Model structures

(Read Roe, Chap. 5)

Remember:

ρ *(r) --> I (q) possible*

I (q) --> ρ *(r)* not possible

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*I (**q**) -->* Γ_ρ *(**r**) only*

Thus, use a reasonable model to fit *I (**q**)* or Γ_ρ *(**r**)*

Model structures

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ρ *(**r**) --> I (**q**) possible*

*I (**q**) --> ρ (**r**)* not possible

*I (**q**) --> Γ_ρ (**r**) only*

Thus, use a reasonable model to fit *I (**q**)* or Γ_ρ *(**r**)*:

dilute particulate system

non-particulate 2-phase system

soluble blend system

periodic system

Model structures

Use reasonable model to fit $I\ (q)$ or $\Gamma_\rho\ (r)$:

Dilute particulate system

polymers, colloids

dilute - particulates not correlated

if particulate shape known, can calc $I\ (q)$

if particulate shape not known, can calc
radius of gyration

Model structures

Use reasonable model to fit *I (q)* or Γ_ρ *(r)*:

Non-particulate 2- phase system

2 matls irregularly mixed - no host or matrix - crystalline & amorphous polymer phases

also, particulate system w/ no dilute species

get state of dispersion, domain size, info on interphase boundary

Model structures

Use reasonable model to fit *I (q)* or Γ_ρ *(r)*:

soluble blend system

single phase, homogeneous but disordered

two mutually soluble polymers, solvent + solute

get solution properties

Model structures

Use reasonable model to fit $I\ (q)$ or $\Gamma_\rho\ (r)$:

periodic system

crystalline matls, semi-crystalline polymers, block copolymers, biomaterials

crystallinity poor

use same techniques as in high angle diffraction, except structural imperfection prominent

Model structures

Dilute particulate system

1. Homogeneous sphere
2. Spherical shell
3. Spherical concentric shells
4. Particles consisting of spherical subunits
5. Ellipsoid of revolution
6. Tri-axial ellipsoid
7. Cube and rectangular parallelepipedons
8. Truncated octahedra
9. Faceted Sphere

9x Lens

10. Cube with terraces
11. Cylinder:
12. Cylinder with elliptical cross section
13. Cylinder with hemi-spherical end-caps

13x Cylinder with 'half lense' end caps

14. Toroid
15. Infinitely thin rod
16. Infinitely thin circular disk
17. Fractal aggregates

Model structures

Dilute particulate system

18. Flexible polymers with Gaussian statistics
19. Polydisperse flexible polymers with Gaussian statistics
20. Flexible ring polymers with Gaussian statistics
21. Flexible self-avoiding polymers
22. Polydisperse flexible self-avoiding polymers
23. Semi-flexible polymers without self-avoidance
24. Semi-flexible polymers with self-avoidance
25. Star polymer with Gaussian statistics
26. Polydisperse star polymer with Gaussian statistics
27. Regular star-burst polymer (dendrimer) with Gaussian statistics
28. Polycondensates of A_f monomers
29. Polycondensates of AB_f monomers
30. Polycondensates of ABC monomers
31. Regular comb polymer with Gaussian statistics
32. Arbitrarily branched polymers with Gaussian statistics
33. Arbitrarily branched semi-flexible polymers
34. Arbitrarily branched self-avoiding polymers
35. Sphere with Gaussian chains attached
36. Ellipsoid with Gaussian chains attached
37. Cylinder with Gaussian chains attached
38. Polydisperse thin cylinder with polydisperse Gaussian chains attached to the ends
39. Sphere with corona of semi-flexible interacting self-avoiding chains of a corona chain

Model structures

Dilute particulate system

40. <u>Very anisotropic particles with local planar geometry</u>:

Cross section:

(a) Homogeneous cross section
(b) Two infinitely thin planes separated by
(c) A layered centro symmetric cross-section
(d) Gaussian chains attached to the surface

