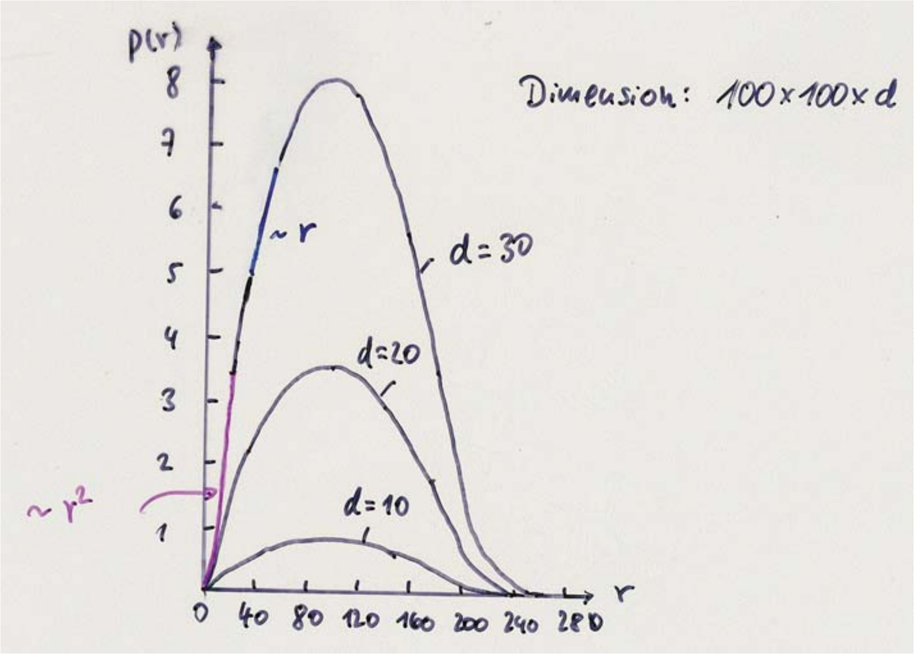
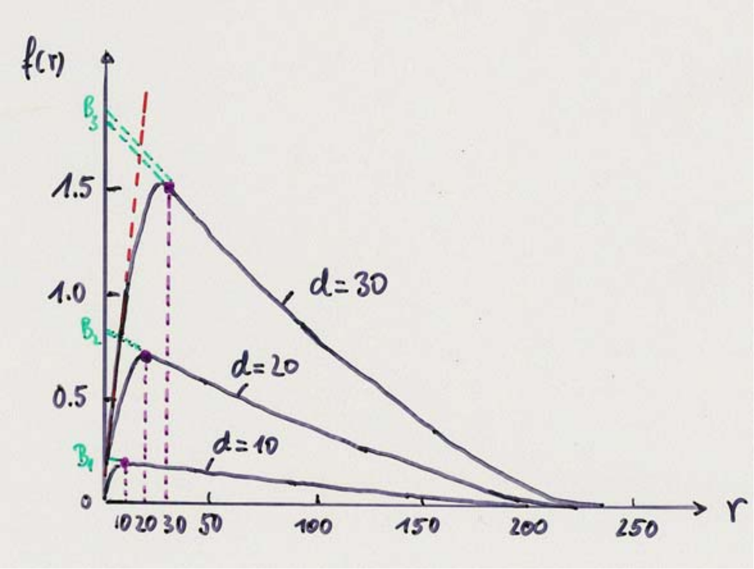
# p(r) for platelet-like particles




Transition from $r^2$ behaviour to $\sim r$ behaviour difficult to localize

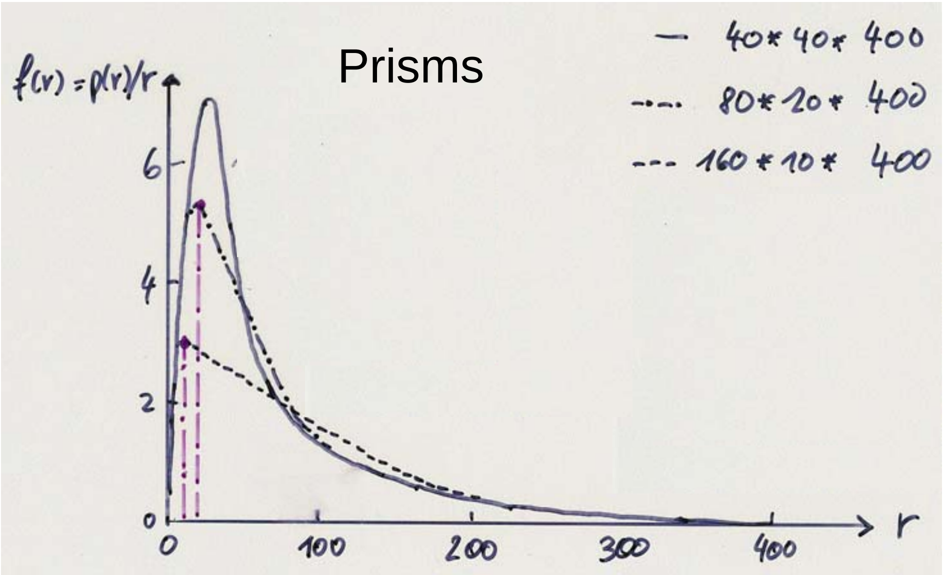
$\rightarrow$ Definition of a new function: $f(r) = p(r)/r$

--- linear initial region

- inflection indicates thickness Dt of platelet

$B = f(0)_{extrapol} = (1/2)(\Delta\rho_s)^2 A\ d^2$
$\Rightarrow$ info about basal area A
(requires data on absolute scale!)

