SMALL-ANGLE NEUTRON SCATTERING

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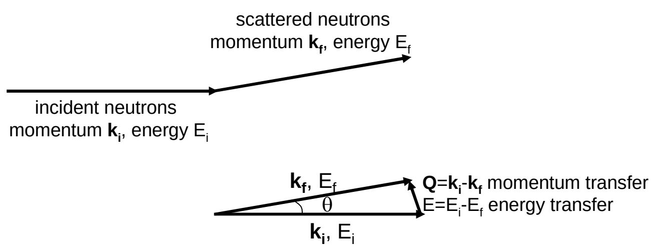
OUTLINE

- 1. Neutron Scattering
- 2. The SANS Technique
- 3. SANS Data Analysis
  Standard Plots
  SANS Models
- 4. SANS Research Topics
  A – Polymer Thermodynamics
  B – Pluronic Micelles
  C – Protein Complex
- 5. Final Points

1. Neutron Scattering

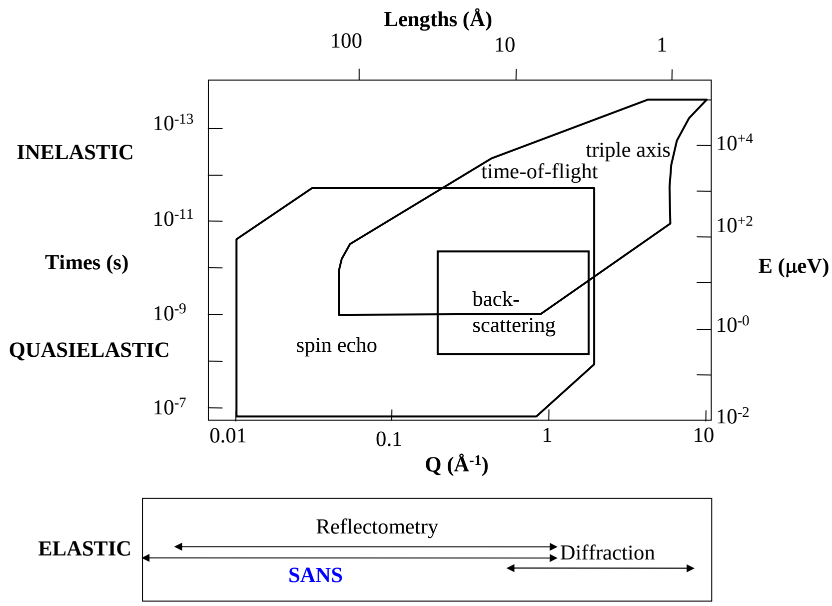
ELASTIC *vs* INELASTIC NEUTRON SCATTERING



Elastic scattering corresponds to E=0. Investigate structures.

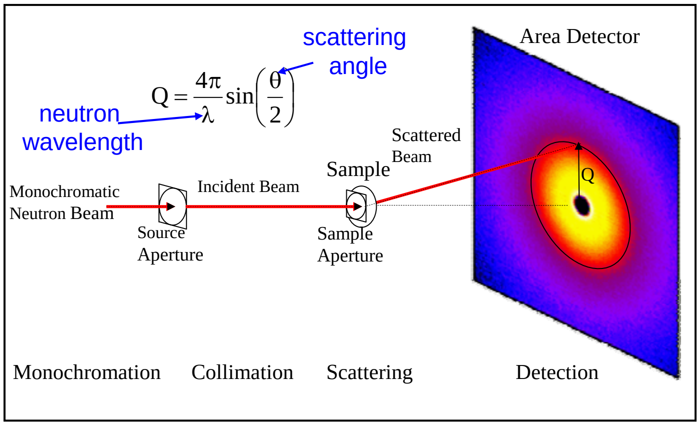
SANS and NR are elastic scattering techniques.

