SANS RESEARCH TOPICS

Boualem Hammouda

National Institute of Standards and Technology
Center for Neutron Research

1. SANS from Pluronics

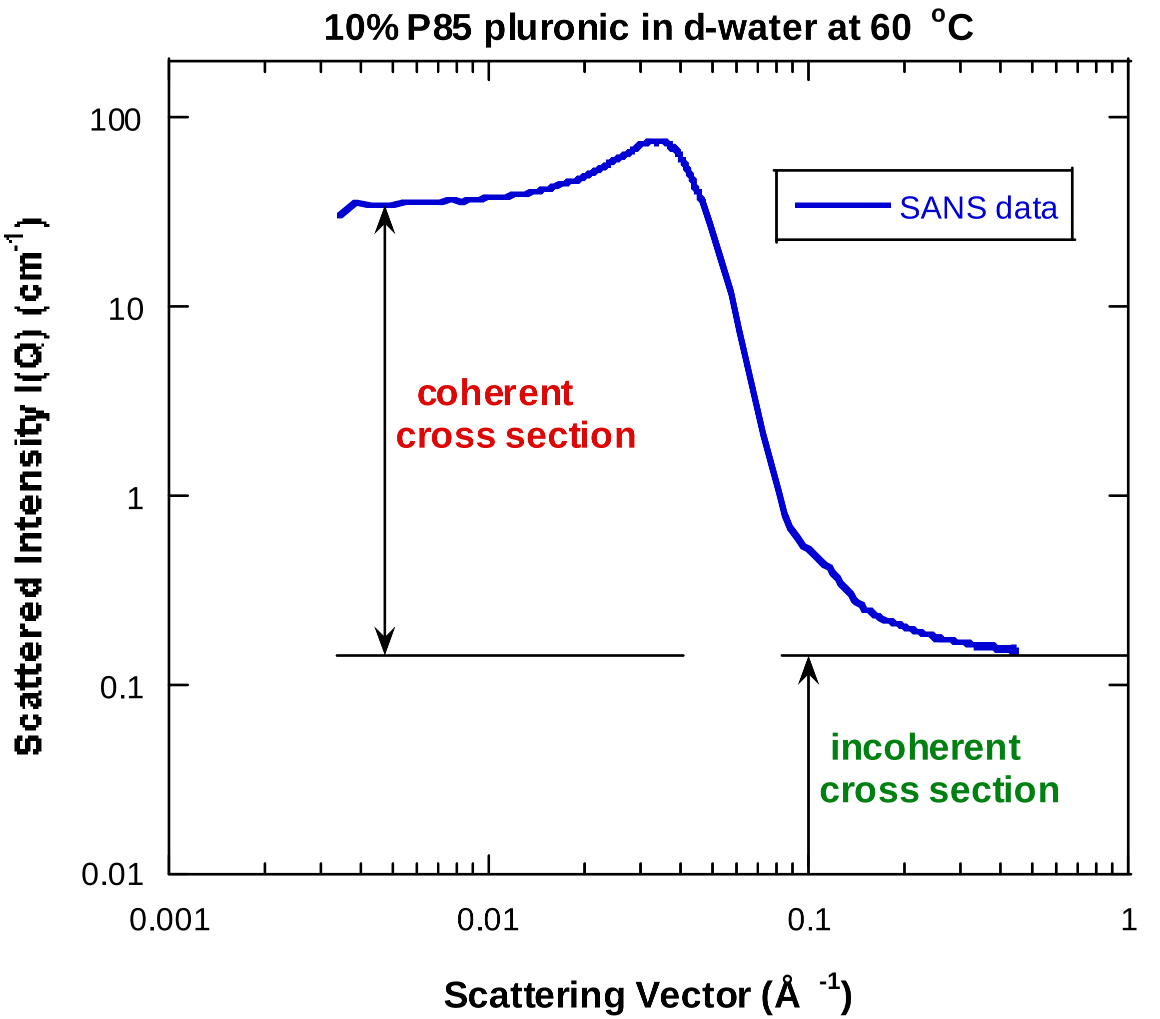