# f(r) functions of other elementary bodies

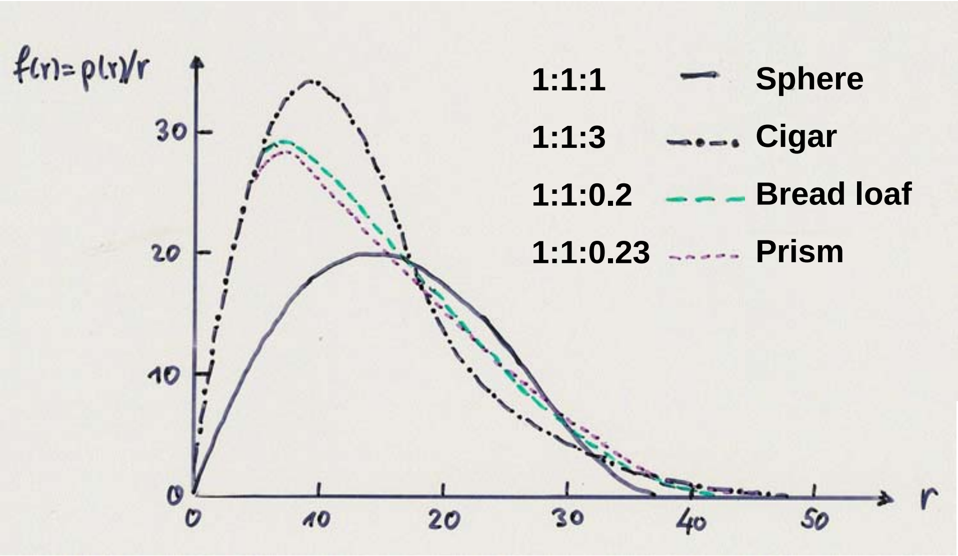



f(r) amplifies lamellar structure elements of an object

Prisms: 40x40 - no lamellar character
80x20 & 160x20 - linear initial slope clear indication of increasing lamellar character

Maximum allows to estimate thickness of "lamella"

Spherical objects →

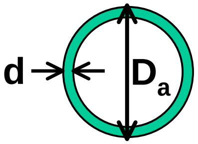


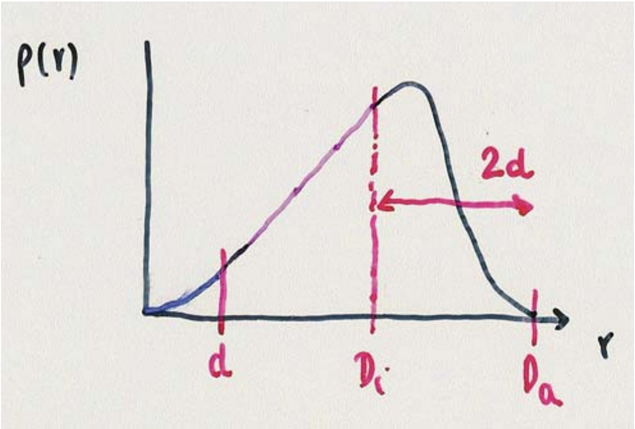

No lamellar character for sphere and cigar

No distinction possible between bread loaf and prism (circular and rectangular base plane) in real experiments; only average thickness can be read off

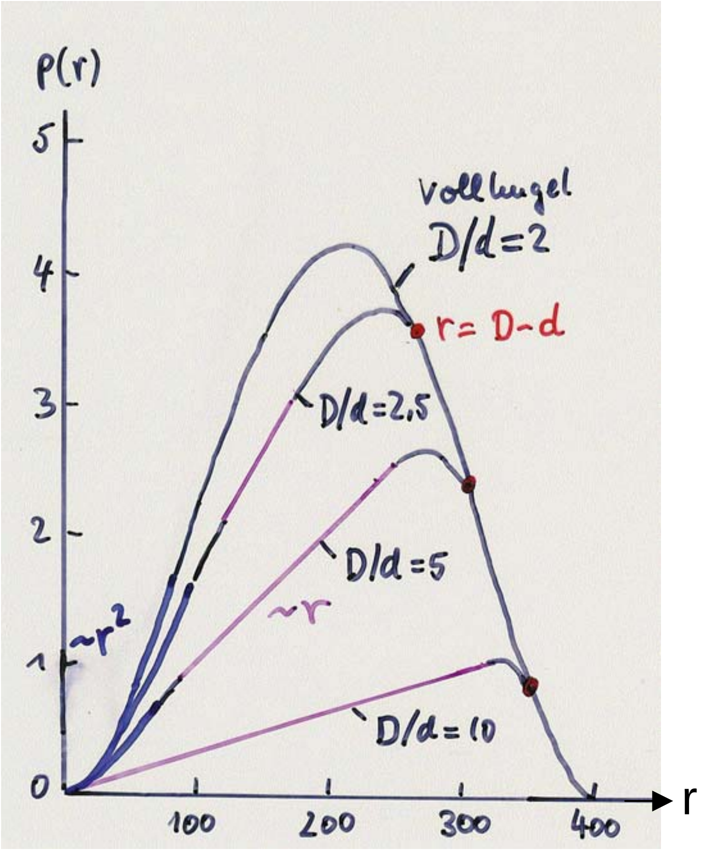
# Hollow and Inhomogeneous Particles: Hollow Spheres

