Neutron scattering presentation series

(3) Data analysis and modeling

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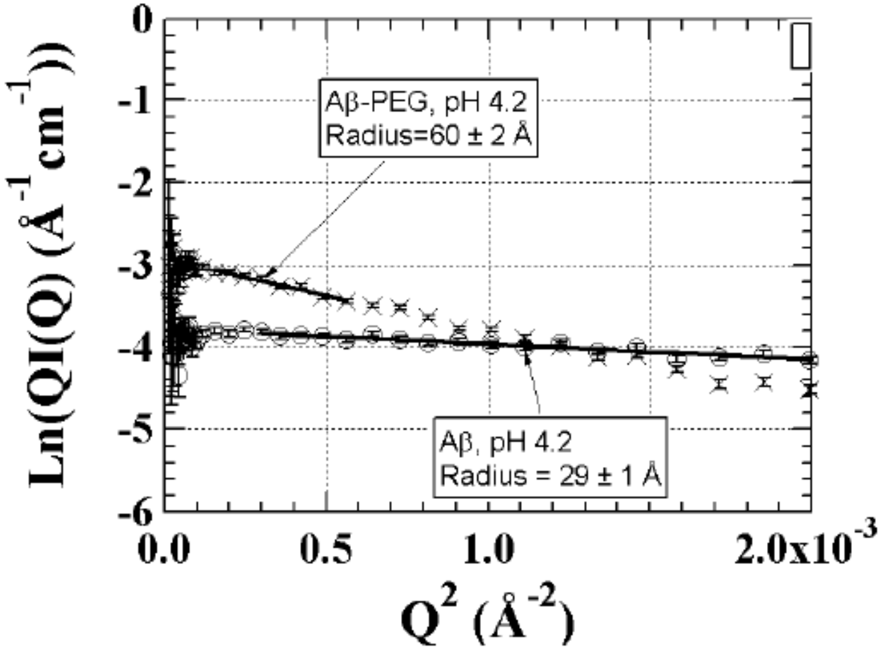
June 1st, 2015

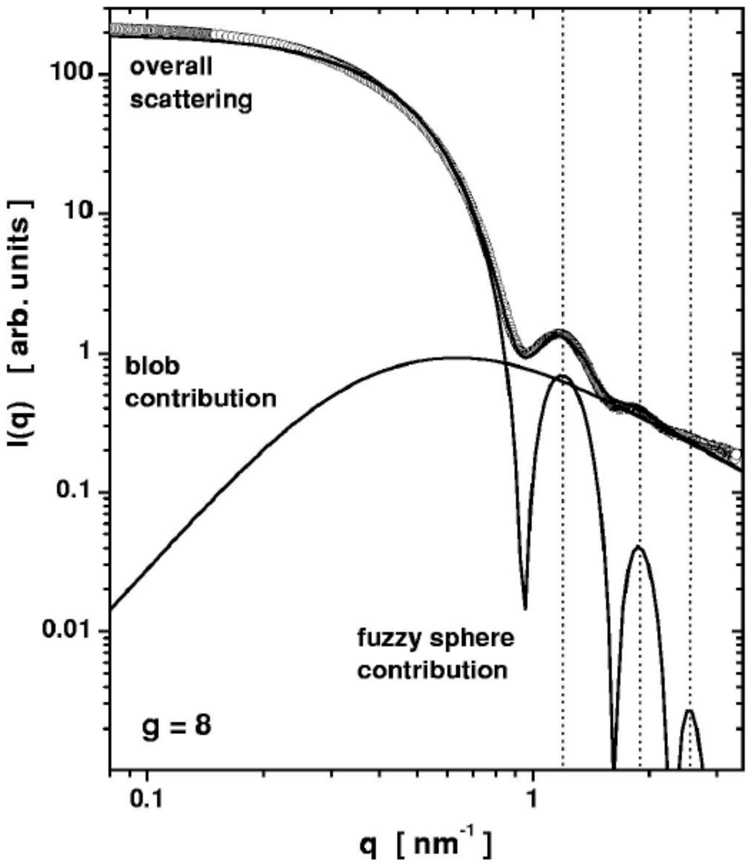
Types of Data Analysis

Standard plots



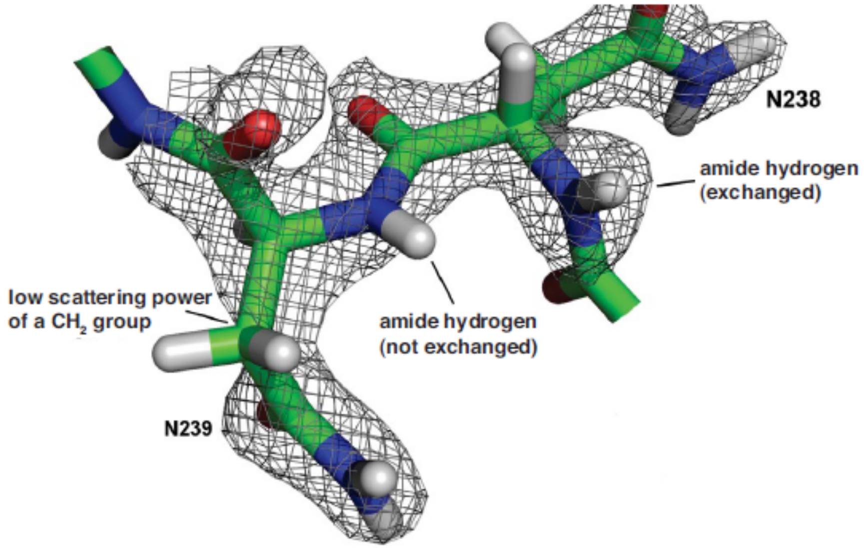
Thiyagarajan et al. JAC 2000

Model fitting



Rathegeber et al. JCP 2000

Refinement and reconstruction



Blum et al. PNAS 2009

Standard Plots

Advantage:

- Convenient
- Model free
- Usable for complicated systems

Disadvantage:

- Qualitative
- Limited Q range
- Single length scale
- No interaction

Model Fitting - Outline

1. P(Q) and S(Q)
2. Polydisperse system
3. Non-spherical system
4. Scattering contrast
5. Derive new scattering functions

Systems: polymers, colloids, microemulsions, superalloys…

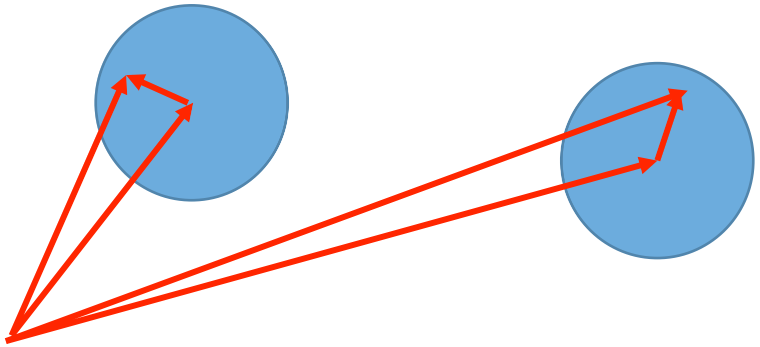
P(Q) and S(Q)