2. Polymer Blend Thermodynamics

3. Helix-to-Coil Transition in DNA

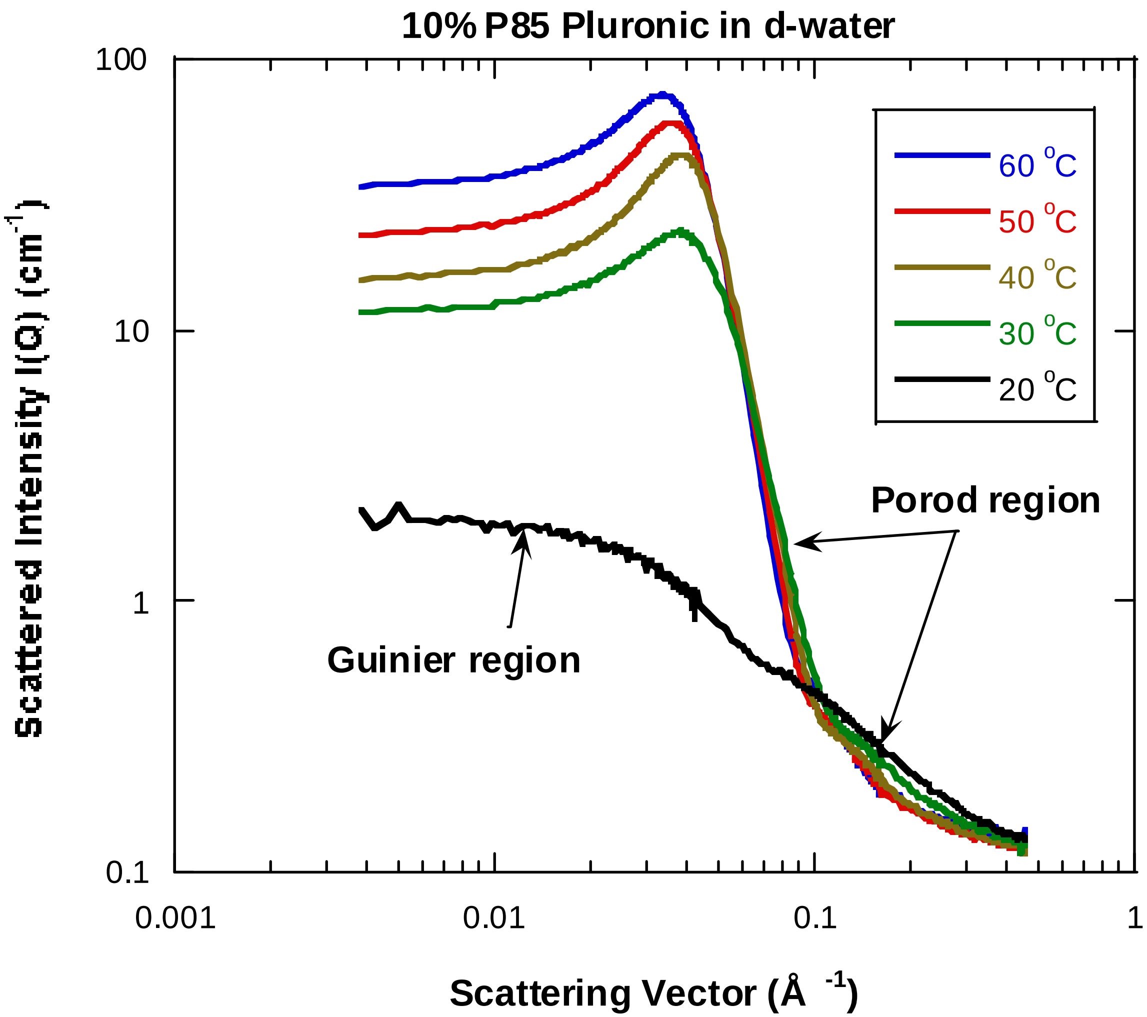
1. SANS FROM PLURONICS

Pluronics are triblock copolymers: PEO-PPO-PEO

PEO: $-CH_2CH_2O-$ is hydrophillic
