 0.00084$ and $\Delta Q_y = 0.00119$ Å$^{-1}$): (a) sample thickness $d = 2$ mm, (b) $d = 5$ mm. (See Fig. 2 for additional notation.)
4. Modelling

In the following paragraphs, we discuss some aspects of the modelling of the SANS curve.

4.1. Influence of collimation

Fig. 2 demonstrates the effect of the instrumental resolution on the anisotropic scattering. Fig. 2(b) corresponds approximately to the usual symmetrical setup of the SANS experiment [i.e. collimation length is equal to the sample-to-detector distance (SDD)] on the V4 instrument of BENS, at the Hahn-Meitner-Institut (HMI), Berlin. The difference between parts (a) and (b) of Fig. 2 clearly shows that the resolution of a SANS instrument should be considered when evaluating strongly anisotropic scattering.

4.2. The effect of multiple SANS

Fig. 3 displays two modelled scattering curves for the same type of particle and the same volume fraction in the matrix, but for samples having different thicknesses. In order to model only multiple scattering and clearly distinguish this effect from a possible influence of interparticle interference, a dilute system \((J_m = 1)\) of nonordered cubes having the same orientation was examined. The total true scattering probabilities were equal to 0.230 and 0.600 for cases (a) and (b), respectively. Computing of apparent scattering probabilities without taking multiple scattering into account would lead to the incorrect values 0.261 and 0.915, respectively.

4.3. Particle-shape modelling

As an example of the particle-shape modelling, we present here the SANS curve of cuboidal particles (Fig. 4). The radii of curvature of the particle surfaces, \(r_1\), and edges, \(r_2\), together with the size of the cube edge, \(a_0\), are parameters that fully describe the morphology of the particle. A detailed description of the model can be found in the papers by Strunz, Wiedenmann, Zrnić & Lukáš (1997) and of Strunz, Zrnić, Wiedenmann & Lukáš (1995).

4.4. Influence of distance between particles

The influence of the distance between particles on the shape of the scattering curve is demonstrated in Fig. 5 for cubic particles. The cubes were positioned on the nodes of a square grid with a lattice parameter \(l\). An example of a scattering curve which is not influenced by interparticle interference can be seen in Fig. 3(a) for the same particle size and the same sample thickness.

![Fig. 4. The scattering curve of the cuboidal particle \((a_0 = 2000 \, \text{Å})\). The ratios \(r_1/a_0\) and \(r_2/a_0\) were equal to 3.07 and 0.160, respectively. The cuboid had the same volume as the cube, the scattering curve of which is drawn in Fig. 2(b); the volume fraction as well as the scattering contrast were also the same as those of the cube. (See Fig. 2 for additional notation.)](image)

![Fig. 5. Modelling of the influence of interparticle interference. The size of the cubes was set to 2000 Å and their distance was \(l = 6000 \, \text{Å}\) and \(l = 3200 \, \text{Å}\). (See Fig. 2 for notation.)](image)
5. Data treatment

The applicability of the fitting procedure is demonstrated using a real-data example. As a testing sample, we used a solution of polystyrene spheres in H$_2$O. Scattering produced by this sample was not anisotropic, but it was sufficient for a test of convergence of parameter refinement in the fitting procedure.

We refined the size and the volume distribution of the spheres using data collected with the V4 pinhole SANS facility of BENSC at HMI, Berlin. The convergence of the fitting procedure was reliable for the input value of the diameter in the range ±50% from the correct diameter of the particles. The resulting value was found to be equal to 1560 (10) Å. Simultaneously, the width of the volume distribution was found to be equal to 17 (2)%.

The result of the fit is displayed in Fig. 6.

Examples of an evaluation of anisotropic SANS data employing this numerical procedure can be found in the papers of Strunz, Zrnik, Wiedenmann & Lukáš (1995) and of Strunz, Wiedenmann, Zrnik & Lukáš (1997).

6. Conclusions

The derivation of analytical expressions for 2D anisotropic scattering curves can be performed only for several special shapes of scattering particles, e.g. octahedra (Hendricks, Schelten & Schmatz, 1974), interacting spheres (Dauger, Fumeron, Guillot & Roth, 1979), cubes (Bellet, Royer et al., 1992), ellipsoids and plate-like shapes (Fratzl, Langmayr & Paris, 1993). The utilization of the numerical approach enables testing of a wider variety of models to fit a measured data set. For example, the scattering curve of a perfect cube differs significantly from that of a cuboid, even for a small rounding of the edges and surfaces [compare Fig. 2(b) and Fig. 4]. It should be pointed out that an appropriate model has to be chosen for such an evaluation of SANS data. Direct imaging of the particles by electron microscopy is thus indispensable.

The presented evaluation procedure is not restricted to low total scattering probabilities and/or densities of particles because the interparticle-interference and multiple-scattering effects are taken into account in the numerical calculations. Contrary to the usual approach to 2D SANS data evaluation (Hendricks, Schelten & Schmatz, 1974; Bellet, Royer, Bastie, Lajzerowicz & Legrand, 1992), this procedure takes into account an influence of $\lambda$-distribution smearing, as well as smearing due to the finite collimation of the neutron beam. It facilitates utilization for evaluation of data measured with different experimental set-ups and/or at different pinhole SANS facilities.

Finally, the evaluation procedure uses all measured points from the PSD at once. It simplifies the evaluation of the data compared with carrying out cuts through the measured 2D SANS data (see, e.g. Bellet, Royer et al., 1992). The second consequence is that the procedure takes full advantage of the 2D PSD.

The program can be used both for isotropic and anisotropic SANS data evaluation. However, the main field of its application is the latter one. An extension of the computer program which would allow modelling of a spatial distribution of particle orientations is in progress.

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