Thin hollow sphere ~ flat, but bent particle
$\rightarrow$p(r) shares some features with lamellar objects




$D_a = 400$

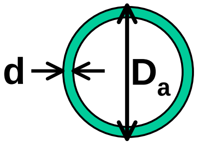



| | |
|---|---|
| p(r) ~ $r^2$ | for $r \leq d = R_a - R_i$ |
| ~ $r$ | for $d < r \leq D_a - 2d = 2R_i$ |
| ~ full sphere | for $r \geq D_a$-d |

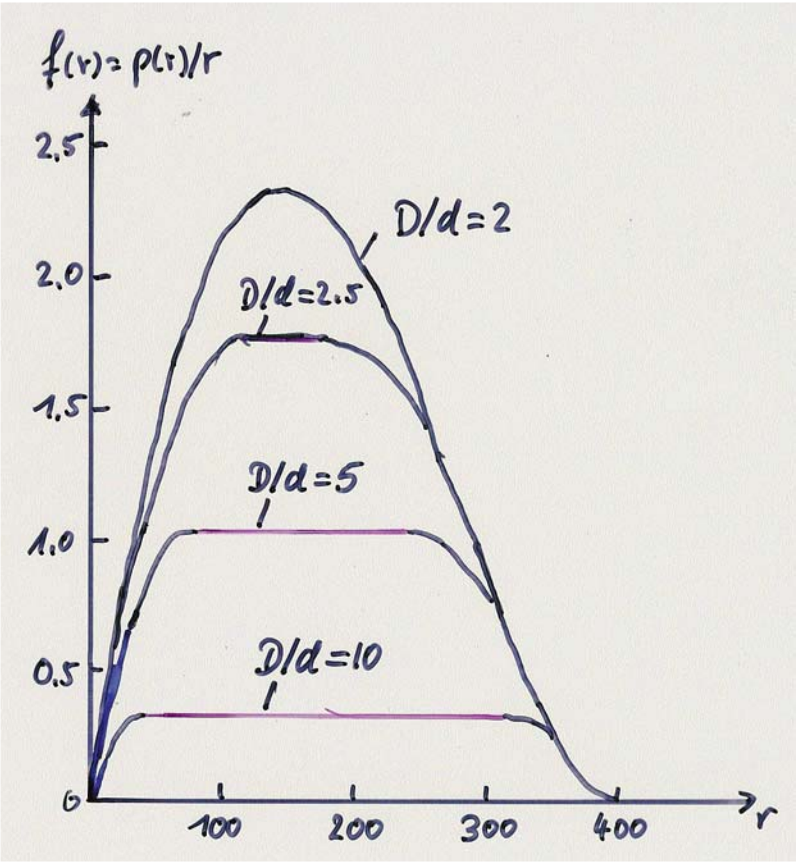
Renormalized PDDF

$$f(r) = p(r)/r$$

exposes the linear region of p(r)