$$I(Q)=nP(Q)S(Q)$$

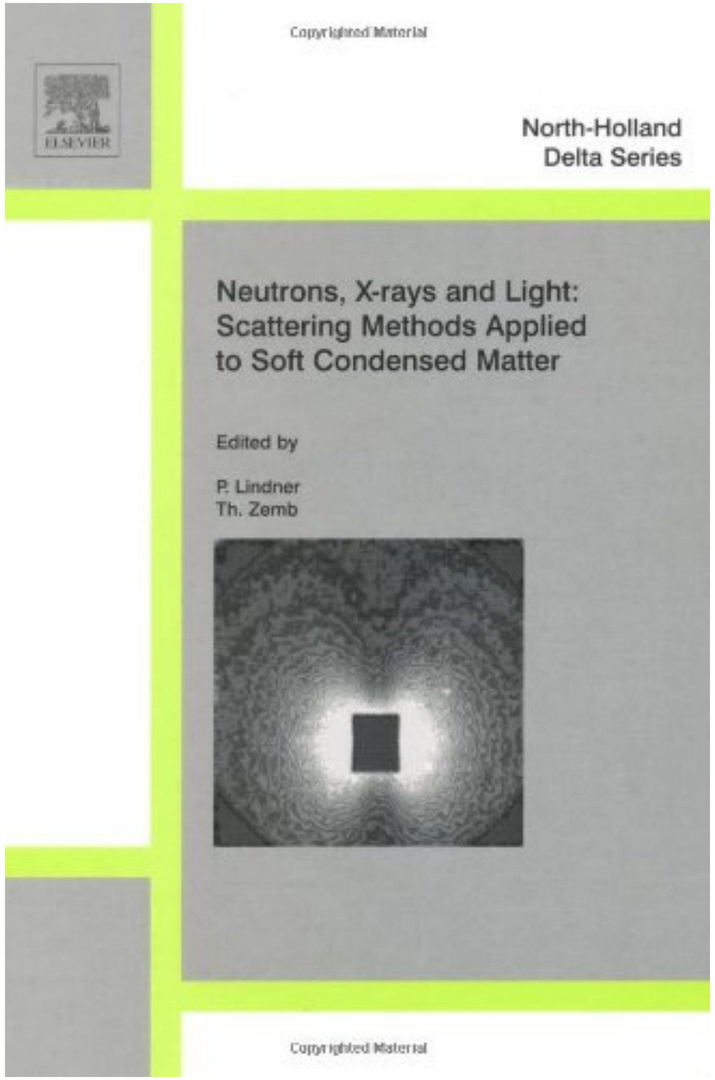
n: number density

P(*Q*): form factor – single molecule structural information

S(*Q*): structure factor – intermolecular relative position

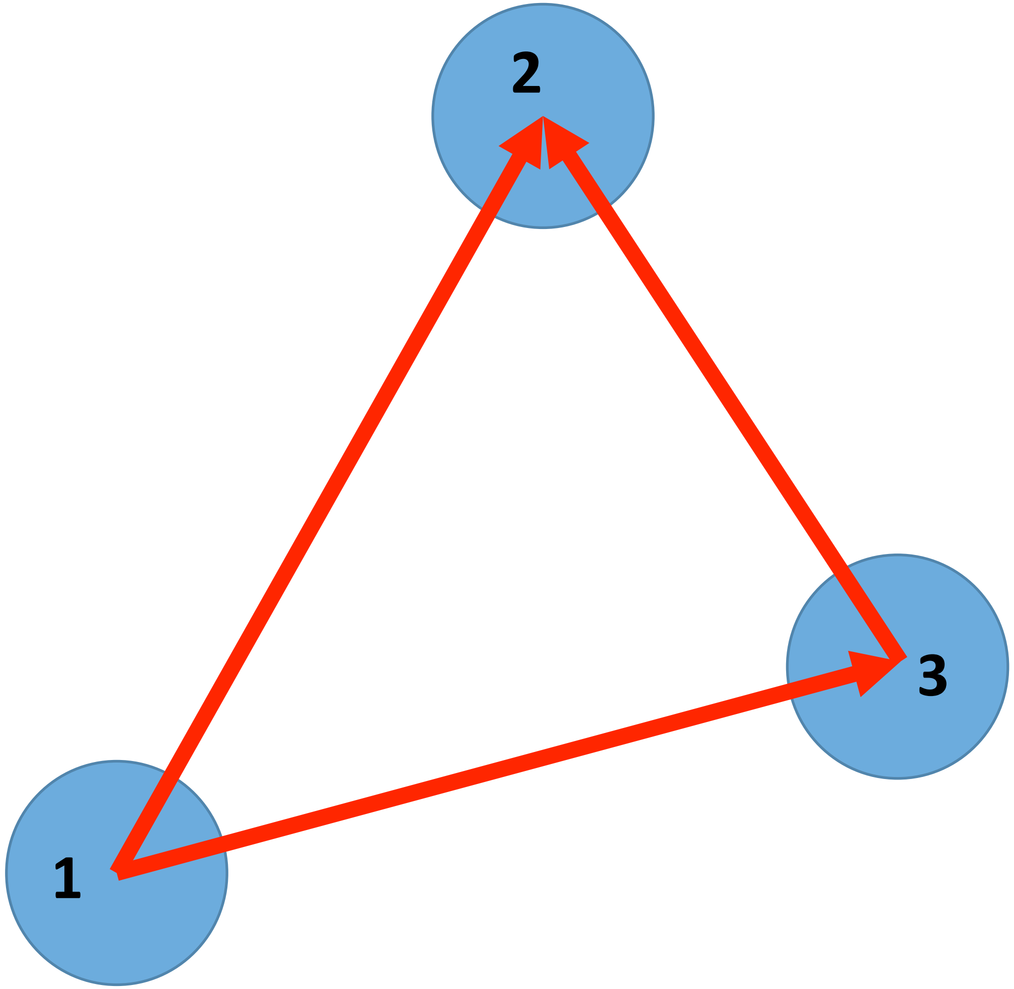


Only valid for **monodisperse spherical** particles in solution.



Chapter 16, J. Pedersen

Solving S(Q)



$$h_{12} = c_{12} + c_{13} * h_{23}$$

Ornstein-Zernike (OZ) Equation

$$h(r) = c(r) + h(r) * c(r)$$

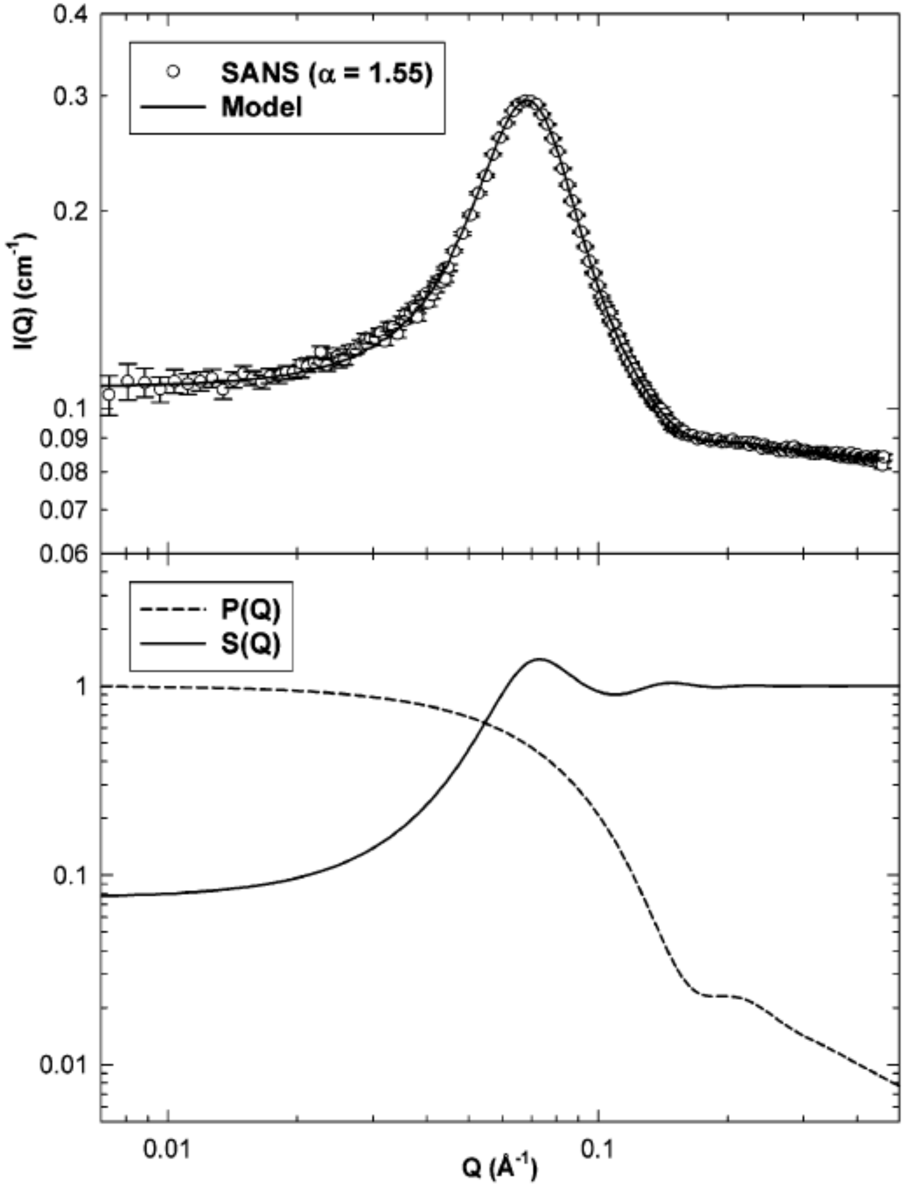
h(*r*): total correlation function
c(*r*): direct correlation function

Closure equation

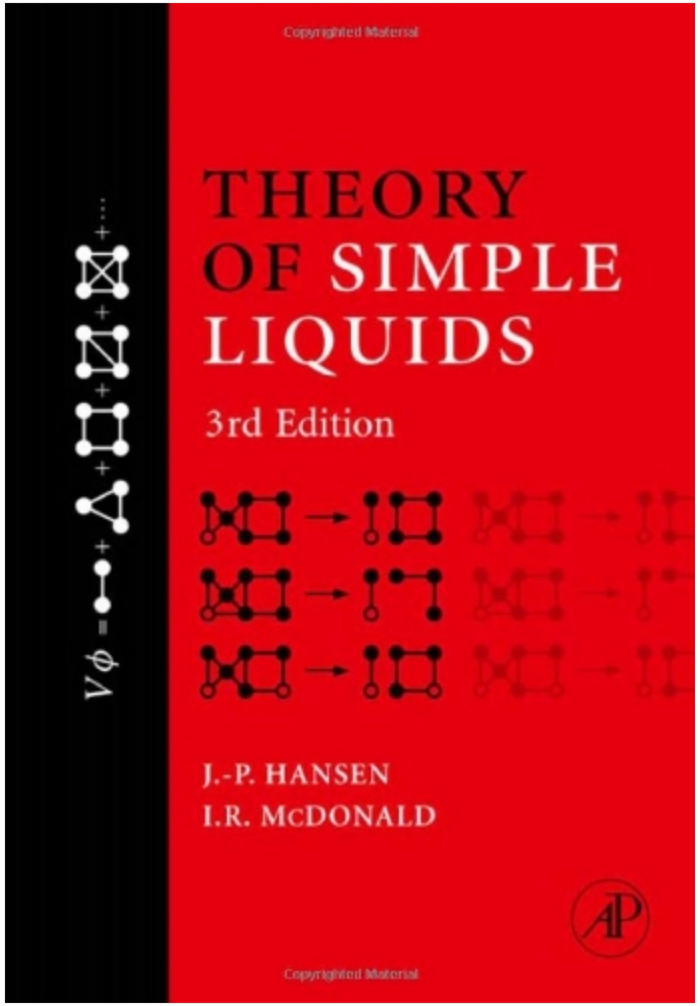
$$F[h(r), c(r), V(r), n] = 0$$

Percus-Yevick, MSA, RMSA, HNC, Rogers-Young, Zerah-Hansen…

Solving S(Q) (cont'd)