NEUTRON SCATTERING TECHNIQUES



2 – The SANS Technique

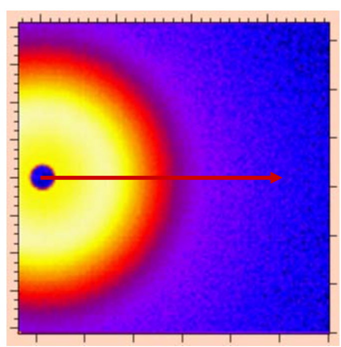
THE SANS TECHNIQUE

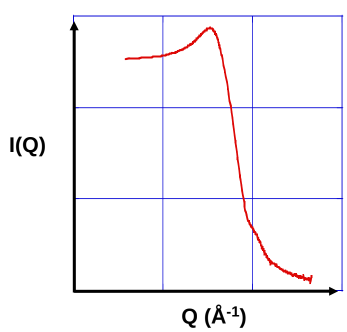


SANS DATA

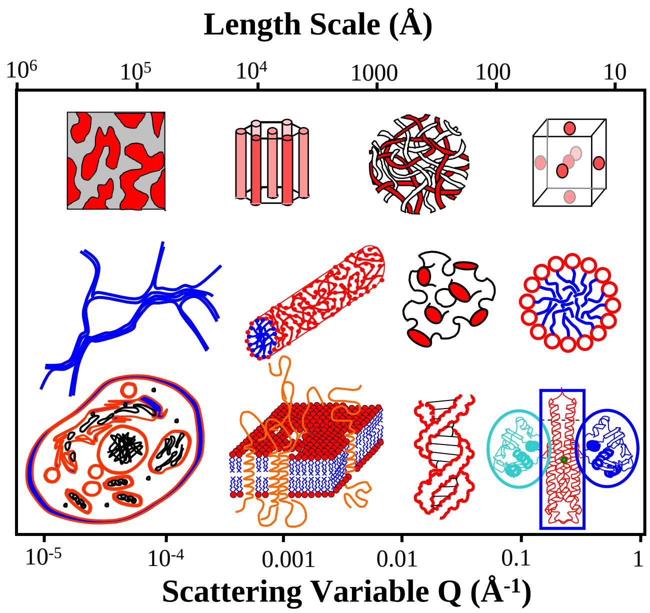
10% P85 Pluronic

in d-water at 60^{o}C

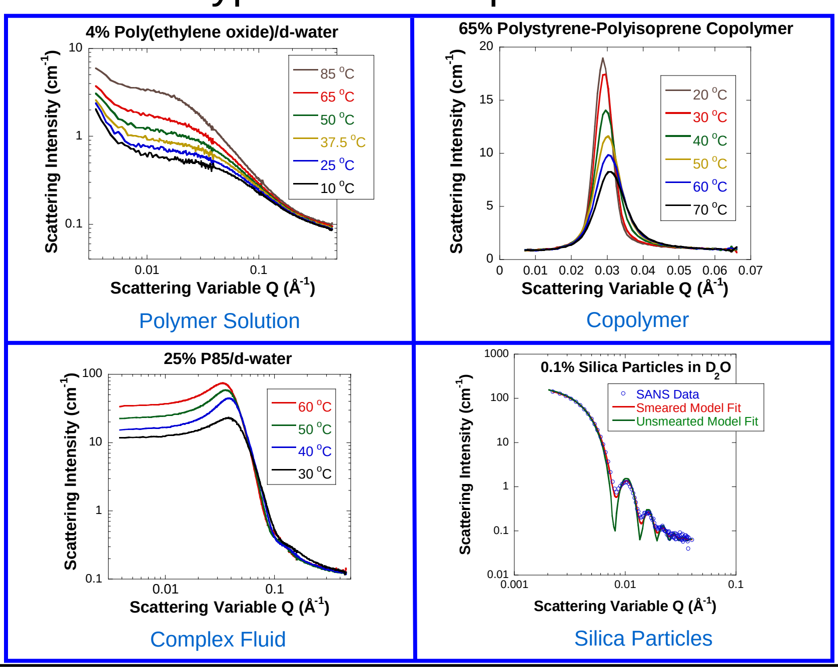




The Nanoscale



Typical SANS Spectra



SANS Cross Sections

$$I(Q) = \frac{d\Sigma_{coh}(Q)}{d\Omega} + \frac{d\Sigma_{incoh}}{d\Omega}$$

COHERENT

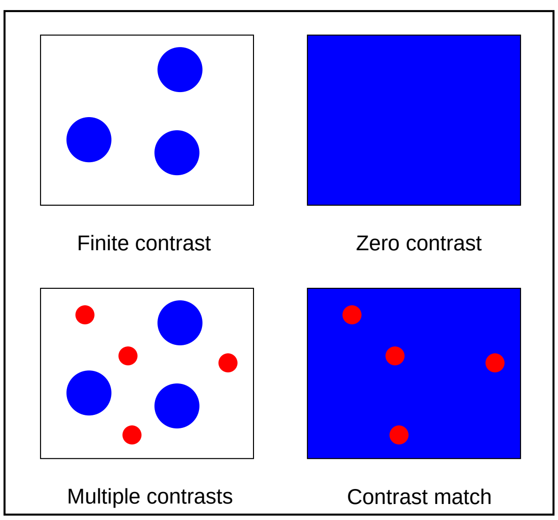
~ Contrast factor = $(\rho_A - \rho_B)^2$
- Info. about structure

INCOHERENT

- Q-independent
- no info. about structure

Scattering length density: $\rho_A = \frac{b_A}{v_A} = \frac{\text{scattering length}}{\text{volume}}$