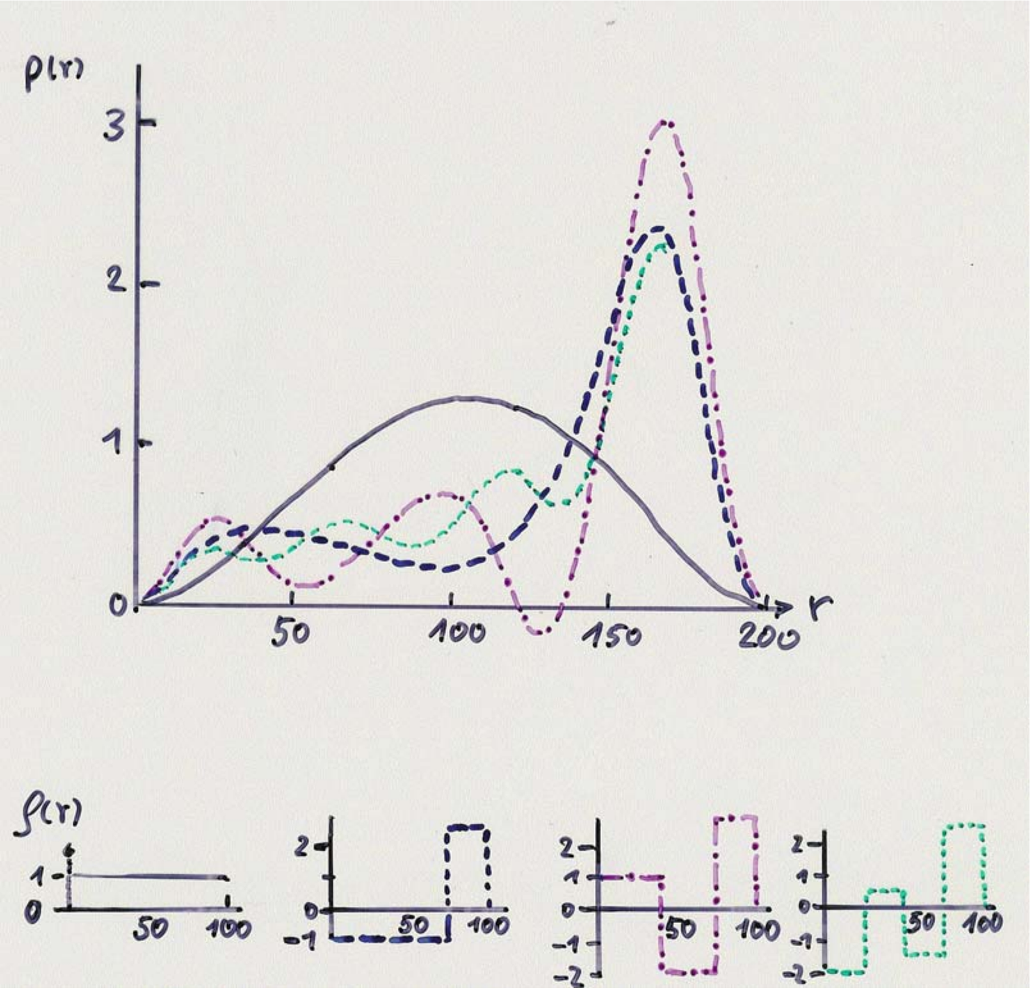

| | | |
|---|---|---|
| $p(r) \sim r^2$ | | for $r \le d = R_a - R_i$ |
| $\sim r$ | | for $d < r \le D_a - 2d = 2R_i$ |
| $\sim$ | full sphere | for $r \ge D_a\text{-}d$ |



# Hollow and Inhomogeneous Particles: Inhomogeneous Spheres

Multilayer Spheres:

Occurrence of minima signals signals existence of layers of alternating sign of difference scattering density $(\Delta\rho_s(r))^2$

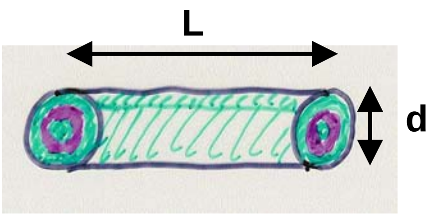



full sphere

multi layer spheres

# Inhomogeneous Rods – long circular cylinders

i) density profile along cross section



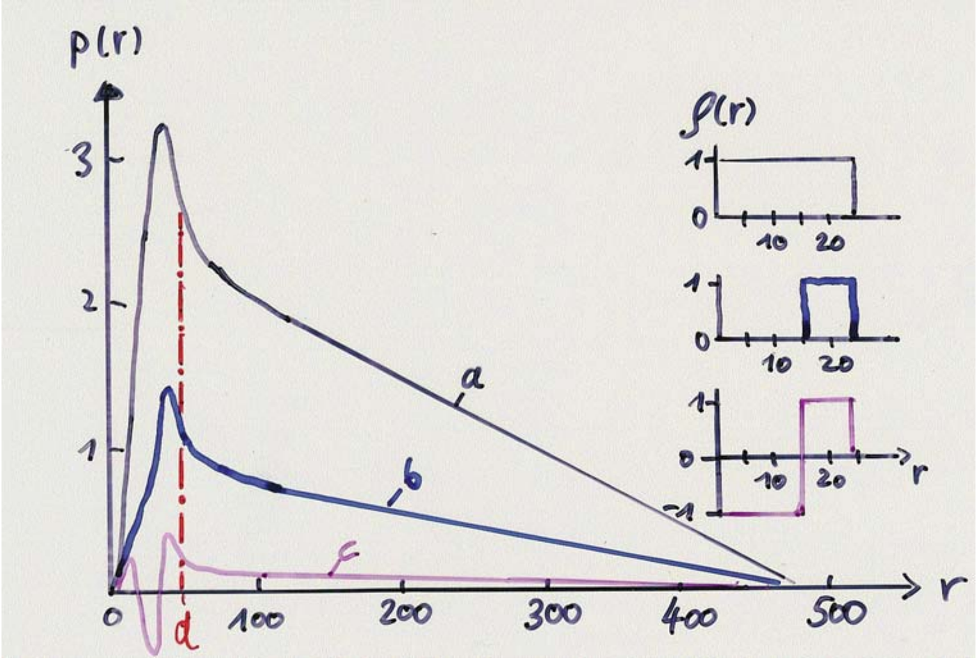

- inhom. cylinder: negative regions in p(r) $\rightarrow$ distances connecting regions with positive and negative contrast (core-shell) dominate