Chen et al. Macromolecules, 2007



Chapter 3, 4, 5

Example 1 – Charge Stabilized Protein

THE JOURNAL OF CHEMICAL PHYSICS 123, 054708 (2005)

Diffusion and microstructural properties of solutions of charged nanosized proteins: Experiment versus theory

J. Gapinski,[a)] A. Wilk, and A. Patkowski
Institute of Physics, A. Mickiewicz University, 61-614 Poznan, Poland

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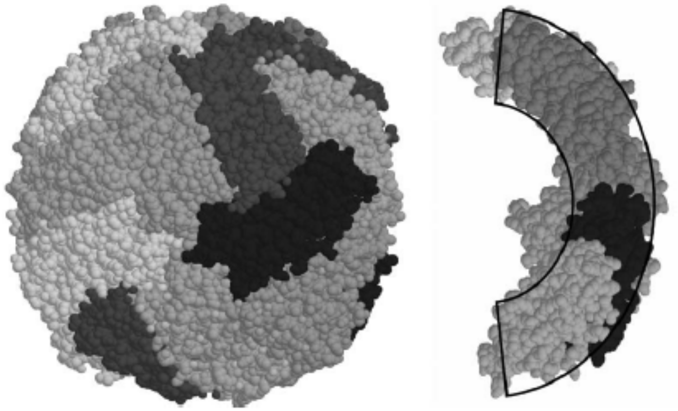
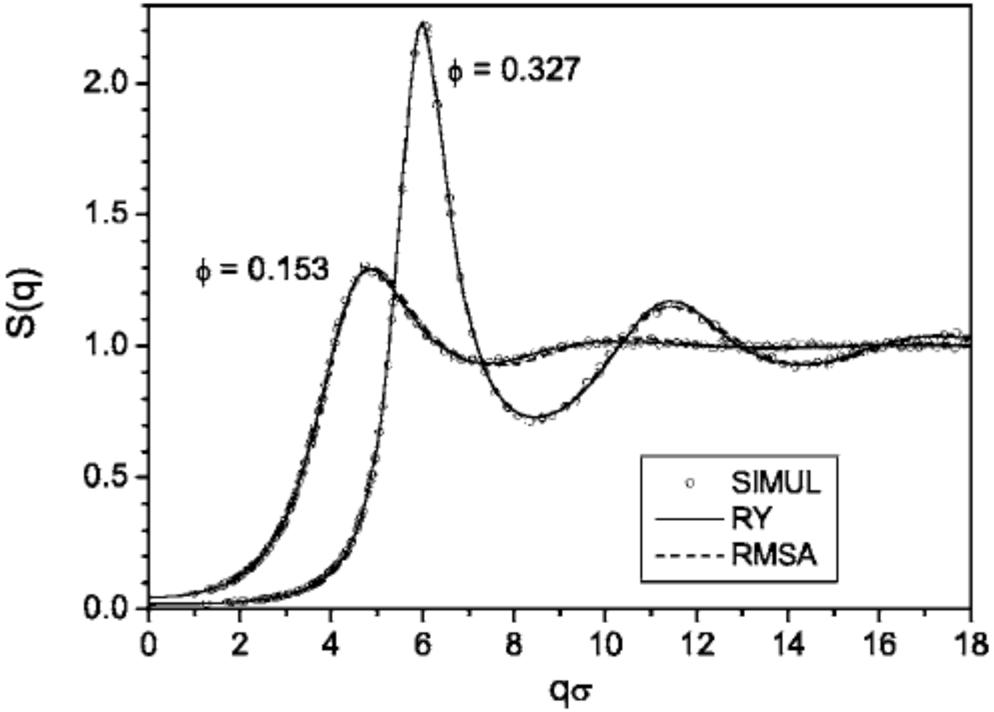
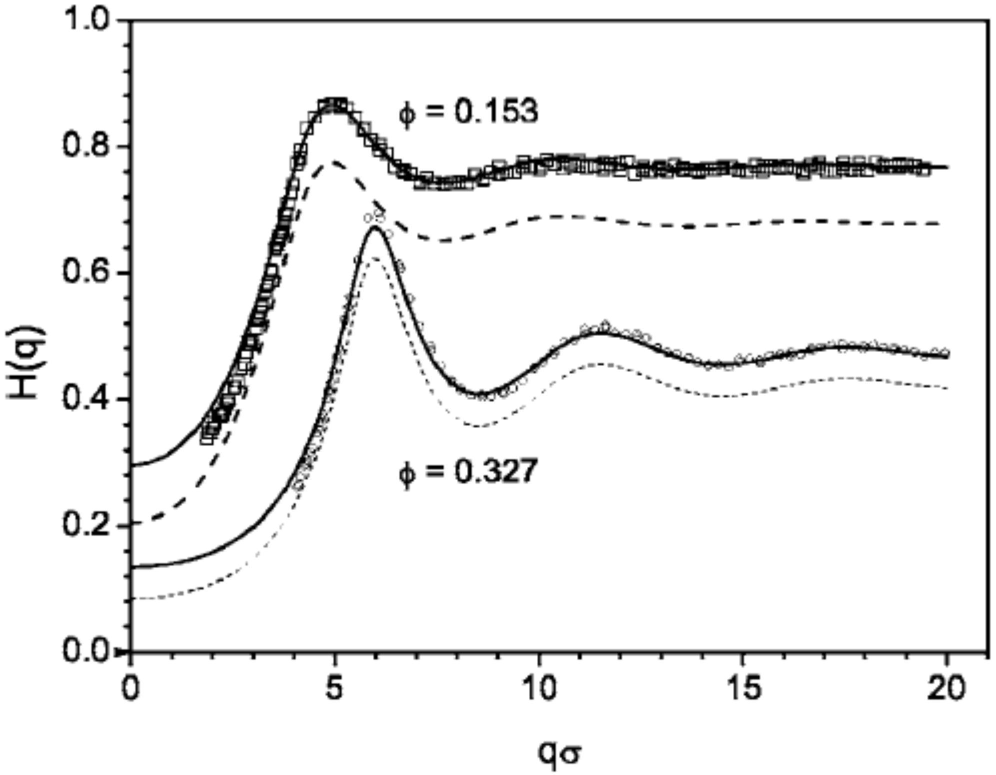
Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

(Received 15 December 2004; accepted 15 June 2005; published online 11 August 2005)



Apoferritin





$$D(Q)=D_0\, H(Q)/S(Q)$$

Example 2 – Core Shell Structure

Macromolecules **2000,** *33,* 542–550

Contrast Variation Small-Angle Neutron Scattering Study of the Structure of Block Copolymer Micelles in a Slightly Selective Solvent at Semidilute Concentrations

Jan Skov Pedersen*

Condensed Matter Physics and Chemistry Department, Risø National Laboratory, Roskilde, DK-4000, Denmark

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Chang Yeol Ryu and Timothy P. Lodge

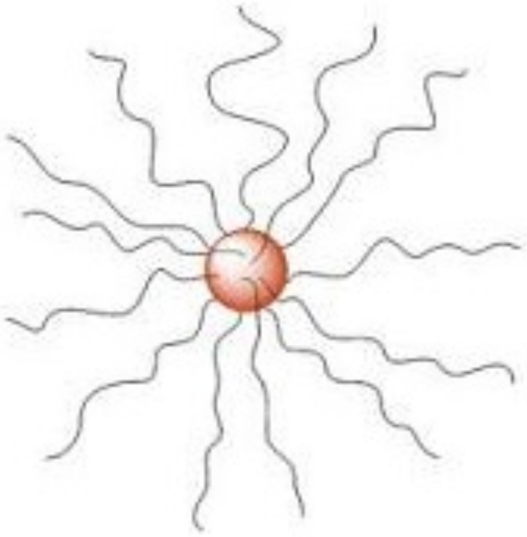
Department of Chemistry and Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, Minnesota 55455

Received May 12, 1999; Revised Manuscript Received October 20, 1999

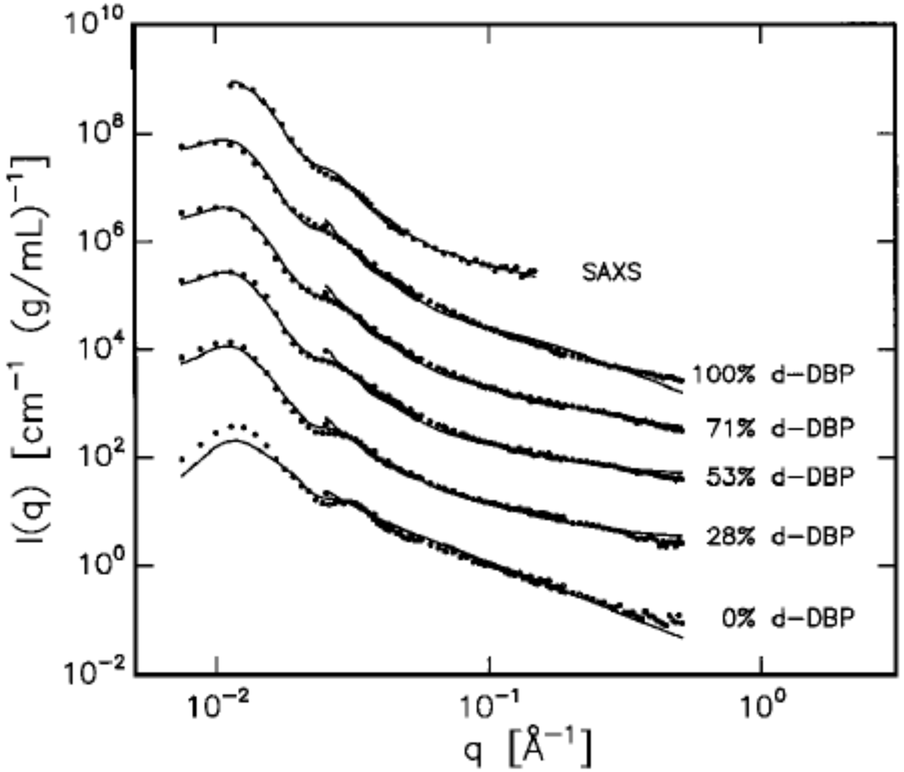
$$F_{\rm mic}(q) = N\beta_{\rm core}{}^2 F_{\rm core}(q) + N\beta_{\rm chain}{}^2 F_{\rm chain}(q) + 2N\beta_{\rm core}\beta_{\rm chain} S_{\rm core-chain}(q) + N(N-1)\beta_{\rm chain}{}^2 S_{\rm chain-chain}(q) \quad (1)$$

$$F_{\rm chain}(q) = \frac{2[\exp(-x) - 1 + x]}{x^2} \quad (2)$$

where $x = q^2 R_g{}^2$.