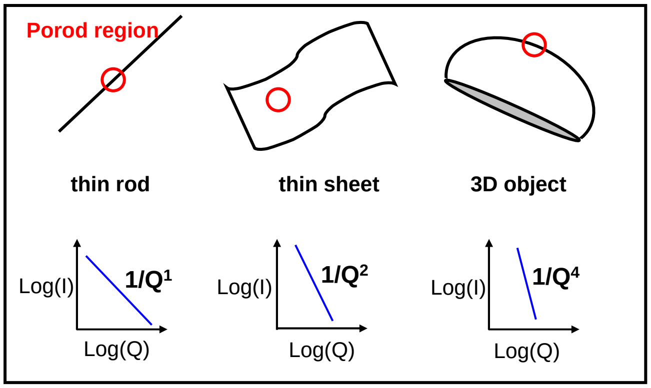
The Contrast Match Method



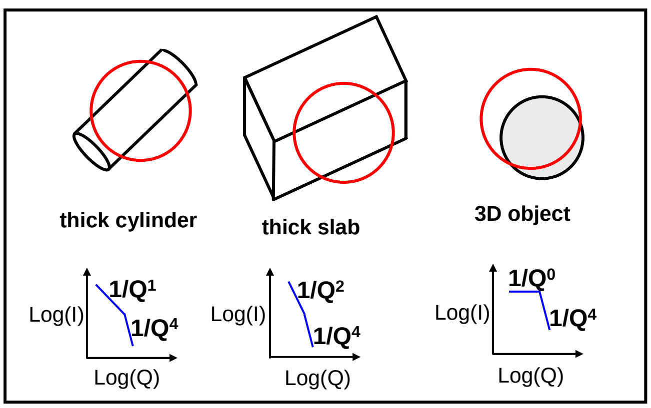
3 –SANS Data Analysis

- Standard Plots (Porod Plot, Guinier Plot)
- SANS Models
- Other Mehods

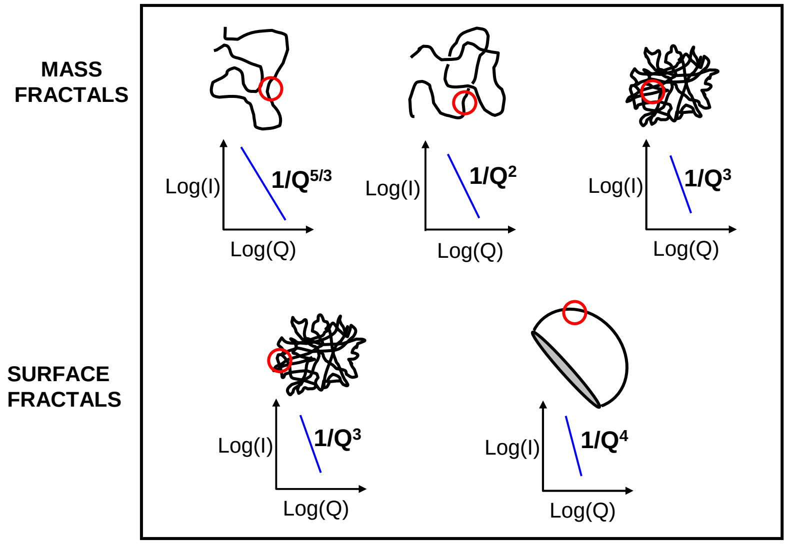
Assortment of Porod Exponents



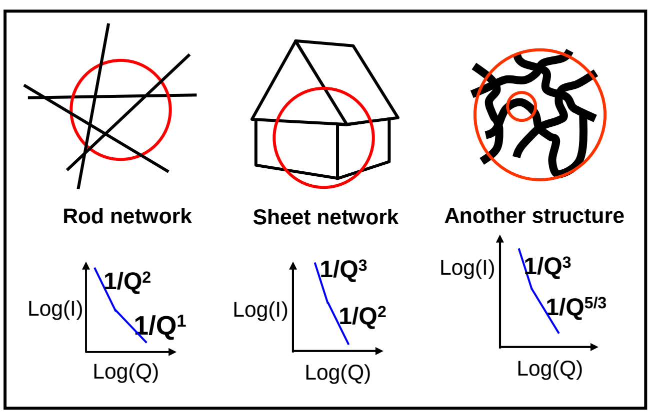
More Porod Exponents

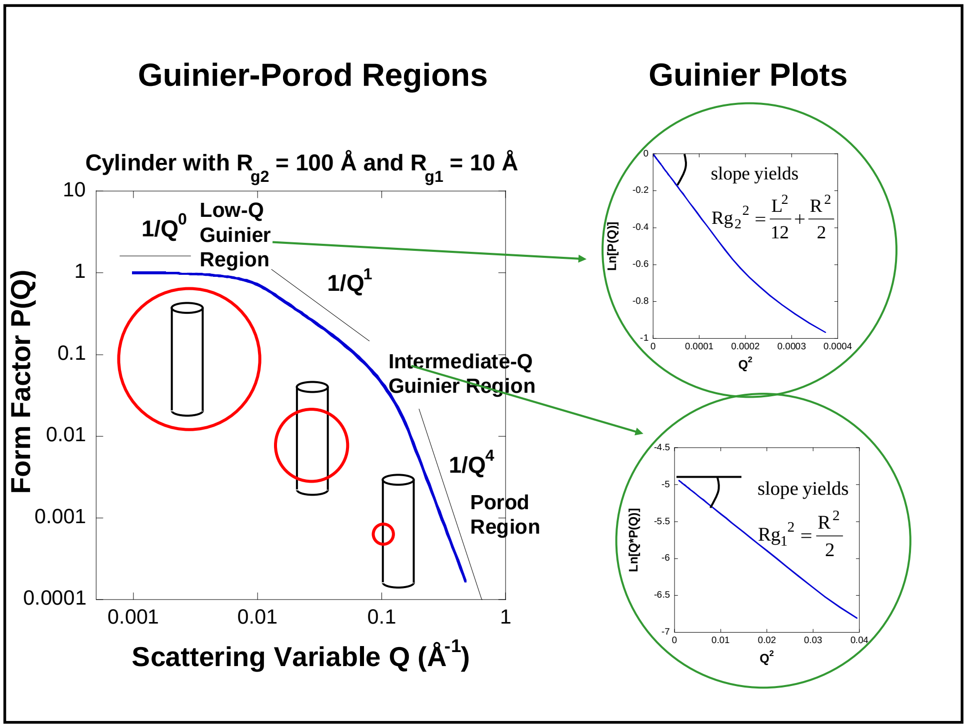


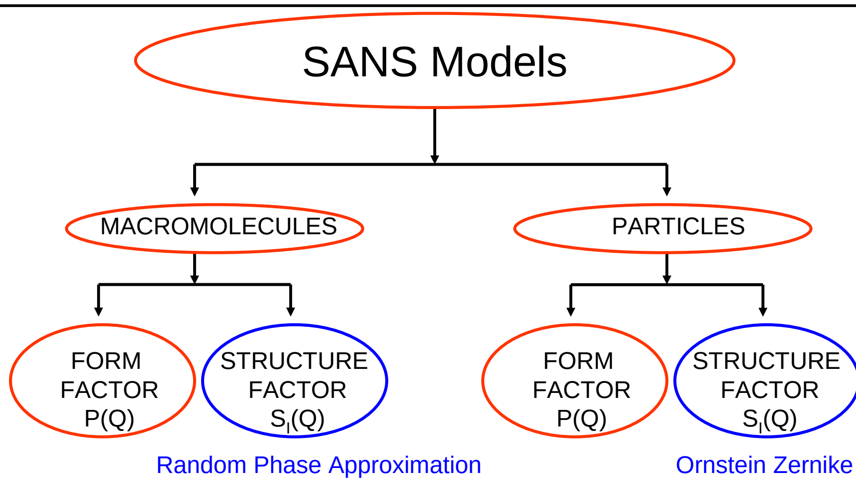
More Porod Exponents



More Porod Exponents



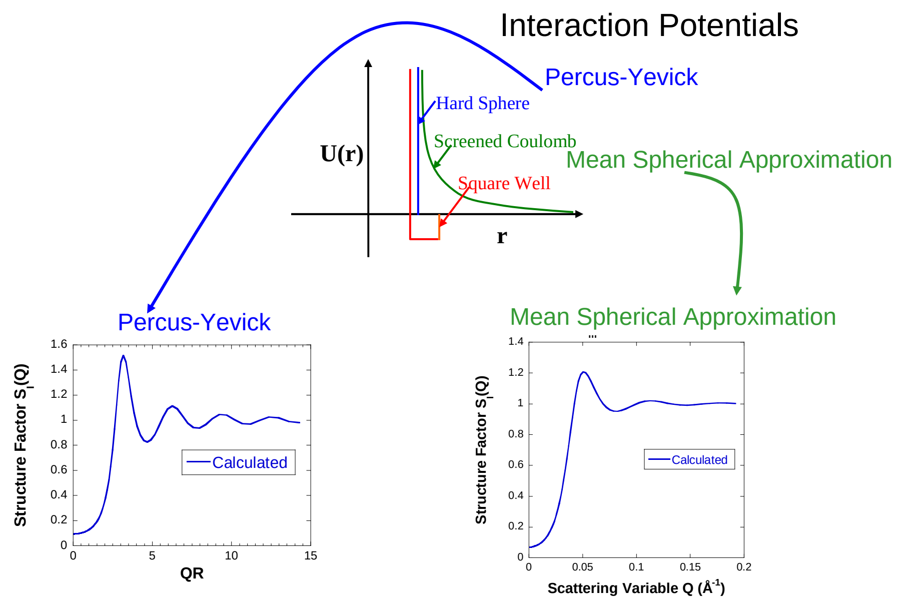




$$\frac{d\Sigma(Q)}{d\Omega} = \phi_A (\rho_A - \rho_B)^2 V_A P(Q) S_I(Q)$$

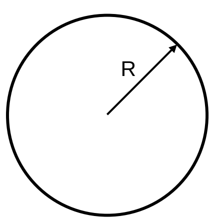
cross section | number density | contrast factor | particle volume | form factor | structure factor

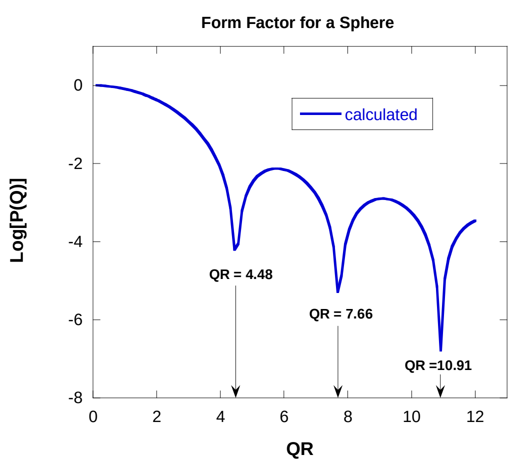
The Ornstein-Zernike Equation



FORM FACTOR FOR A SPHERE

$$P(Q) = \left[\frac{3j_1(QR)}{QR}\right]^2 = \left[\frac{3}{QR}\left(\frac{\sin(QR)}{(QR)^2} - \frac{\cos(QR)}{QR}\right)\right]^2$$