- linearly decreasing region is retained – only slope is changing

$$p(r) = (1/2\pi)\ (\Delta\rho_s(r))^2\ A^2\ (L\text{-}r)$$

- $\Delta\rho_s(r) = 0 \rightarrow$ linear region coincides with abszissa; oscillations corresponding to internal density fluctuations remain

- differences in p(r) most clearly for r < d



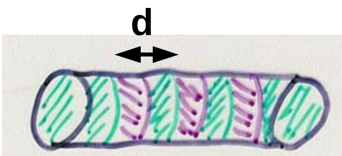

a) homogeneous cylinder

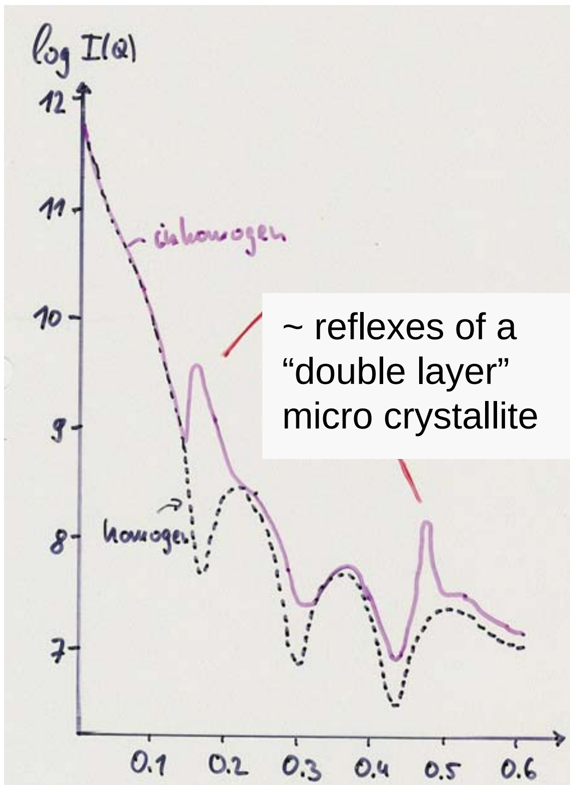
b) hollow cylinder

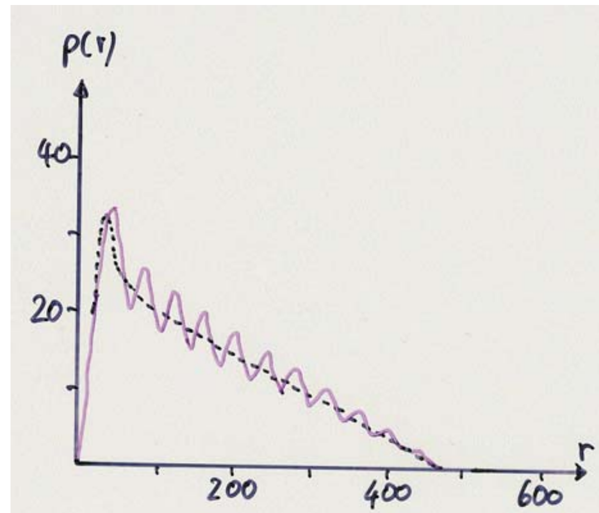
c) inhomogeneous cylinder

# Inhomogeneous Rods – long circular cylinders

ii) density profile along cylinder axis



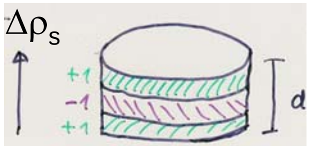

- oscillations in p(r) with period d of the “double layer” (2x20 = 40)
- cylinder = micro crystallite; double layer = unit cell
  $\rightarrow$ reflexes in I(q): position $\leftrightarrow$ distance of unit cells ($q = 2\pi/40 \approx 0.16$)
  width $\leftrightarrow$ number of unit cells

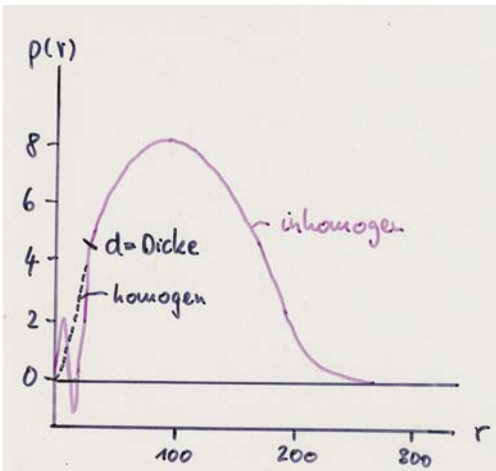
- Guinier region of I(q) identical $\leftrightarrow$ identical outer shape