Polystyrene-polyisoprene (PS-PI) diblock copolymer in di-n-butyl phthalate (DBP)



Example 3 – Star-like Polymer

JOURNAL OF CHEMICAL PHYSICS VOLUME 117, NUMBER 8 22 AUGUST 2002

Dynamics of star-burst dendrimers in solution in relation to their structural properties

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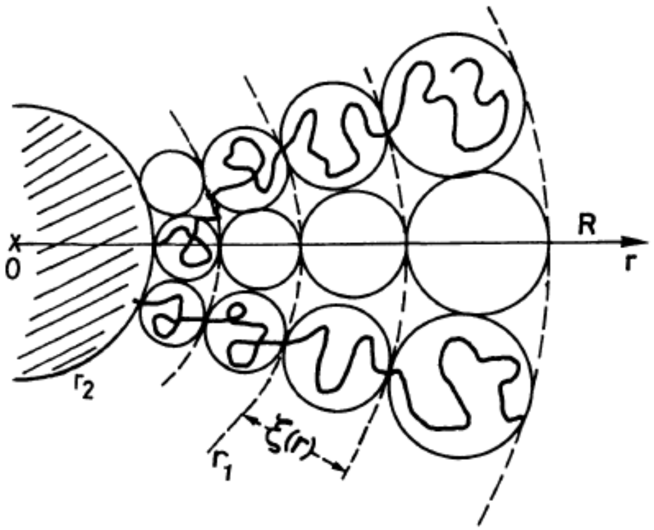
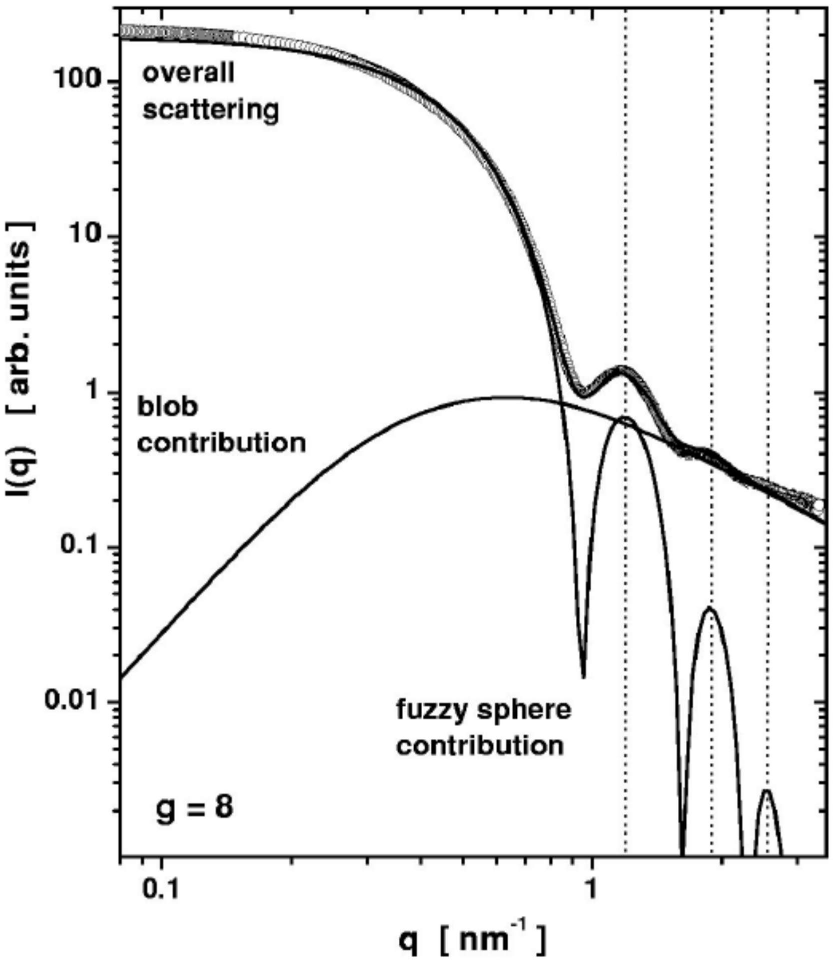
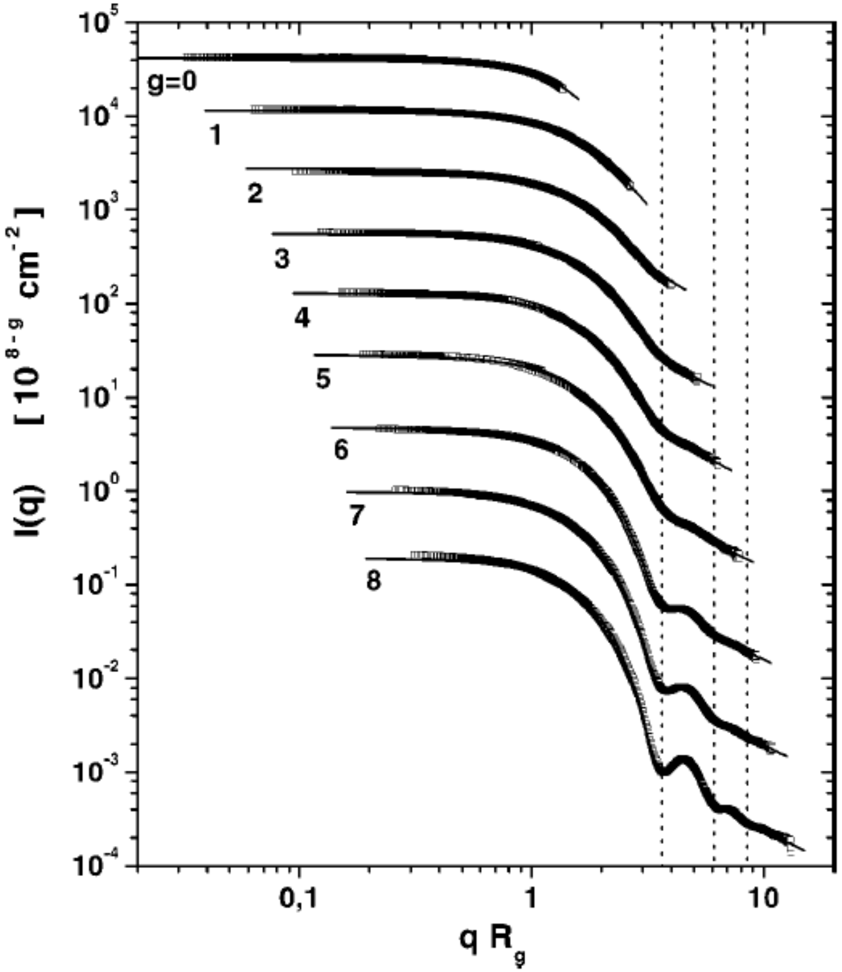
(Received 8 January 2002; accepted 22 May 2002)



(Daoud and Cotton J. Phys. 1982)





Polydisperse System

Monodisperse: $I(Q)=nP(Q)S(Q)$

Polydisperse dilute: $I(Q)=\int_0^{\infty} n(R)P(Q,R)dR$ with $\int_0^{\infty} n(R)dR=1$

Polydisperse interacting (binary mixture):

$$I(Q)=\begin{bmatrix}\sqrt{n_1}P(Q,R_1) & \sqrt{n_2}P(Q,R_2)\end{bmatrix}\begin{bmatrix}S_{11}(Q,R_1) & S_{12}(Q,R_1,R_2)\\ S_{21}(Q,R_1,R_2) & S_{22}(Q,R_1)\end{bmatrix}\Big[$$

$$=n_1P(Q,R_1)S_{11}(Q,R_1)+n_2P(Q,R_2)S_{22}(Q,R_2)+2\sqrt{n_1 n_2}P(Q,R_1)P(Q,R_2)S_{12}(Q,R_1,R_2)$$

$S_{12}(Q,R_1,R_2)=S_{12}(Q,R_1,R_2)$ is the cross correlation between species 1 and 2 as the partial structure factor.