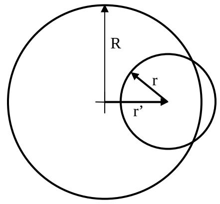




FORM FACTOR FOR A SPHERE

Density-density correlation function:

$$P(Q) = \frac{<n(-Q)n(Q)>}{n^2} = \int d\vec{r} \int d\vec{r}' \frac{<n(r)n(r')>}{n^2} \exp[i\vec{Q}.(\vec{r}'-\vec{r})]$$

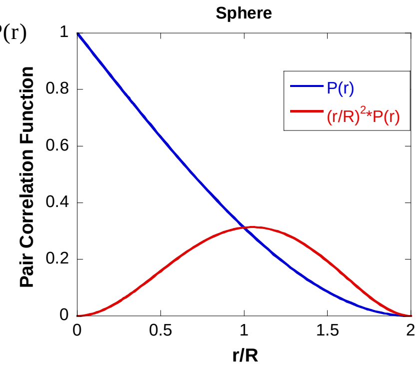


Fourier transform:

$$P(Q) = \int d^3r \exp[-i\vec{Q}.\vec{r}]\, P(\vec{r}) = \frac{1}{V_P} \int_0^{\infty} dr 4\pi r^2 \frac{\sin(Qr)}{Qr} P(r)$$

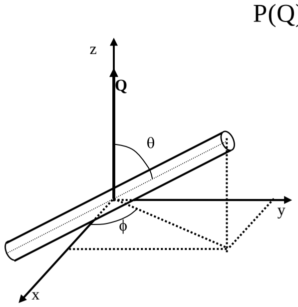
Radial pair correlation function:

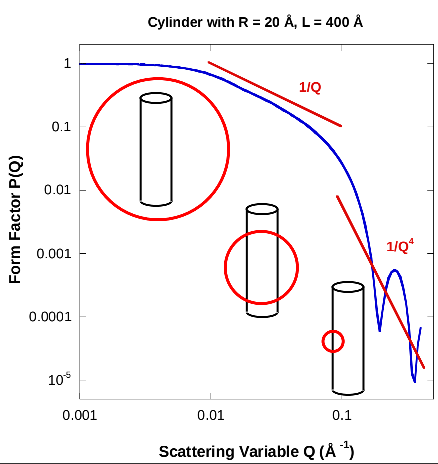
$$P(r) = 1 - \frac{3}{4}\left(\frac{r}{R}\right) + \frac{1}{16}\left(\frac{r}{R}\right)^3$$



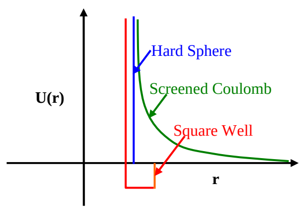
FORM FACTOR FOR A CYLINDER

$$P(Q) = \frac{1}{2} \int_{-1}^{1} d\mu \left[\frac{\sin(Q\mu L/2)}{Q\mu L/2}\right]^2 \left[\frac{2J_1(Q\sqrt{1-\mu^2}R)}{Q\sqrt{1-\mu^2}R}\right]^2$$

