

## 2.6. SMALL-ANGLE TECHNIQUES

thickness of the lamella. An example is given in Fig. 2.6.1.10 where we compare a homogeneous lamellar particle (with  $\rho = +\frac{1}{3}$ ) with an inhomogeneous one,  $\rho_r(x)$  being a three-step function alternating between the values  $+1, -1, +1$ .

*Flat particles. In-plane inhomogeneity.* Lamellae with a homogeneous cross section but inhomogeneities along the basal plane have a PDDF that deviates from that of a homogeneous lamella in the whole range  $0 < r < D$ . These deviations are a measure of the in-plane inhomogeneities; a general evaluation method does not exist. Even more complicated is the situation that occurs in membranes: these have a pronounced cross-sectional structure with additional in-plane inhomogeneities caused by the membrane proteins (Laggner, 1982; Sadler & Worcester, 1982).

*Contrast variation and labelling.* An important method for studying inhomogeneous particles is the method of contrast variation (Stuhrmann, 1982). By changing the contrast of the solvent, we can obtain additional information about the inhomogeneities in the particles. This variation of the contrast is much easier for neutron scattering than for X-ray scattering because hydrogen and deuterium have significantly different scattering cross sections. This technique will therefore be discussed in the section on neutron small-angle scattering.

A method for distance determination with X-rays by heavy-atom labelling was developed by Kratky & Worthman (1947). These ideas are now used for the determination of distances between deuterated subunits of complex macromolecular structures with neutron scattering.

*High-resolution experiments.* A special type of study is the comparison of the structures of the same molecule in the crystal and in solution. This is done to investigate the influence of the crystal field on the polymer structure (Krigbaum & Kügler, 1970; Damaschun, Damaschun, Müller, Ruckpaul & Zinke, 1974; Heidorn & Trewhella, 1988) or to investigate structural changes (Ruckpaul, Damaschun, Damaschun, Dimitrov, Jänig, Müller, Pürschel & Behlke, 1973; Hubbard, Hodgson & Doniach, 1988). Sometimes such investigations are used to verify biopolymer structures predicted by methods of theoretical physics (Müller, Damaschun, Damaschun, Misselwitz, Zirwer & Nothnagel, 1984). In all cases, it is necessary to measure the small-angle scattering curves up to relatively high scattering angles ( $h \approx 30 \text{ nm}^{-1}$ , and more). Techniques for such experiments have been developed during recent years (Damaschun, Gernat, Damaschun, Bychkova & Ptitsyn, 1986; Gernat, Damaschun, Kröber, Bychkova & Ptitsyn, 1986; I'anson, Bacon, Lambert, Miles, Morris, Wright & Nave, 1987) and need special evaluation methods (Müller, Damaschun & Schrauber, 1990).

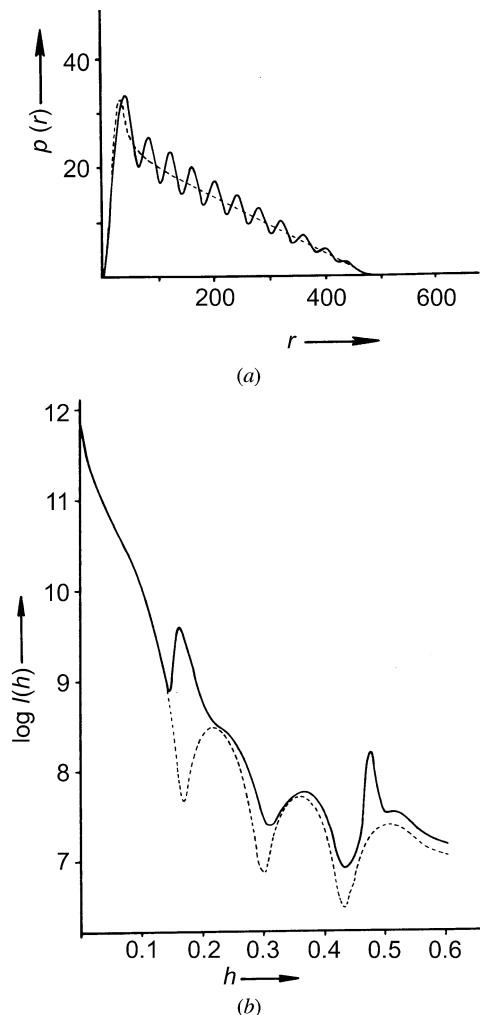


Fig. 2.6.1.9. Inhomogeneous circular cylinder with periodical changes of the electron density along the cylinder axis compared with a homogeneous cylinder with the same mean electron density. (a)  $p(r)$  function; (b) scattering intensity; — inhomogeneous cylinder; - - - homogeneous cylinder.

## 2.6.1.3.3. Interparticle interference, concentration effects

So far, only the scattering of single particles has been treated, though, of course, a great number of these are always present. It has been assumed that the intensities simply add to give the total diffraction pattern. This is true for a very dilute solution, but with increasing concentration interference effects will contribute. Biological samples often require higher concentrations for a sufficient signal strength. We can treat this problem in two different ways:

-We accept the interference terms as additional information about our system under investigation, thus observing the spatial arrangement of the particles.

-We treat the interference effect as a perturbation of our single-particle concept and discuss how to remove it.

The first point of view is the more general, but there are many open questions left. For many practical applications, the second point of view is important.

*The radial distribution function.* In order to find a general description, we have to restrict ourselves to an isotropic assembly of monodisperse spheres. This makes it possible to

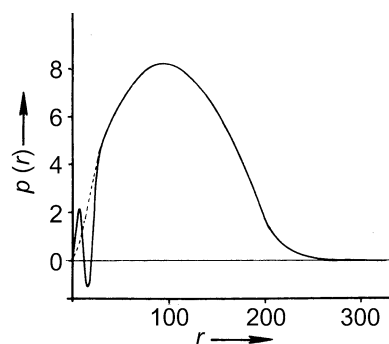


Fig. 2.6.1.10.  $p(r)$  function of a lamellar particle. The full line corresponds to an inhomogeneous particle,  $\rho_r(x)$  is a three-step function with the values  $+1, -1, +1$ . The broken line represents the homogeneous lamella with  $\rho = +\frac{1}{3}$ .