PPO: $-CH_2CH_2(CH_3)O-$ is hydrophobic

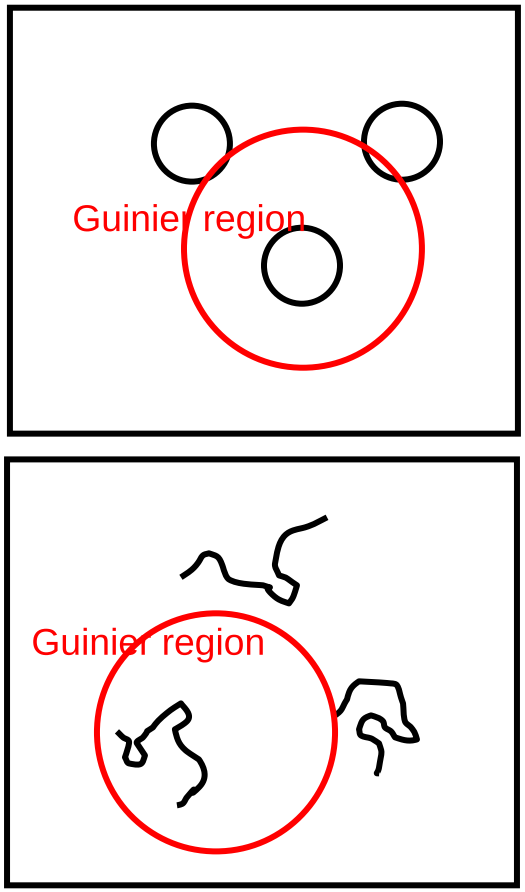


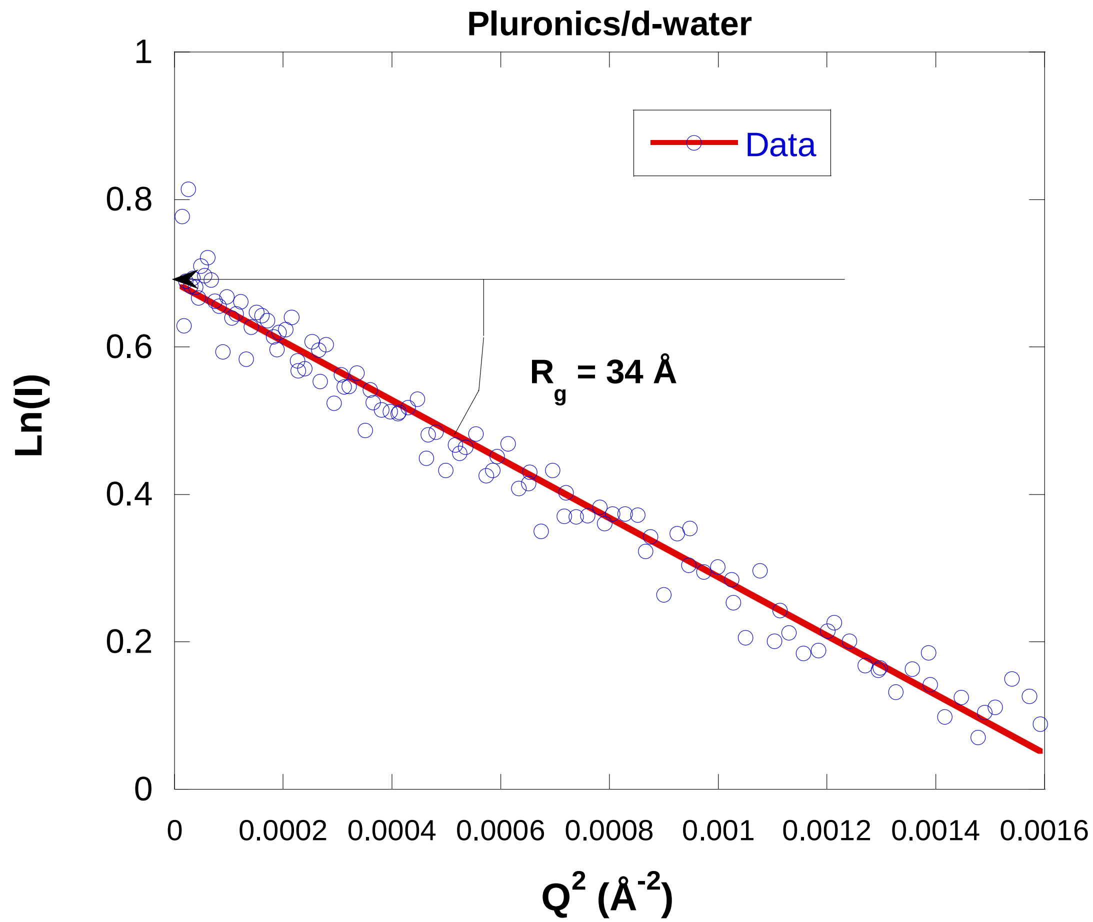
P85 Pluronic forms micelles at high temperatures