Overall shape:

(a) Infinitely thin spherical shell
(b) Elliptical shell
(c) Cylindrical shell
(d) Infinitely thin disk

41. <u>Very anisotropic particles with local cylindrical geometry:</u>

Cross section:

(a) Homogeneous circular cross-section
(b) Concentric circular shells
(c) Elliptical Homogeneous cross section.
(d) Elliptical concentric shells
(e) Gaussian chains attached to the surface and

Overall shape:

(a) Infintely thin rod
(b) Semi-flexible polymer chain with or without excluded volume

Model structures

Dilute particulate system

dilute - particulates not correlated

matrix presents only uniform bkgrd

$I_{total} = \Sigma I_{individual\ particle}$

isotropic

Radius of gyration, R_g:

$$R_g^2 = \int \mathbf{r}^2 \rho(\mathbf{r})\, d\mathbf{r} / \int \rho(\mathbf{r})\, d\mathbf{r}$$

$\rho(\mathbf{r})$ = scattering length density distribution in particle

Model structures

Dilute particulate system

Radius of gyration, R_g:

$$R_g^2 = \int r^2 \rho(\mathbf{r})\, d\mathbf{r} / \int \rho(\mathbf{r})\, d\mathbf{r}$$

$\rho(\mathbf{r})$ = scattering length density distribution in particle

If scattering length density is constant thru-out particle:

$$R_g^2 = (1/v) \int r^2 \sigma(\mathbf{r})\, d\mathbf{r}$$

$\sigma(\mathbf{r})$ = shape fcn of particle; v = particle volume

Model structures

Dilute particulate system

Simple shapes

For a single particle

$$A(\mathbf{q}) = \int_V \rho(\mathbf{r}) \exp(-i\mathbf{q}\mathbf{r})\, d\mathbf{r}$$

$$I(\mathbf{q}) = A^2(\mathbf{q})$$

Average over all orientations of the particle

Model structures

Dilute particulate system

For a single particle

$$A(\mathbf{q}) = \int_V \rho(\mathbf{r}) \exp(-i\mathbf{qr})\, d\mathbf{r}$$

$$I(\mathbf{q}) = A^2(\mathbf{q})$$

Sphere:

$\rho(r) = \rho$ for $r \leq R$ & 0 elsewhere

Then

$$A(q) = \int_o^\infty \rho(\mathbf{r})\, 4\pi r^2 \,(\sin(qr))/qr\, dr$$

$$A(q) = \rho/q \int_o^R \rho(\mathbf{r})\, 4\pi r \sin(qr)\, dr$$

$$A(q) = (3\rho v/(qR)^3)(\sin(qR) - qR\cos(qR))$$

Model structures

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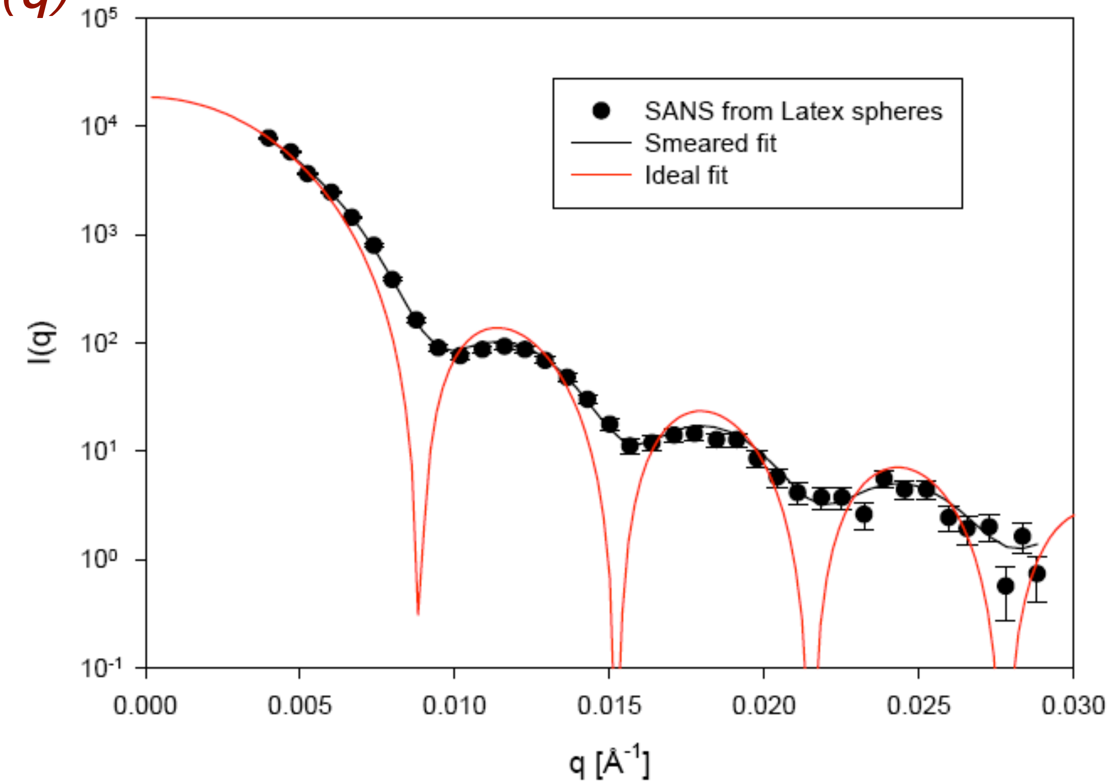
Sphere:



Model structures

Dilute particulate system

Thin rod, length L, ∠ betwn $\boldsymbol{q}$ & rod axis = ϑ

$$I(\boldsymbol{q}) = (\rho v)^2 (2/qL \cos\vartheta)^2 \sin^2((qL/2)\cos\vartheta)$$

Model structures

Dilute particulate system

Thin rod, length L, ∠ betwn $\boldsymbol{q}$ & rod axis = ϑ

$$I(\boldsymbol{q}) = (\rho v)^2 (2/qL \cos\vartheta)^2 \sin^2((qL/2)\cos\vartheta)$$

Averaging over all orientations

$$I(\boldsymbol{q}) = (\rho v)^2\, 2/qL \left(\int_o^{qL} (\sin u)/u \, du - (1 - \cos qL)/\, qL \right)$$

Model structures

Dilute particulate system

Thin disk, radius R

1st order Bessel fcn

$$I(\mathbf{q}) = (\rho v)^2\ 2/(qR)^2\ (1 - (J_1(2qR))/qR)$$

Model structures

Dilute particulate system

Polymer chain w/ N + 1 independent scattering "beads"

Gaussian - w/ one end of polymer chain at origin,
probability of other end at $d\mathbf{r}$ obeys Gaussian distribution

bead volume is v_u ; chain volume is $v = (N + 1)\, v_u$

Model structures

Dilute particulate system

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scattering length of each bead is ρv_u

$$A(\boldsymbol{q}) = \rho v_u \sum_{j=0}^{N+1} exp\ (-i\boldsymbol{q}\boldsymbol{r}_j)$$

Model structures

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$$A(\mathbf{q}) = \rho v_u \sum_{j=0}^{N+1} exp\,(-i\mathbf{q}\mathbf{r}_j)$$

$$I(\mathbf{q}) = (\rho v_u)^2 \int P(\mathbf{r})\, exp\,(-i\mathbf{q}\mathbf{r}) d\mathbf{r}$$

$P(\mathbf{r})$ is # bead pairs $\mathbf{r}$ apart

Model structures

Dilute particulate system

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Averaging over all such chains:

$$I(\mathbf{q}) = (\rho v_u)^2 \int P(r)\, exp\,(-i\mathbf{q}r)dr$$