section in this application, *i.e.* the maximum dimension of the cross section must not be larger than $D_{\max}$.

The situation is quite similar for flat particles. If we combine (2.6.1.47) and (2.6.1.49), we obtain

$$I(h) = 4\pi A \int_0^\infty p_t(r) \frac{\cos(hr)}{h^2}\, \mathrm{d}r, \qquad (2.6.1.66)$$

$p_t(r)$ being the distance distribution function of the thickness. We have to check that the particles are flat with a constant thickness with maximum thickness $T \leq D_{\max}$. A is the area of the particles and would be needed only for experiments on an absolute scale.

2.6.1.6.4. *Direct structure analysis*

It is impossible to determine the three-dimensional structure $\rho(\mathbf{r})$ directly from the one-dimensional information $I(h)$ or $p(r)$. Any direct method needs additional *a priori information* – or assumptions – on the system under investigation. If this information tells us that the structure only depends on one variable, *i.e.* the structure is in a general sense *one dimensional*, we have a good chance of recovering the structure from our scattering data.

Examples for this case are particles with spherical symmetry, *i.e.* ρ depends only on the distance r from the centre, or particles with cylindrical or lamellar symmetry where ρ depends only on the distance from the cylinder axis or from the distance from the central plane in the lamella. We will restrict our discussion here to the spherical problem but we keep in mind that similar methods exist for the cylindrical and the lamellar case.

Spherical symmetry. This case is described by equations (2.6.1.51) and (2.6.1.52). As already mentioned in §2.6.1.3.2.2, we can solve the problem of the calculation of $\rho(r)$ from $I(h)$ in two different ways. We can calculate $\rho(r)$ *via* the distance distribution function $p(r)$ with a *convolution square-root* technique (Glatter, 1981; Glatter & Hainisch, 1984). The other way goes through the amplitude function $A(h)$ and its Fourier transform. In this case, one has to find the right phases (signs) in the square-root operation $\{A(h) = \pm[I(h)^{1/2}]\}$.The *box-function refinement* method by Svergun, Feigin & Schedrin (1984) is an iterative technique for the solution of the phase problem using the *a priori* information that $\rho(r)$ is equal to zero for $r \geq R_{\max}$ ($D_{\max}/2$). The same restriction is used in the convolution square-root technique. Under ideal conditions (perfect spherical symmetry), both methods give good results. In the case of deviations from spherical symmetry, one obtains better results with the convolution square-root technique (Glatter, 1988). With this method, the results are less distorted by non-spherical contributions.

Multipole expansions. A wide class of homogeneous particles can be represented by a boundary function that can be expanded into a series of spherical harmonics. The coefficients are related to the coefficients of a power series of the scattering function $I(h)$, which are connected with the moments of the PDDF (Stuhrmann, 1970*b*,*c*; Stuhrmann, Koch, Parfait, Haas, Ibel & Crichton, 1977). Of course, this expansion cannot be unique, *i.e.* for a certain scattering function $I(h)$ one can find a large variety of possible expansion coefficients and shapes. In any case, additional *a priori* information is necessary to reduce this number, which in turn influences the convergence of the expansion. Only compact, globular structures can be approximated with a small number of coefficients.

This concept is not restricted to the determination of the shape of the particles. Even inhomogeneous particles can be described using all possible radial terms in a general expansion (Stuhrmann, 1970*a*). The information content can be increased by contrast variation (Stuhrmann, 1982), but in any event one is left with the problem of how to find additional *a priori* information in order to reduce the possible structures. Any type of symmetry will lead to a considerable improvement. The case of axial symmetry is a good example. Svergun, Feigin & Schedrin (1982) have shown that the quality of the results can be further improved when upper and lower limits for $\rho(\mathbf{r})$ can be used. Such limits can come from a known chemical composition.

2.6.1.6.5. *Interpretation of results*

After having used all possible data-evaluation techniques, we end up with a desmeared scattering function $I(h)$, the PDDF $p(r)$ or the size-distribution function $D(R)$, and some special functions discussed in the previous subsections. Together with the particle parameters, we have a data set that can give us at least a rough classification of the substance under investigation.

The interpretation can be performed in reciprocal space (scattering function) or in real space (PDDF *etc*.). Any symmetry can be detected more easily in reciprocal space, but all other structural information can be found more easily in real space (Glatter, 1979, 1982*b*).

When a certain structure is estimated from the data and from *a priori* information, one has to test the corresponding model. That means one has to find the PDDF and $I(h)$ for the model and has to compare it with the experimental data. Every model that fits within the experimental errors can be true, all that do not fit have to be rejected. If the model does not fit, it has to be refined by trial and error. In most cases, this process is much easier in real space than in reciprocal space. Finally, we may end up with a set of possible structures that can be correct. Additional *a priori* information will be necessary to reduce this number.

2.6.1.7. *Simulations and model calculations*

2.6.1.7.1. *Simulations*

Simulations can help to find the limits of the method and to estimate the systematic errors introduced by the data-evaluation procedure. Simulations are performed with exactly known model systems (test functions). These systems should be similar to the structures of interest. The model data are transformed according to the special experimental situation (collimation profiles and wavelength distribution) starting from the theoretical PDDF (or scattering function). '*Experimental data points*' are generated by sampling in a limited h range and adding statistical noise from a random-number generator. If necessary, a certain amount of background scattering can also be added. This simulated data set is subjected to the data-evaluation procedure and the result is compared with the starting function. Such simulation can reveal the influence of each approximation applied in the various evaluation routines.

On the other hand, simulations can also be used for the optimization of the experimental design for a special application. The experiment situation is characterized by several contradictory effects: a large width for the functions $P(t)$, $Q(x)$, and $W(\lambda')$ leads to a high statistical accuracy but considerable smearing effects. The quality of the results of the desmearing procedure is increased by high statistical accuracy, but decreased by large smearing effects. Simulations can help to find the optimum for a special application.

references