# Inhomogeneous platelets

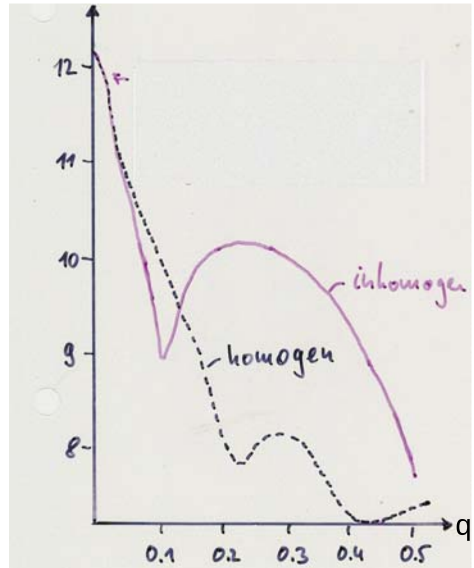
(i) Density profile perpendicular to base plane

$\Delta\rho_s$




log I(q)

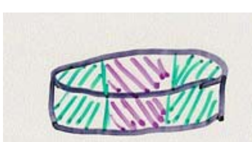



q

comparison of a homogeneous (---) and an inhomogeneous (—) lamella with dimensions 200x200x30 Å; $\Delta\rho_{inhomog}$ is a three-step function (3x10 Å) with $\Delta\rho$ = +1, -1, +1

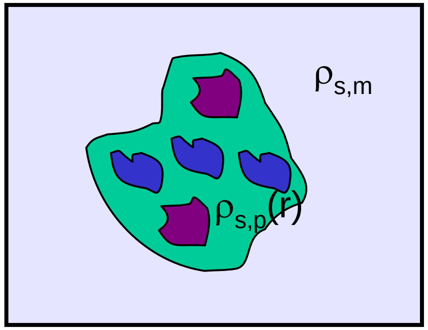
Differences only visible for r < d

(ii) Density profile parallel to base plane



p(r) of this chess board like structure shows oscillations for all r

## Study of particle inhomogeneities via contrast variation




Contrast: $$\Delta\rho_s(r,\rho_{s,m}) = \rho_{s,p}(r) - \rho_{s,m}$$

Average contrast: $$\langle \Delta\rho_s \rangle = \frac{1}{V_p}\int \Delta\rho_s(r,\rho_{s,m})\,dV_p$$

Decomposition of particle contrast in its average and fluctuations around this average:

$$\Delta\rho_s(r,\rho_{s,m}) = \langle \Delta\rho_s \rangle + \delta(\Delta\rho_s(r))$$

$\Rightarrow$ Scattering intensity contains three contributions:

$$I(q) = I_\delta(q) + \langle \Delta\rho_s \rangle I_{c\delta}(q) + \langle \Delta\rho_s \rangle^2 I_c(q)$$

Fluctuation contribution from internal inhomogeneities

Cross term

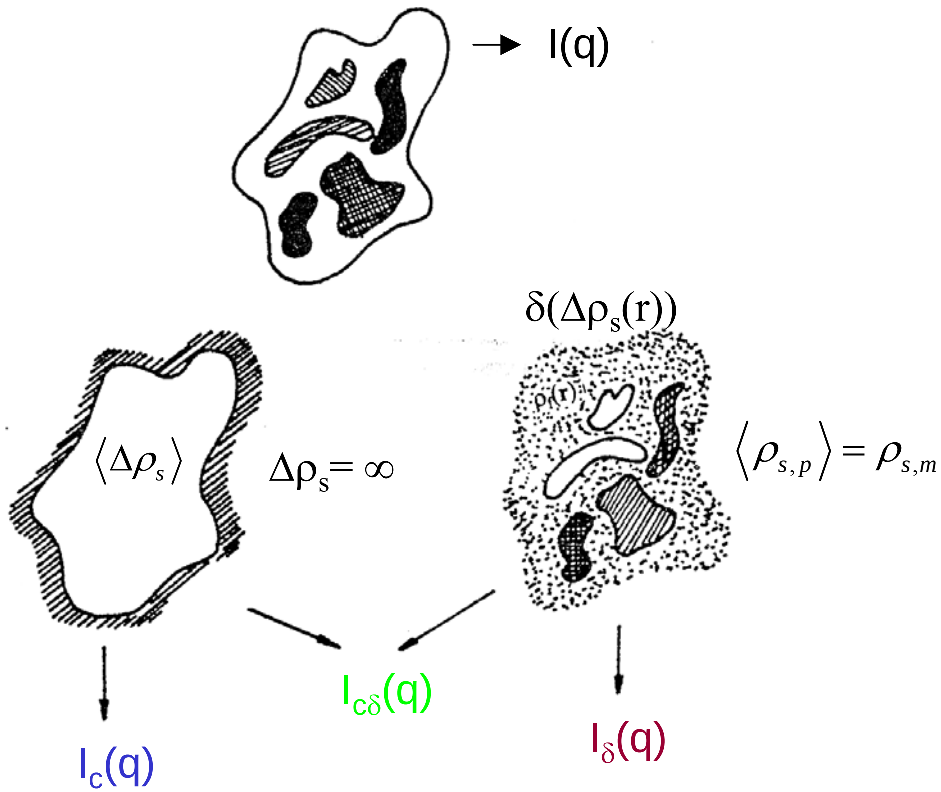
Average contrast contribution from particle shape (“envelope”)