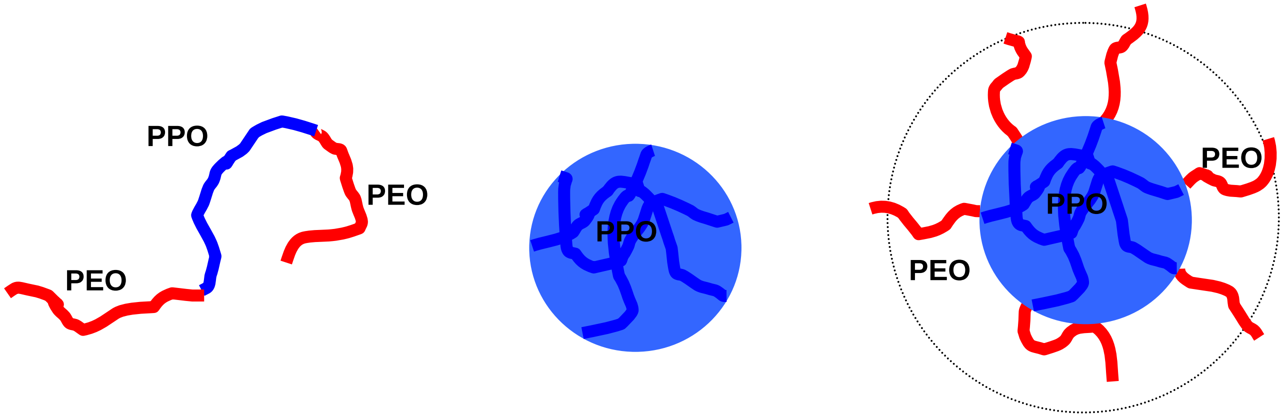
The Guinier Plot

$$I(Q) = I(0)\exp(-Q^2R_g^2/3)$$

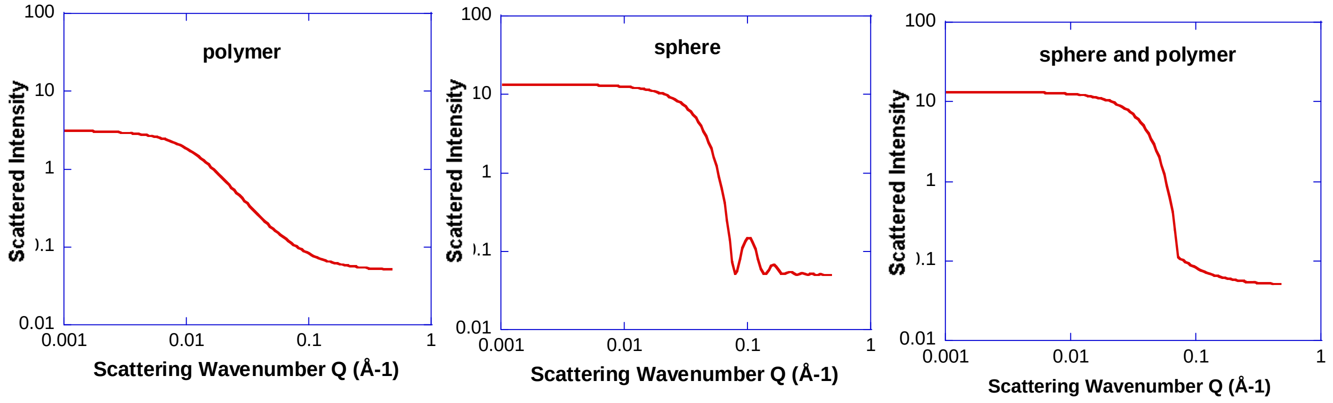




SANS from Pluronics Micelles



low temperature **high temperature**



Polymer Sphere Sphere and polymer

Single-Particle Form Factors and Inter-Particle Structure Factors

$I(Q) = (N_A/V)V_A^2 (b_A/v_A - b_B/v_B)^2 P(Q) S_I(Q)$

N_A: number of particles, V_A: particle volume, V: sample volume

$(b_A/v_A - b_B/v_B)^2$ = contrast factor

P(Q): single-particle structure factor