Example 4 – Binary Mixture

PHYSICAL REVIEW E **73**, 031407 (2006)

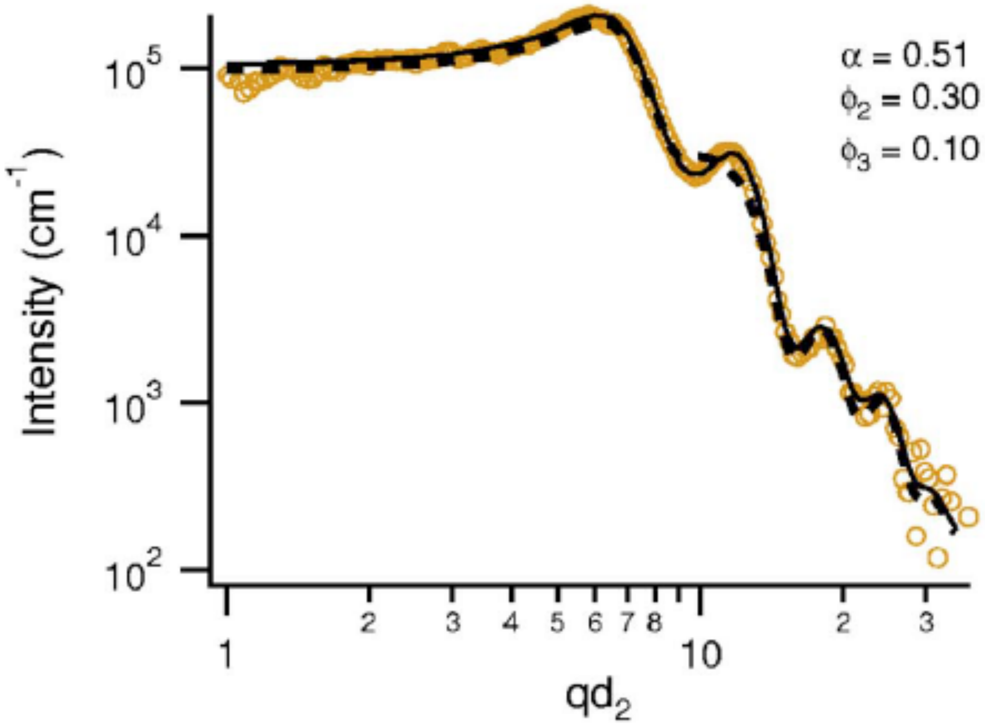
Scattering for mixtures of hard spheres: Comparison of total scattering intensities with model

B. J. Anderson,[1] V. Gopalakrishnan,[1] S. Ramakrishnan,[2] and C. F. Zukoski[1,*]
[1]*Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA*
[2]*Department of Chemical and Biomedical Engineering, Florida A&M–Florida State University, Tallahassee, Florida 32310, USA*
(Received 18 October 2005; published 23 March 2006)

$$S_{11}(q) = \frac{[1 - n_2 C_{22}(q)]}{[1 - n_1 C_{11}(q) - n_2 C_{22}(q) + n_1 n_2 C_{11}(q) C_{22}(q) - n_1 n_2 C_{12}^2(q)]},$$

$$S_{22}(q) = \frac{[1 - n_1 C_{11}(q)]}{[1 - n_1 C_{11}(q) - n_2 C_{22}(q) + n_1 n_2 C_{11}(q) C_{22}(q) - n_1 n_2 C_{12}^2(q)]},$$

$$S_{12}(q) = \frac{n_1 n_2 C_{12}(q)}{[1 - n_1 C_{11}(q) - n_2 C_{22}(q) + n_1 n_2 C_{11}(q) C_{22}(q) - n_1 n_2 C_{12}^2(q)]}.$$



Non-spherical System

$$\beta(Q)=|\langle F(Q)\rangle|^2/\langle|F(Q)|^2\rangle=|\langle F(Q)\rangle|^2/P(Q)$$

$$I(Q)=nP(Q)[1+\beta(Q)(S(Q)-1)]$$

$\beta(Q)$ can be caused by both the asphericity and polydispersity. This method can also be applied to the case of a small polydispersity ($|\beta(Q)-1|<0.1$).

Ann. Rev. Phys. Chem. 1986. 37 : 351–99

SMALL ANGLE NEUTRON SCATTERING STUDIES OF THE STRUCTURE AND INTERACTION IN MICELLAR AND MICROEMULSION SYSTEMS

S. H. Chen

Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Example 5 – Ellipsoidal Micelle

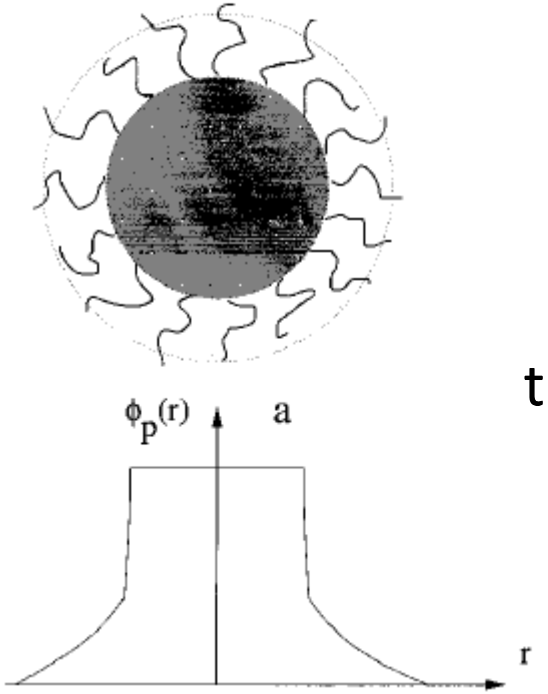
Macromolecules **1998**, *31*, 2236–2244

Small-Angle Neutron Scattering Analysis of the Structure and Interaction of Triblock Copolymer Micelles in Aqueous Solution

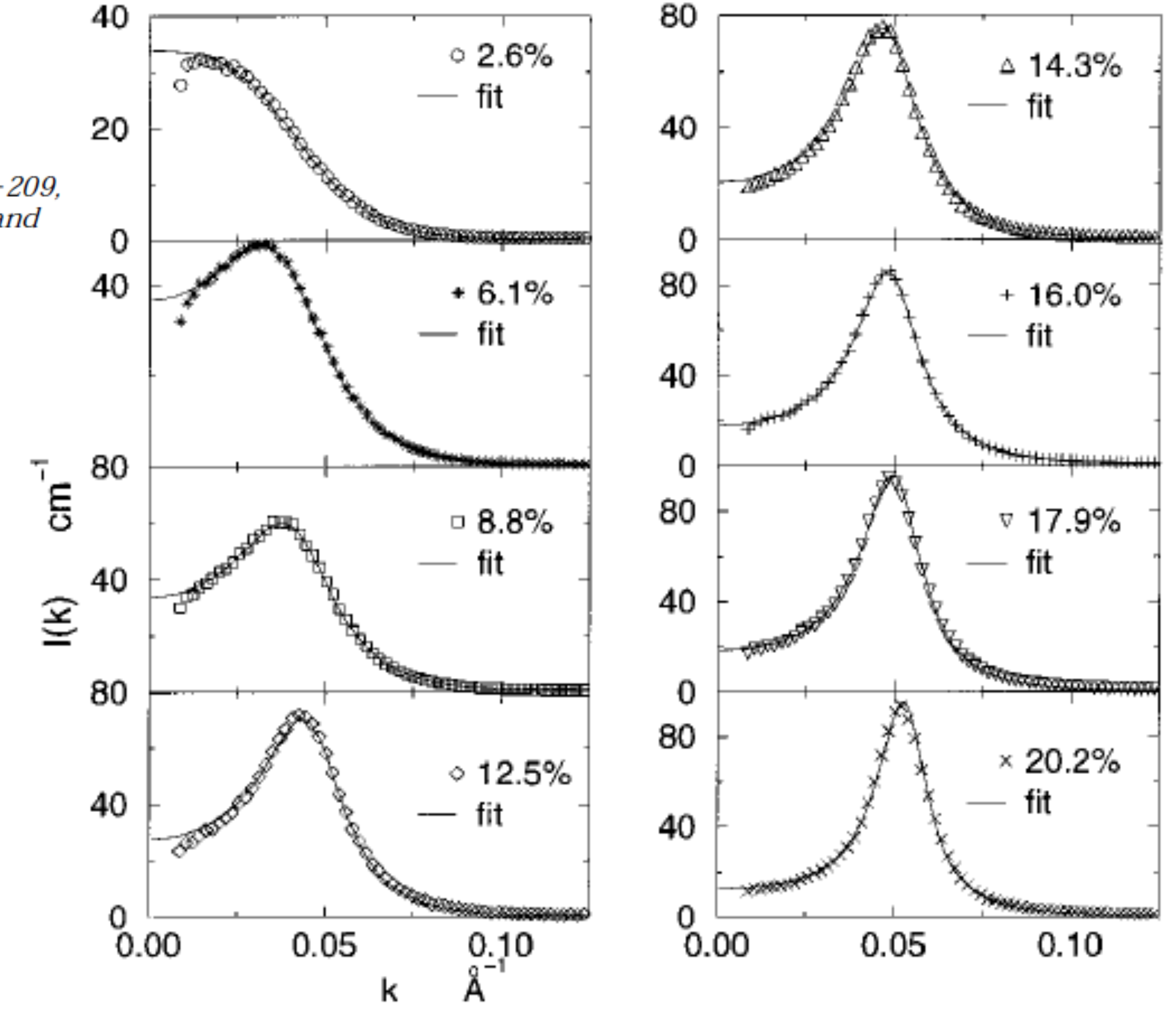
Yingchun Liu,[†] Sow-Hsin Chen,[*,‡] and John S. Huang[§]

Department of Materials Science and Engineering and Department of Nuclear Engineering, 24–209, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, and Exxon Research and Engieering Company, Annandale, New Jersey 08801