Similar contributions $\gamma(r)$ and p(r):

$$p(r) = p_{\delta}(r) + \langle \Delta\rho_s \rangle p_{c\delta}(r) + \langle \Delta\rho_s \rangle^2 p_c(r)$$

Separation of contributions:

Measurements at n≥3 contrasts
and solution of the set of n linear
equations for each q-value (r-value)



Contrast variation of $R_g$:

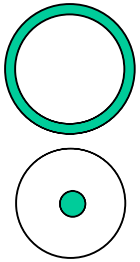
$$R_g^2 = R_c^2 - \frac{\alpha}{\langle \Delta\rho_s \rangle} - \frac{\beta}{\langle \Delta\rho_s \rangle^2}$$

$$\alpha = V^{-1} \int \delta(\Delta\rho_s(\vec{r}))\, r^2 d\vec{r}$$

$$\beta = V^{-2} \iint \delta(\Delta\rho_s(\vec{r}_1))\, \delta(\Delta\rho_s(\vec{r}_2))\, \vec{r}_1\, \vec{r}_2\, d\vec{r}_1\, d\vec{r}_2$$

$R_c = R_g$ of particle shape; $R_g = R_c$ for homogeneous particles
$\Rightarrow R_g \neq f(\langle \Delta\rho_s \rangle) \rightarrow$ homogeneous particle

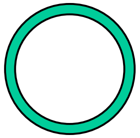
$\alpha$: describes arrangement of regions of higher and lower scattering density with respect to "center of mass" of envelope



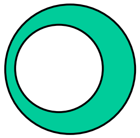
$\alpha > 0$

$\alpha < 0$

$\beta$: measure of separation of "center of mass" of envelope and of inhomogeneities



$\beta = 0$



$\beta \neq 0$

# Examples:

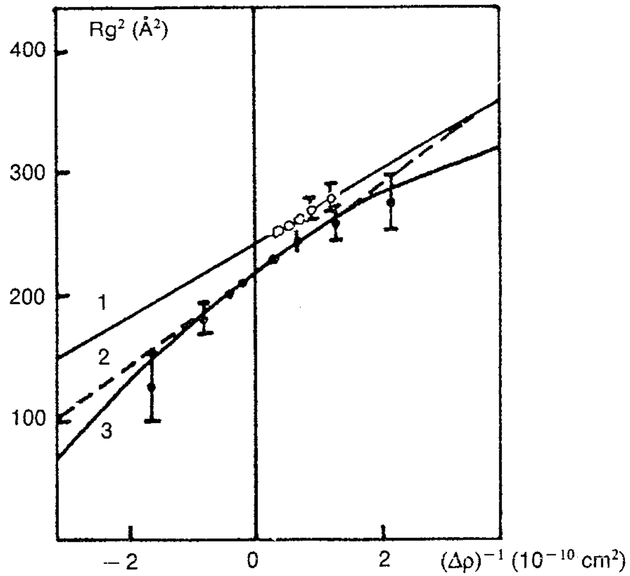



***Figure 4.10.*** Radius of gyration of myoglobin as a function of contrast (after Ibel and Stuhrmann, 1975). Open circles denote X-ray data and shaded circles, neutron data. (1), (2) straight lines with slope $\alpha$ calculated near $(\Delta\rho)^{-1} = 0$; (3) calculated from the myoglobin model (neutrons).

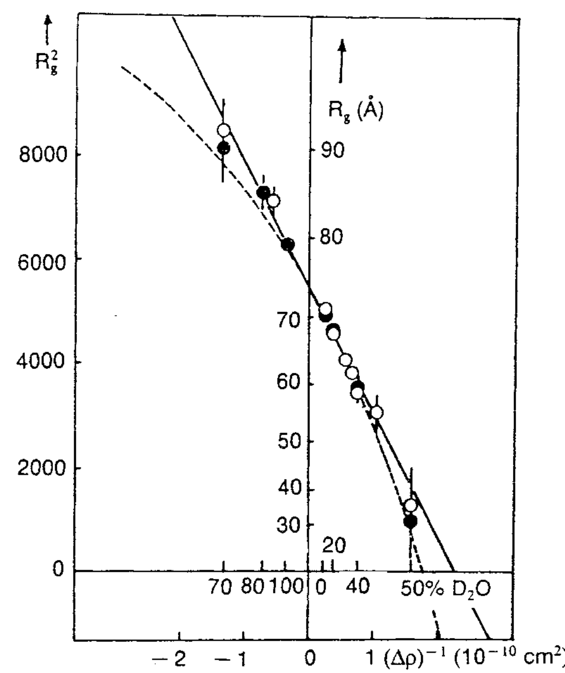



***Figure 4.12.*** Radius of gyration as a function of contrast for the 50 S ribosomal sub-particle (after Stuhrmann *et al.*, 1976a). Open and shaded circles correspond to measurements in different solvents.