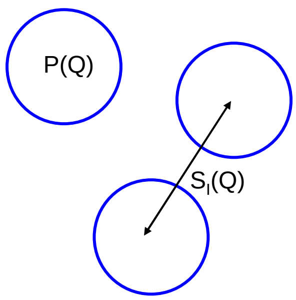


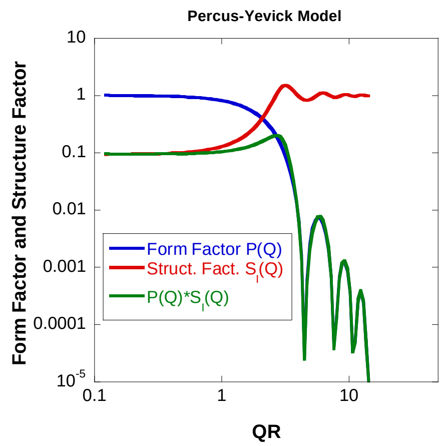


STRUCTURE FACTOR – THE ORNSTEIN-ZERNIKE EQUATION



$$\frac{d\Sigma(Q)}{d\Omega} = \phi_A \left(\rho_A - \rho_B\right)^2 V_A \, P(Q) \, S_I(Q)$$



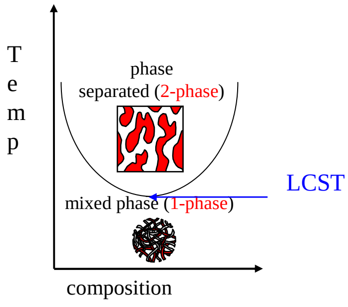


4. SANS Research Topics

A – Polymer Thermodynamics
B – Pluronic Micelles
C - Protein Complex

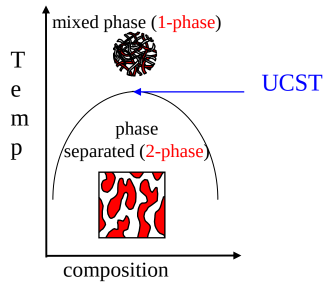
A – Polymer Thermodynamics

POLYMER DEMIXING TRANSITIONS



LCST

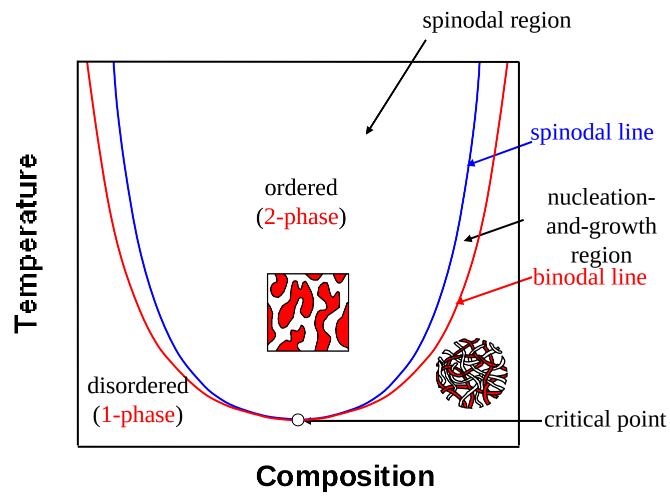
Lower Critical Solution Temp.



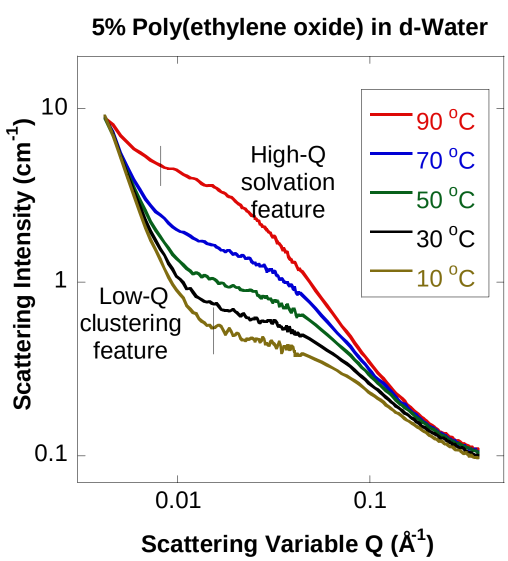
UCST

Upper Critical Solution Temp.