Received August 19, 1997; Revised Manuscript Received January 3, 1998



PEO-PPO-PEO
triblock copolymer

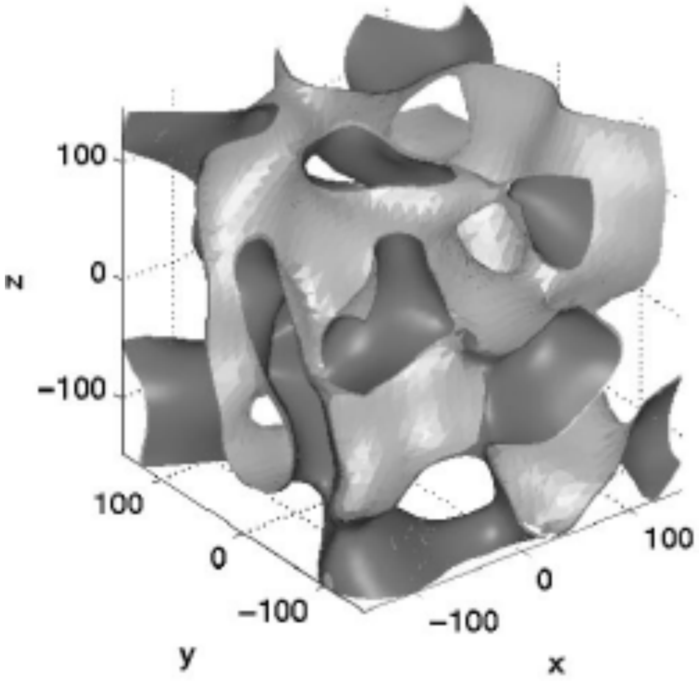


Example 6 – Microemulsion

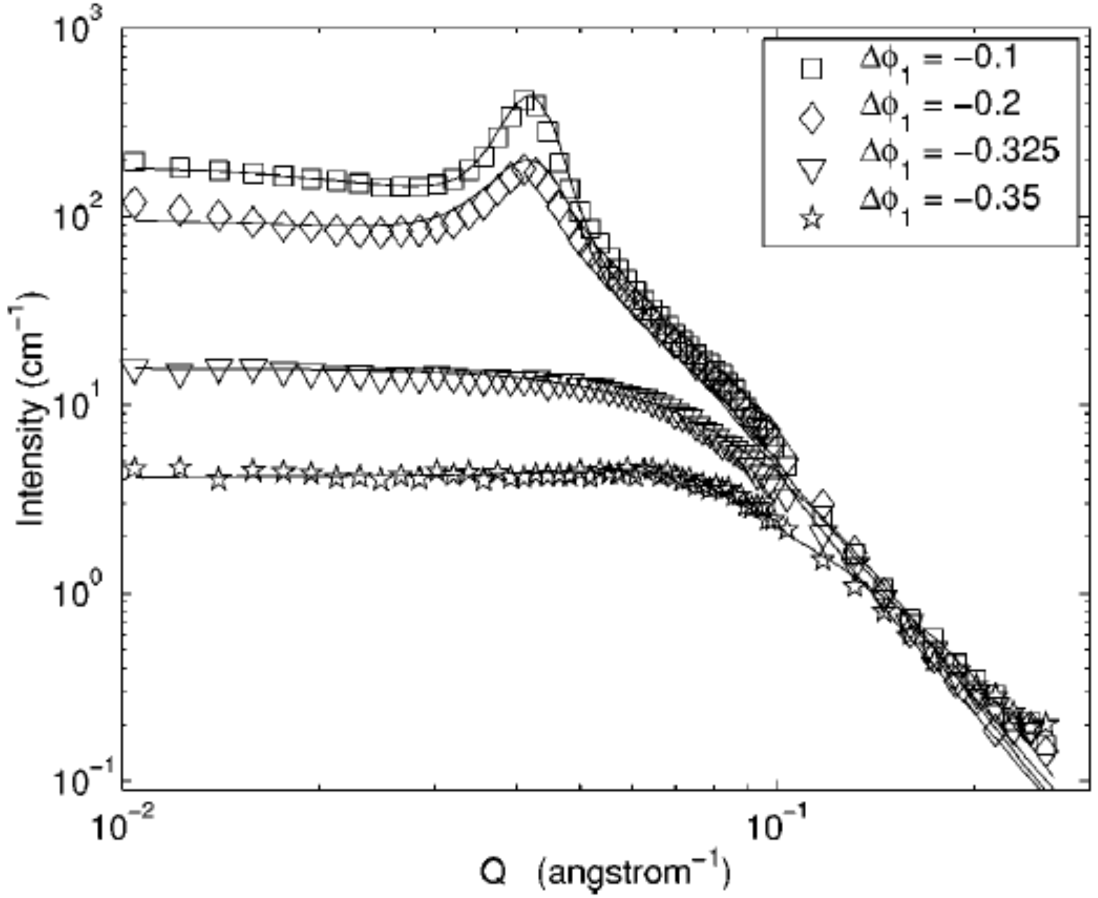
PHYSICAL REVIEW E, VOLUME 63, 021401

Clipped random wave analysis of anisometric lamellar microemulsions

Dawen Choy[1] and Sow-Hsin Chen[2,*]
[1]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
[2]*Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
(Received 28 May 2000; published 10 January 2001)



C12E4-D2O-octane



Example 7 – Carbon Nanotube

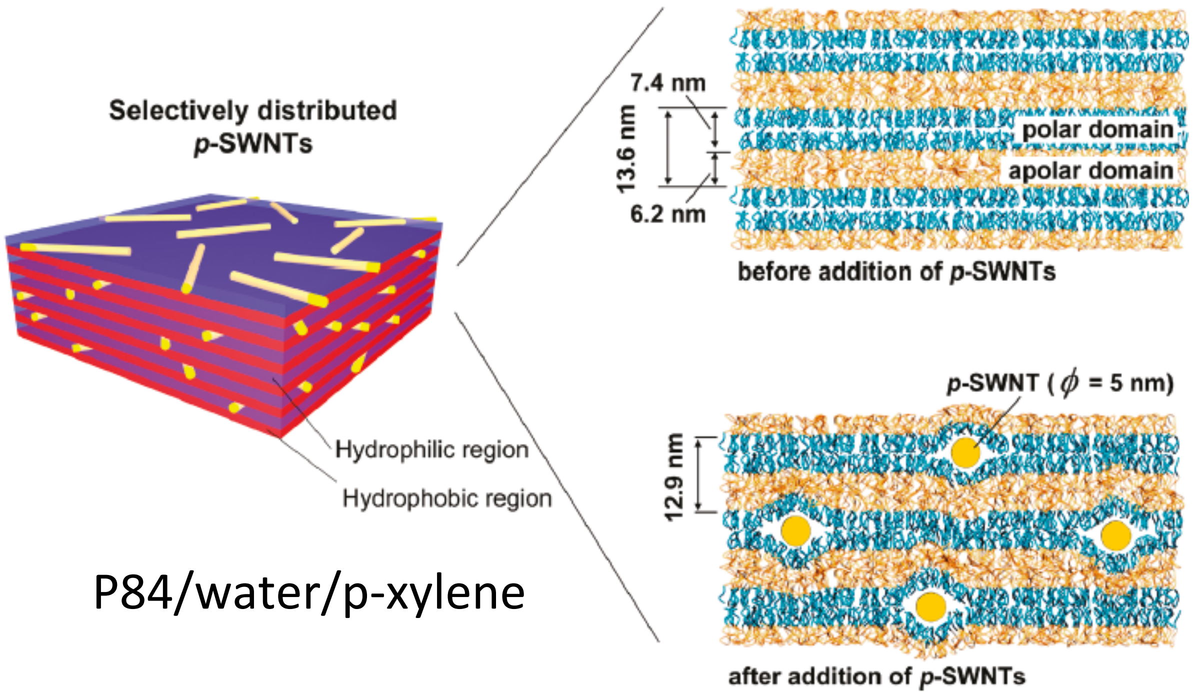
Macromolecules
ARTICLE

SANS Investigation of Selectively Distributed Single-Walled Carbon Nanotubes in a Polymeric Lamellar Phase

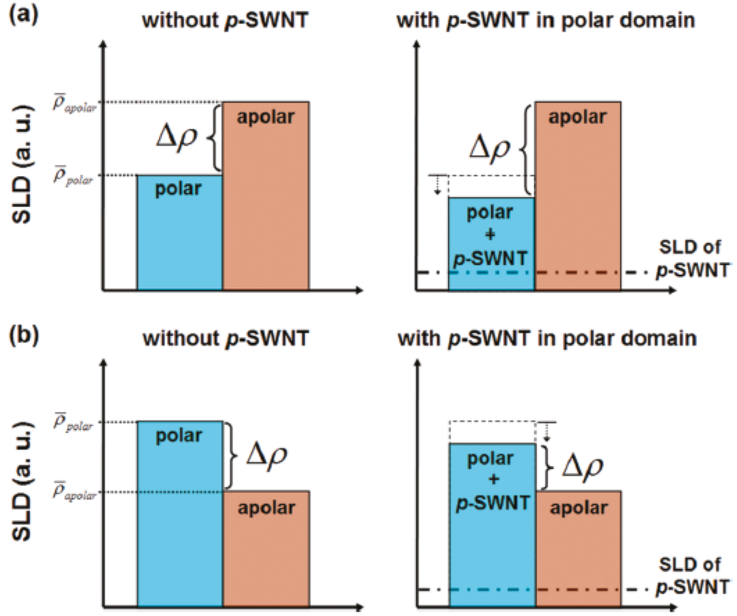
Changwoo Doe,[†] Hyung-Sik Jang,[†] Steven R. Kline,[‡] and Sung-Min Choi*[,†]