Contrast variation of I(0): $I(0) = \langle \Delta\rho_s \rangle^2 I_c(0) = \langle \Delta\rho_s \rangle^2 V_p^2$

$\sqrt{I(0)}$ vs $\langle \Delta\rho_s \rangle$ $\Rightarrow$ Straight line with slope $V_p$

I(0) = 0 for $\langle \rho_{s,p} \rangle = \rho_{s,m}$
(contrast match condition)

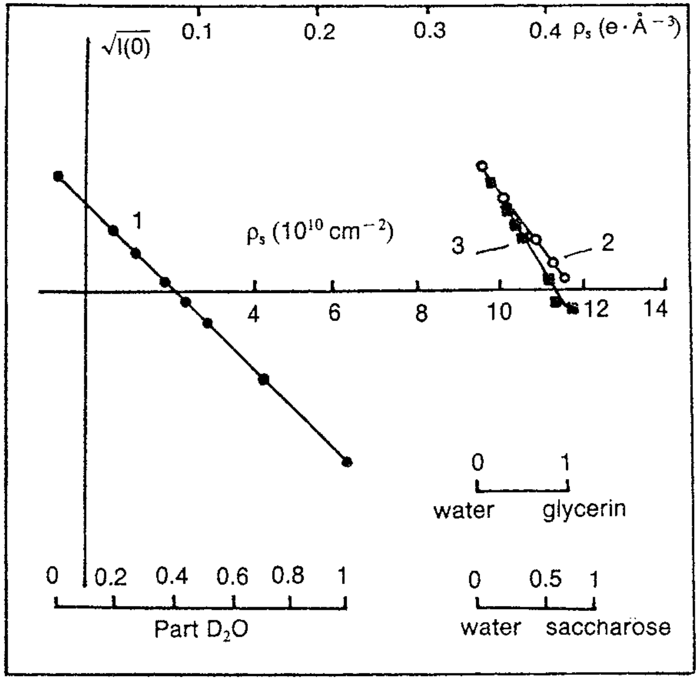



***Figure 4.9.*** Zero-angle scattering of myoglobin solutions (after Ibel and Stuhrmann, 1975): (1) neutron scattering; (2) X-ray scattering (water/glycerol mixtures); (3) X-ray scattering (sugar solutions).

# Indirect Fourier Transformation Method

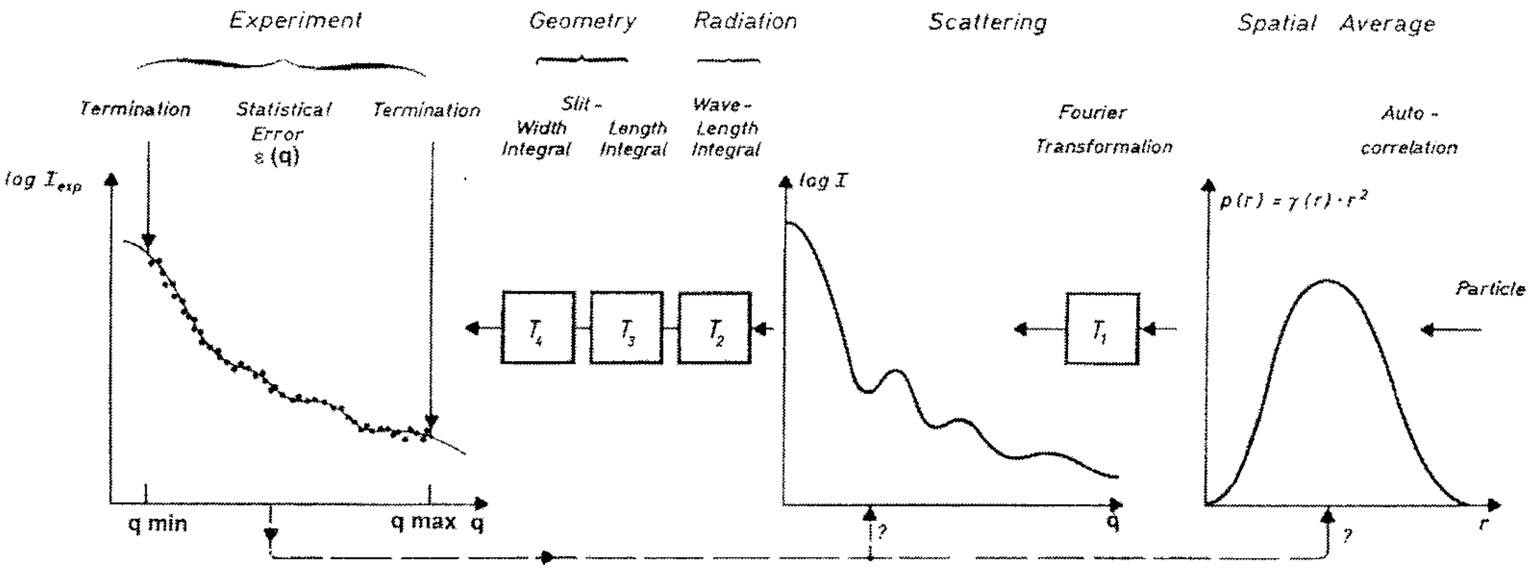



Fig. 1. Schematic representation of the correlation between a particle and its observable experimental scattering data.