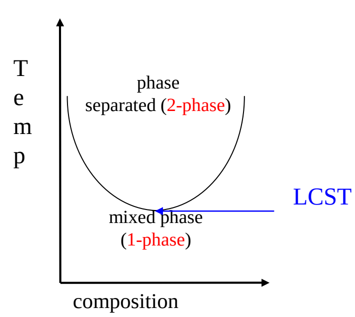
LOWER CRITICAL SPINODAL TEMPERATURE



POLY(ETHYELENE OXIDE) IN D-WATER



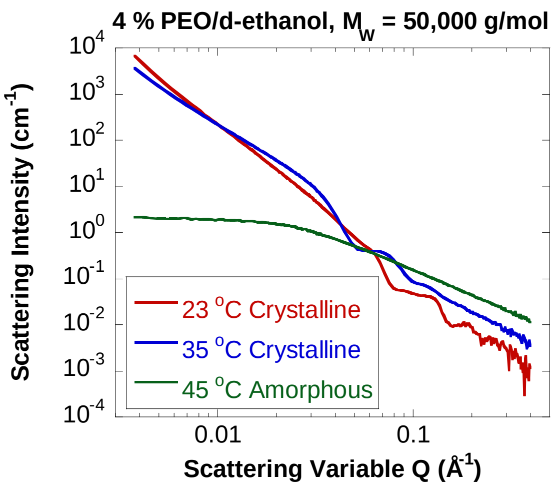
Amorphous



LCST

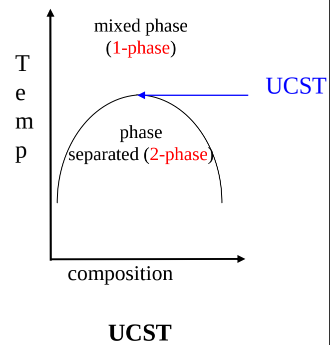
Lower Critical Spinodal Temperature

POLY(ETHYELENE OXIDE) IN D-ETHANOL



Crystalline

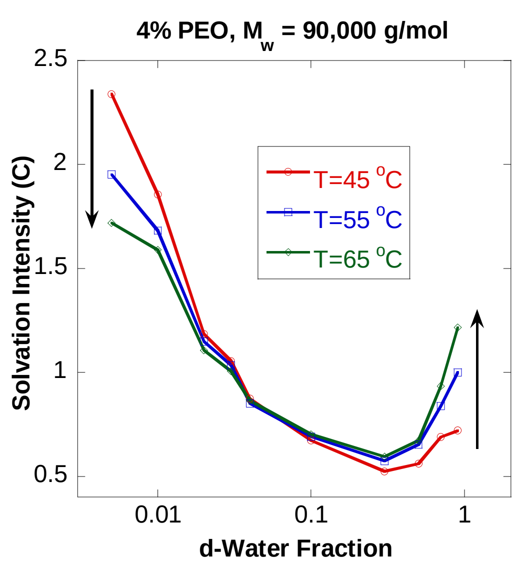
Amorphous



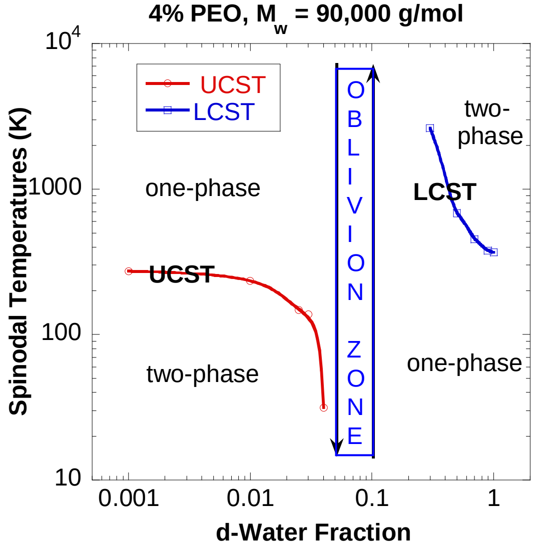
UCST

Upper Critical Spinodal Temperature

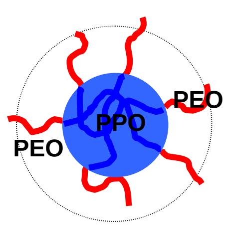
POLY(ETHYELENE OXIDE) IN SOLVENT MIXTURES