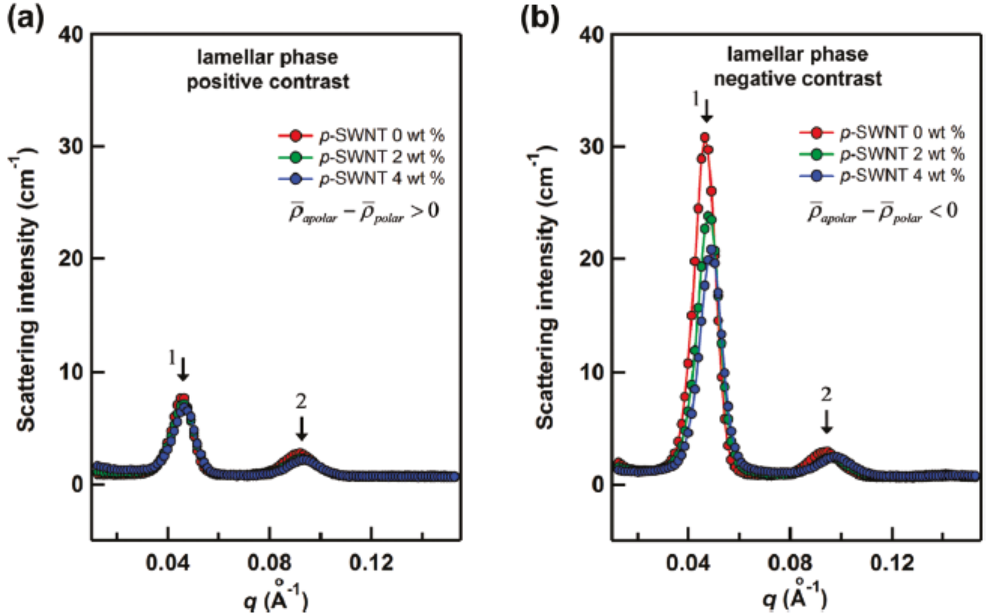
[†]*Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, Daejeon, 305-701, Republic of Korea, and* [‡]*NIST Center for Neutron Research, Gaithersburg, Maryland 20899-6102*

Received February 11, 2010; Revised Manuscript Received May 3, 2010



P84/water/p-xylene





Example 8 – Micellization Kinetics

ACS Macro Letters

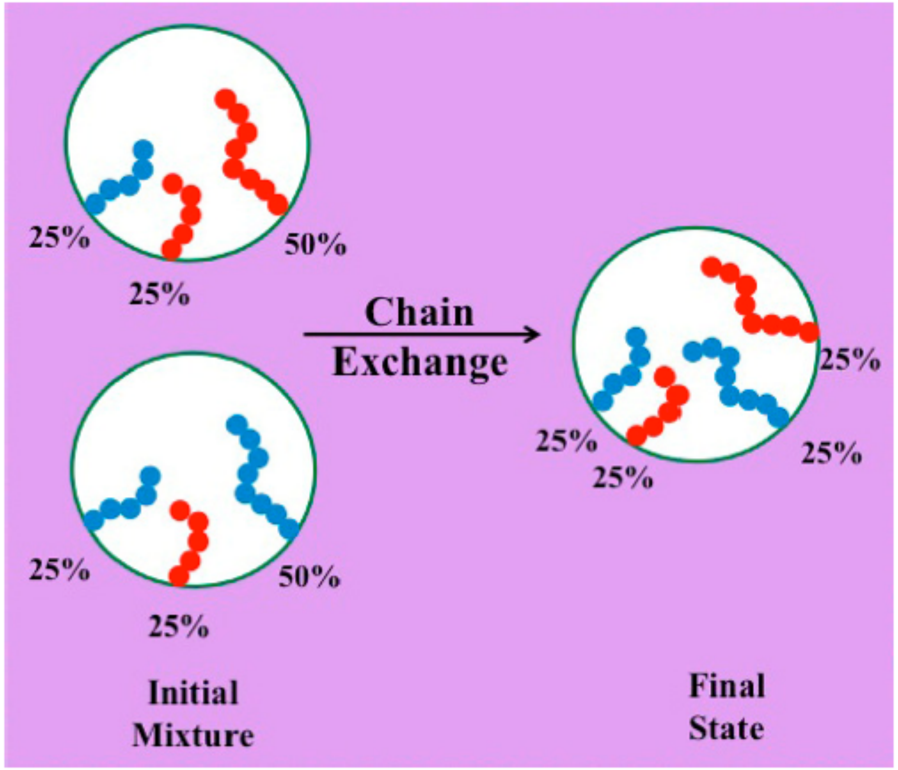
Letter

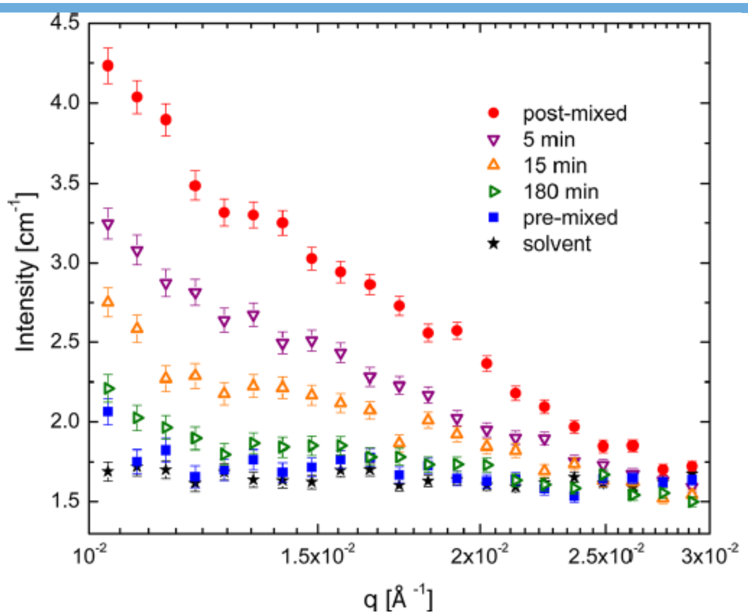
pubs.acs.org/macroletters

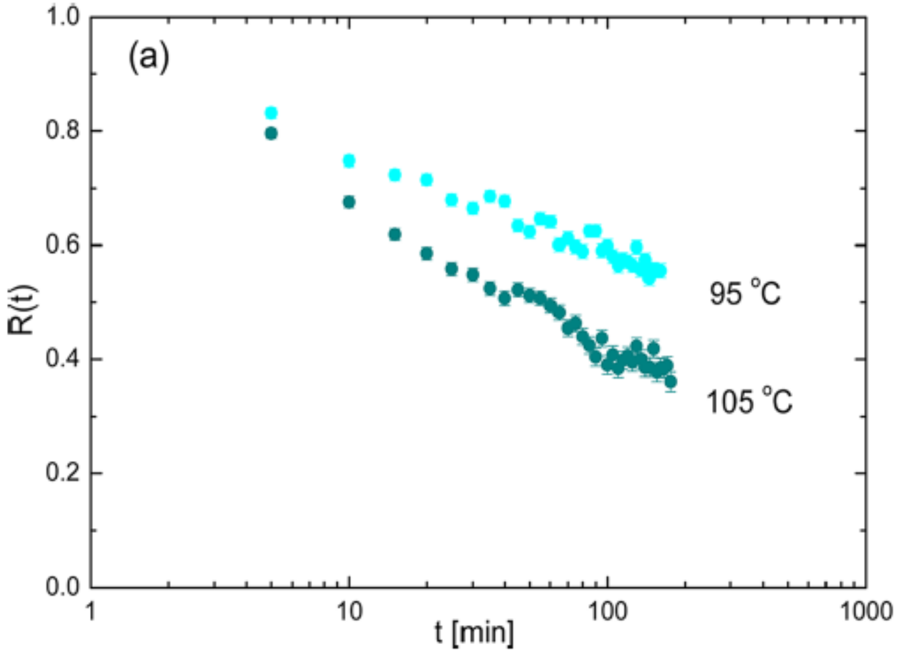
Chain Exchange in Binary Copolymer Micelles at Equilibrium: Confirmation of the Independent Chain Hypothesis

J. Lu,[†] F. S. Bates,[*,†] and T. P. Lodge[*,†,‡]

[†]Department of Chemical Engineering and Materials Science and [‡]Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455, United States