$S_I(Q)$: inter-particle structure factor

$$P(Q) = \left[\frac{3j_1(QR)}{QR}\right]^2 = \left[\frac{3}{QR}\left(\frac{\sin(QR)}{(QR)^2} - \frac{\cos(QR)}{QR}\right)\right]^2$$ for sphere of radius R.

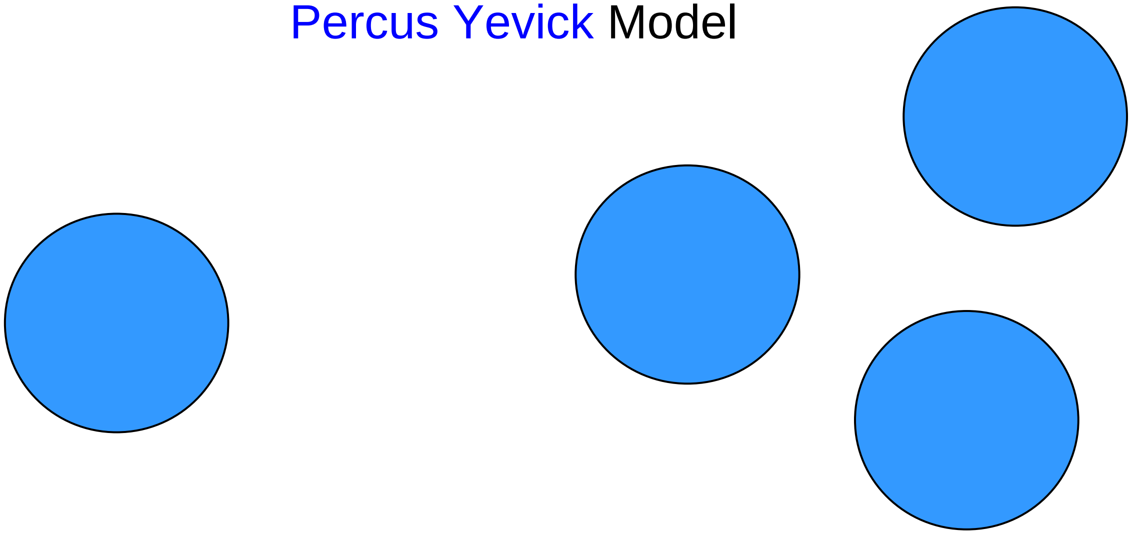
$$P(Q) = \frac{2}{Q^4 R_g^{\,4}}\left[\exp(-Q^2 R_g^{\,2}) - 1 + Q^2 R_g^{\,2}\right]$$ for polymer of radius of gyration R_g.

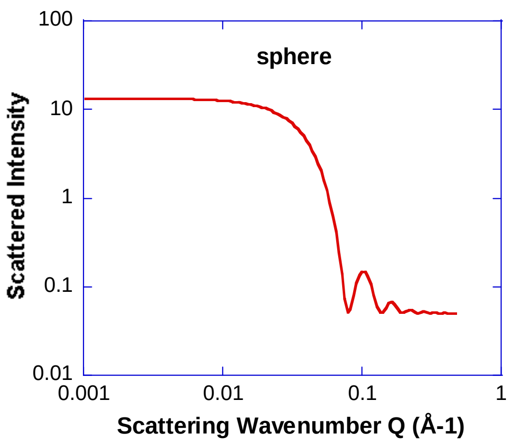
$S_I(Q)$ given by Percus Yevick model for solution of hard spheres.

$S_I(Q)$ given by the Random Phase Approximation model for polymer mixtures.