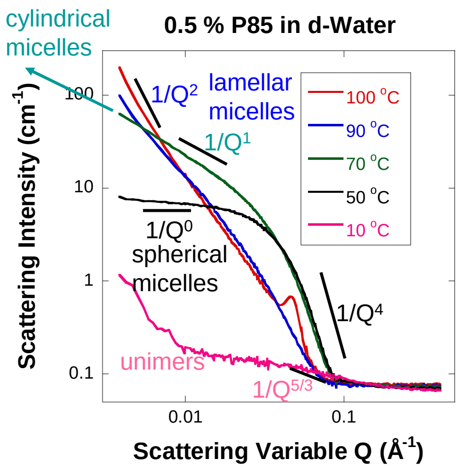
POLY(ETHYELENE OXIDE) IN MIXED SOLVENTS

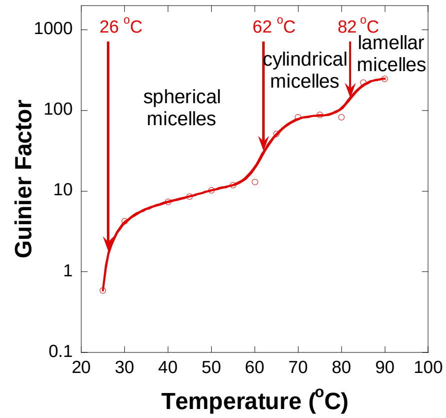


B – Pluronic Micelles

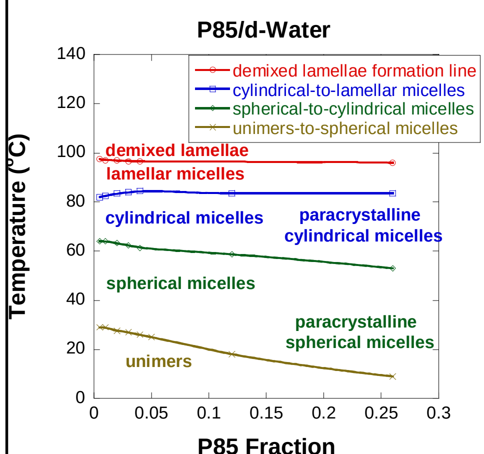


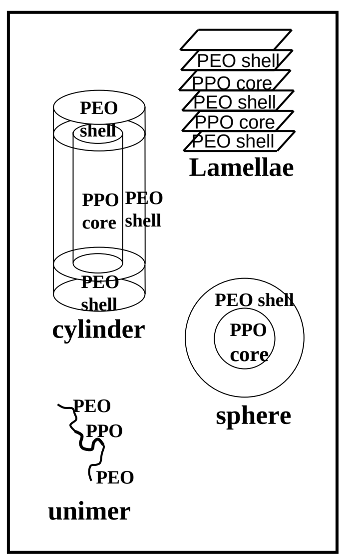
Micelles Phases



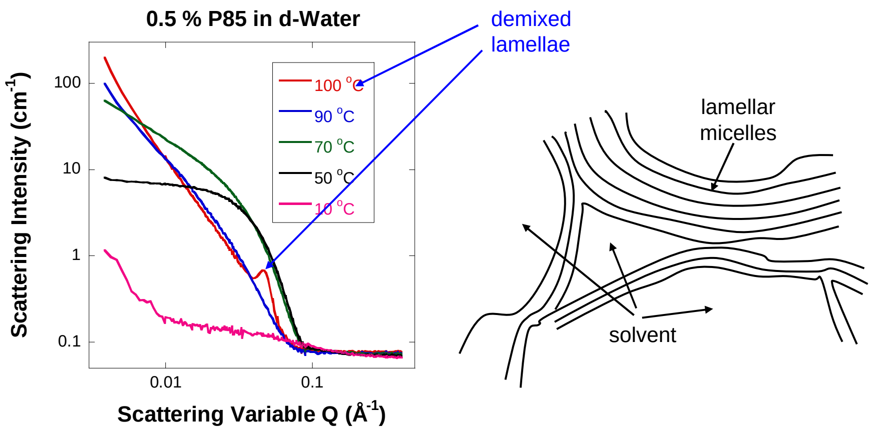


Phase Diagram

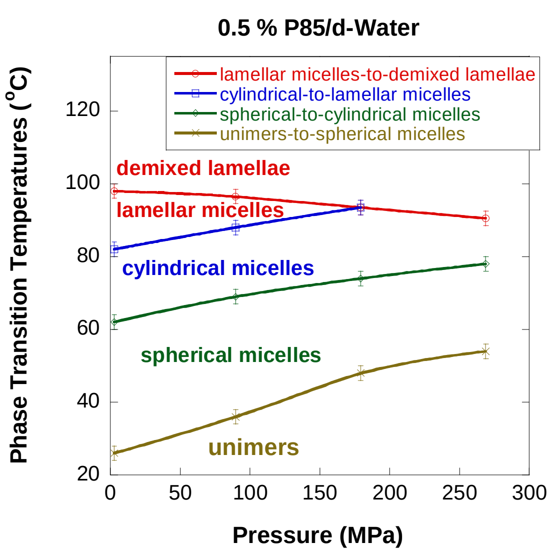




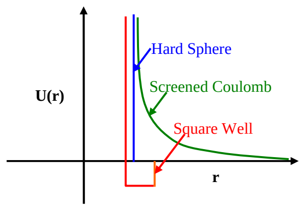
THE DEMIXED LAMELLAE PHASE

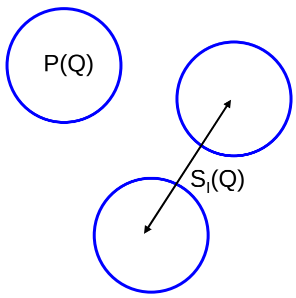


P85/D-Water Under Pressure

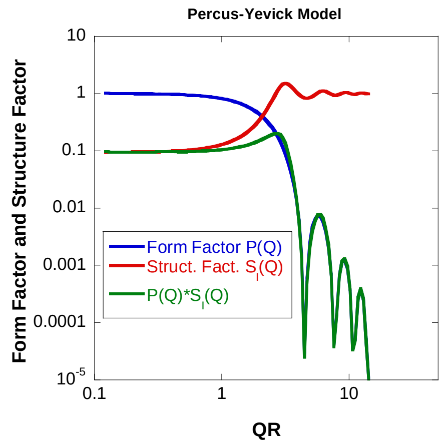


Particle Structure Factor –
The Ornstein-Zernike Equation





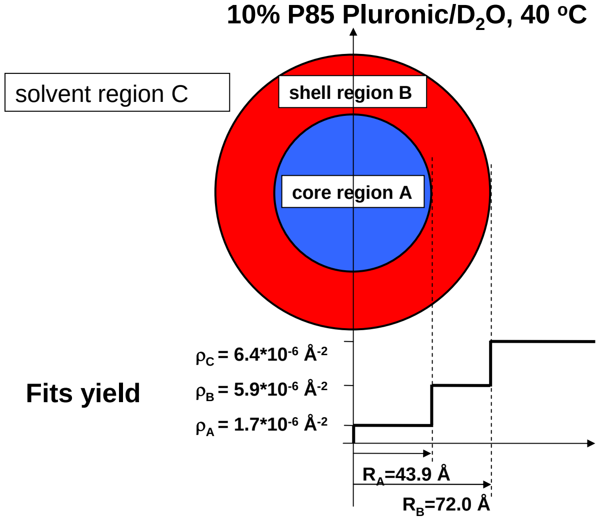
$$\frac{d\Sigma(Q)}{d\Omega} = \phi_A(\rho_A - \rho_B)^2 V_A P(Q)\, S_I(Q)$$



Core-Shell Spherical Particles

$$\frac{d\Sigma(Q)}{d\Omega} = \frac{N}{V}\left[(\rho_A - \rho_B)V_A \frac{3j_1(QR_A)}{QR_A} + (\rho_B - \rho_C)V_{A+B}\left(\frac{3j_1(QR_B)}{QR_B}\right)\right]^2 S_I(Q)$$

10% P85 Pluronic/D_2O, 40 ^oC



Core-Shell Spherical Particles

Material Balance Equations:

$$\frac{4\pi}{3}R_A{}^3 = N_{ag}.\left[40.v_{PO} + 52.f.v_{EO} + 52.f.v_{D_2O}.y_A\right]$$

$$\frac{4\pi}{3}(R_B - R_A)^3 = N_{ag}.\left[52.(1-f).v_{EO} + 52.(1-f).v_{D_2O}.y_B\right]$$

$$\rho_A = \frac{N_{ag}[40b_{PO} + 52.b_{EO}.f + 52b_{D_2O}.f.y_A]}{\frac{4\pi}{3}R_A{}^3}$$

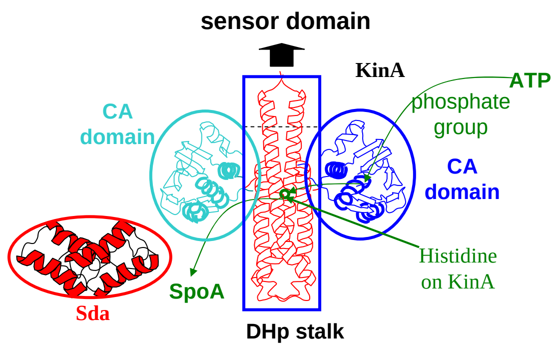
$$\rho_B = \frac{N_{ag}[52.b_{EO}.(1-f) + 52.b_{D_2O}.(1-f).y_B]}{\frac{4\pi}{3}\left(R_B{}^3 - R_A{}^3\right)}$$

Results for 10% P85 at 40 ^oC:

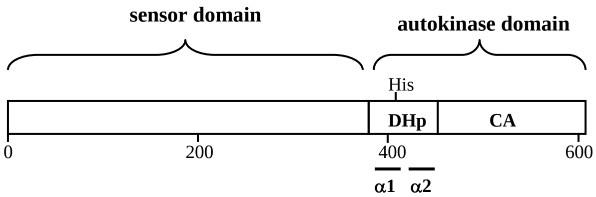
In the core:
2,795 PPO monomers
690 PEO monomers
490 D_2O molecules