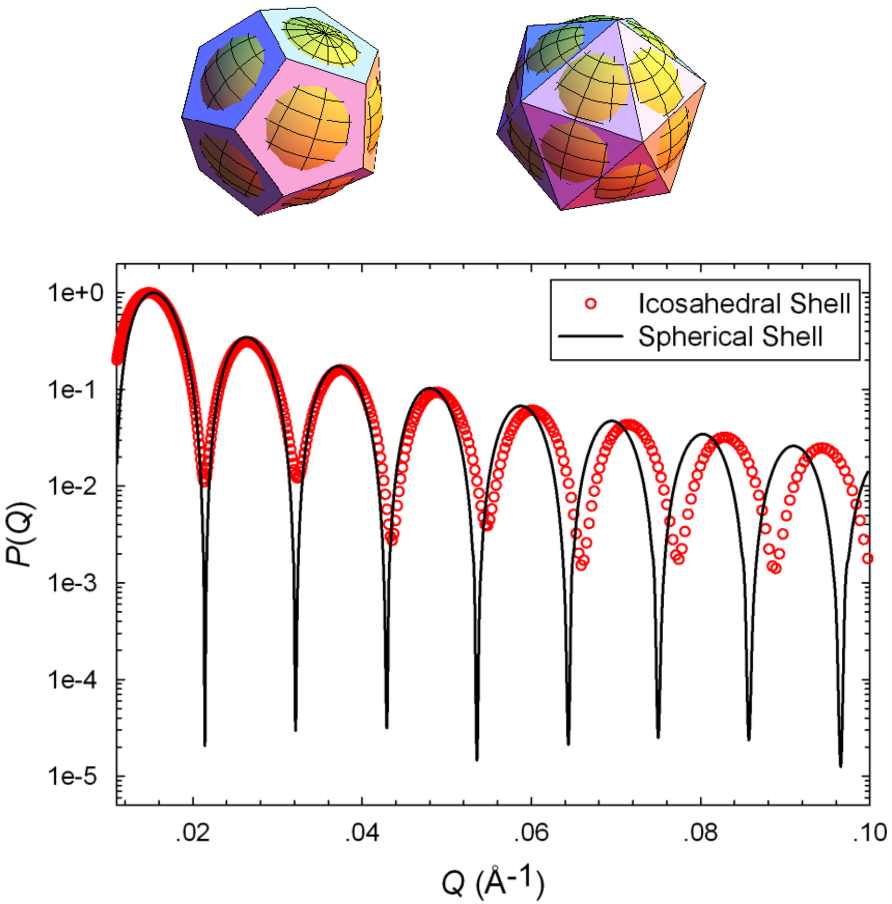




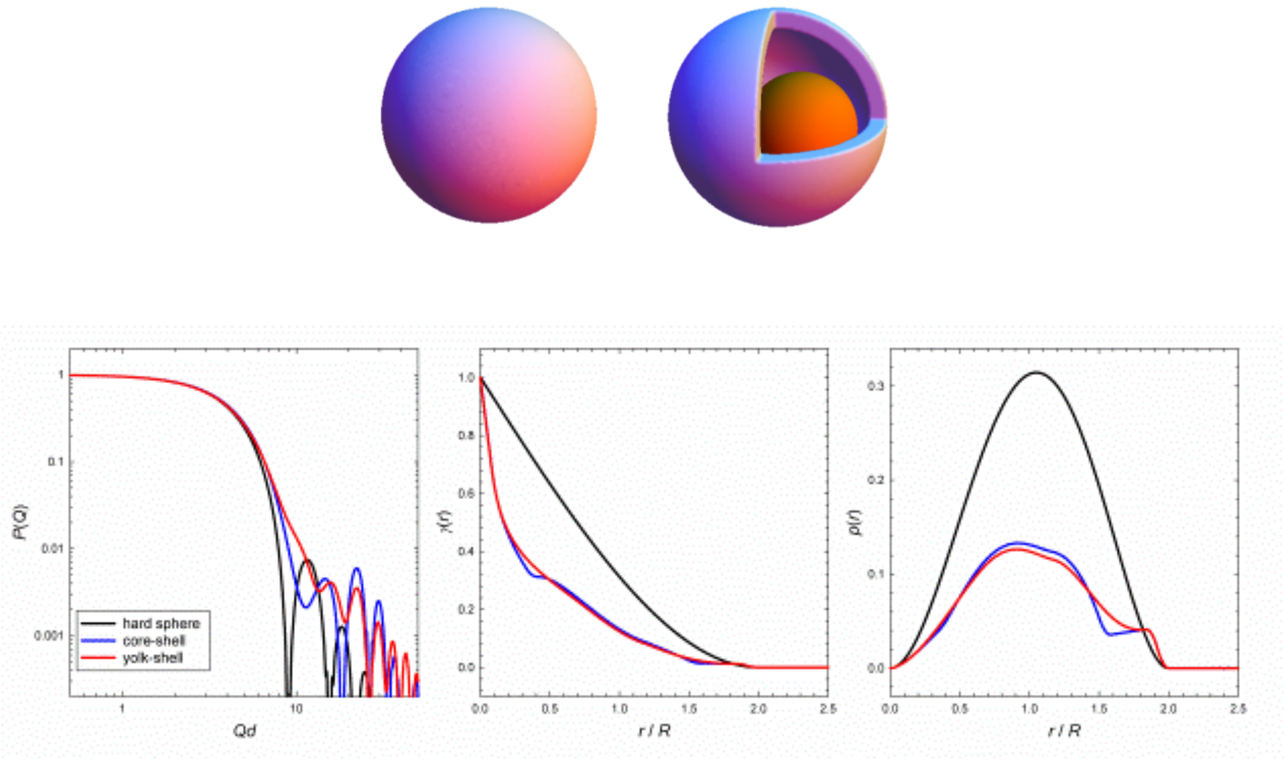


Derive New Scattering Functions

$$P(Q)=\langle |F(Q)|^2 \rangle=\langle |\int_V 4\pi\rho(r)e^{-iQ\cdot r}\,d^3r|^2\rangle$$



Li *et al.* *J. Appl. Cryst.* **44** 545 (2011)



Li *et al.* *J. Appl. Cryst.* **46** 1551 (2013)

Requirements for Model Fitting

Selection on systems for **quantitative** analysis using scattering techniques:

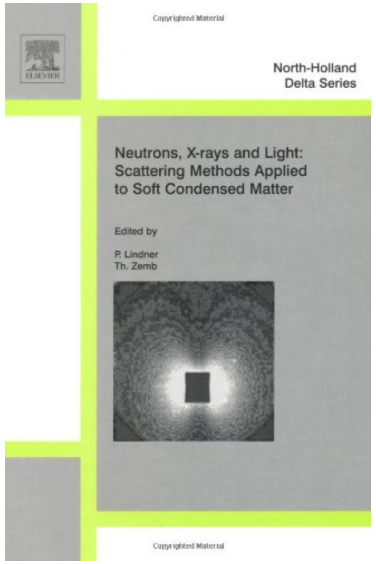
1. Single component in a certain length/time scale

2. Monodisperse ($\beta(Q)$ in S.-H. Chen, *Ann. Rev. Phys. Chem.* **1986** 37, 351-399.)

3. No aggregation (Aggregation does not dominate the scattering.)

4. Not too dilute, not too concentrated ($1\% < \phi_v < 40\%$)

References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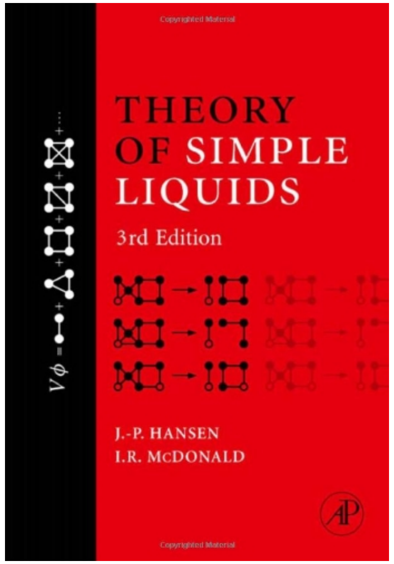
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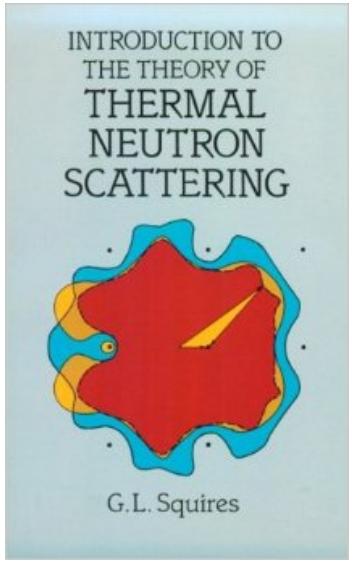
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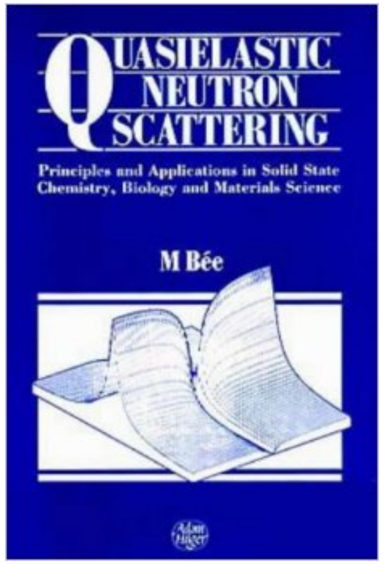
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Principles and Applications in Solid State
Chemistry, Biology and Materials Science
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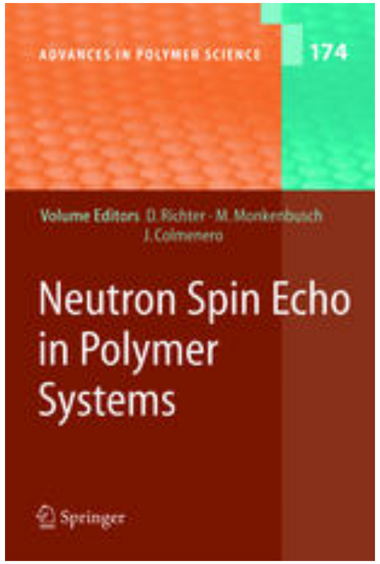
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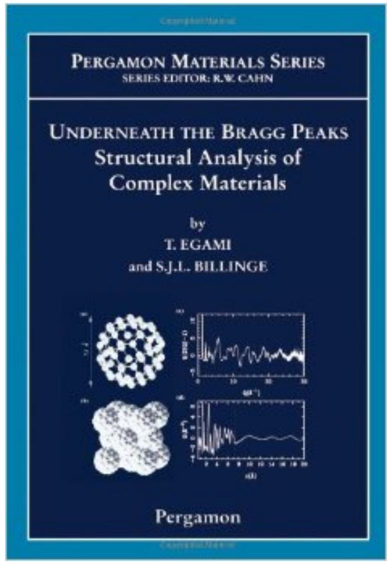
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