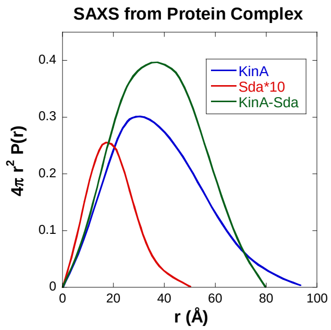
In the shell:
2,943 PEO monomers
34,167 D_2O molecules

C – Protein Complex



KinA-Sda Complex





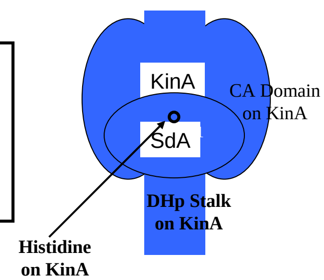
His

TEELMLKSEKLS-------IAGQLAAGIAHEIRNPLTAIKGFLQ-----LMKPTMEGNEHYFDIVFSELSRIELILSELLMLAKPQQNAV

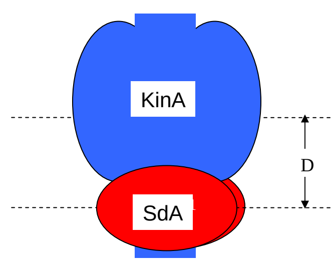
α1 α2

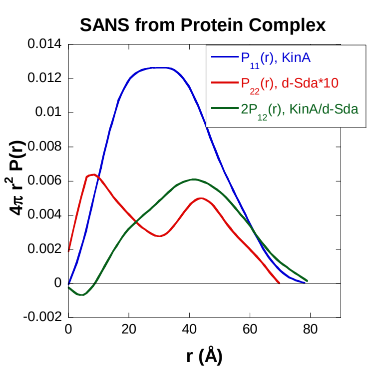
---KEYLNLKKLI-GEVSALLE—TQANLNGIFIRTSYEKDSIYINGDQNQLKQVFINLIKNAV----ESMPDGGTVDIIITEDEHSVHV

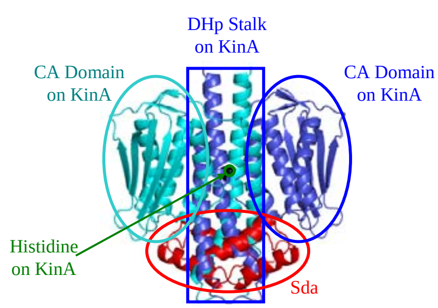
TVKDEGEGIPEKVLNRIGEPF------LTTKEKGTGLGLMVTFNIIENHQGVIHVDSHPEKGTAFKISFPKK



KinA-Sda Complex

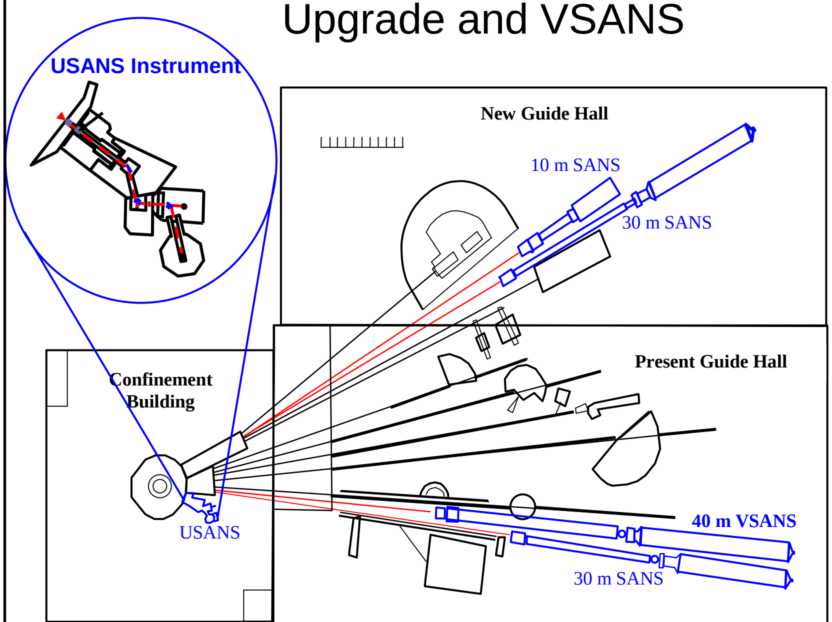




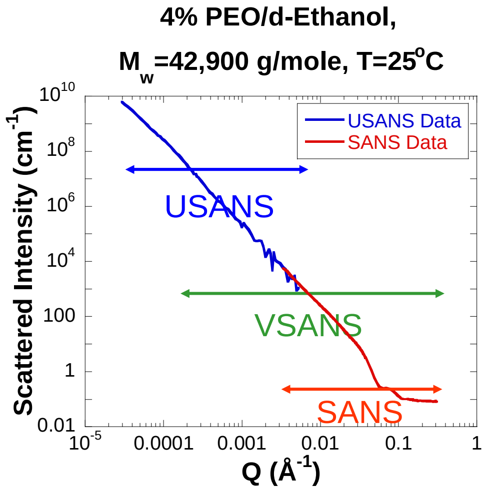


5. FINAL POINTS

Upgrade and VSANS



SANS, VSANS and USANS Ranges



Final Words

THE SANS PROGRAM AT NIST

200 experiments per year

15 theses per year

80 publications per year

FUTURE OUTLOOK

Past 20 years – NCNR development

Next 20 years – NCNR expansion

ACKNOWLEDGMENTS

Derek Ho, Rob Briber, Steve Kline, Jill Trewhella

RECENT REFERENCES

- B. Hammouda “SANS from Polymers - Review of the Recent Literature”, Polymer Reviews 50, 14-39 (2010)

- B. Hammouda, “Probing Nanoscale Structures – The SANS Toolbox”. Book available online. Google it

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