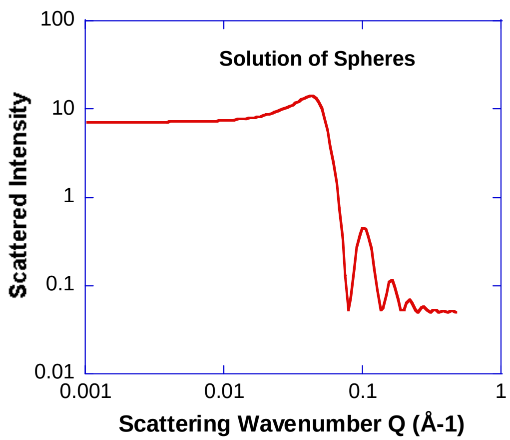
Solution of Spheres

Percus Yevick Model



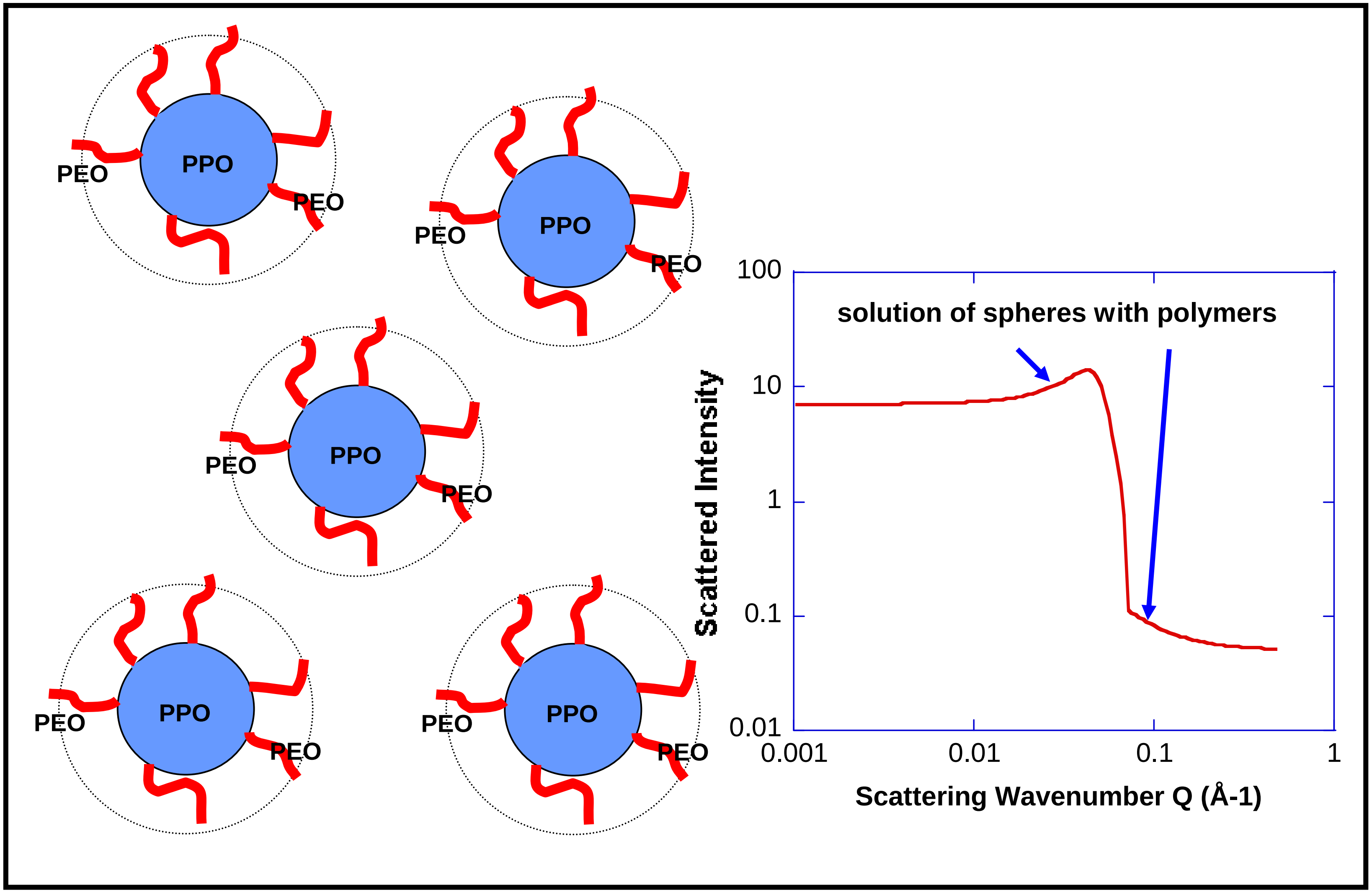


Single sphere



Solution of spheres

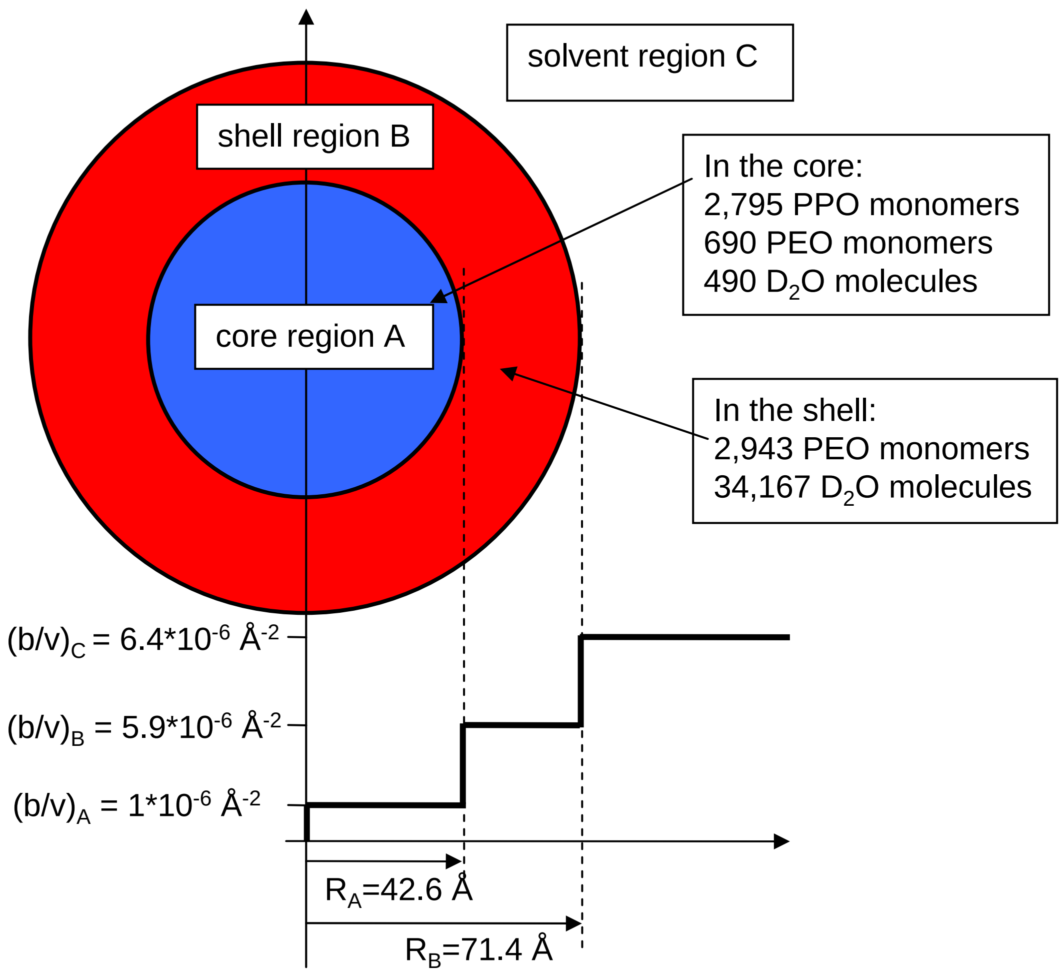
Solution of Spheres with Polymers



Fit SANS Data to a Model of Concentrated Core-Shell Particles

$$\frac{d\Sigma(Q)}{d\Omega} = \frac{N}{V}\left[\left(\frac{b_A}{v_A} - \frac{b_C}{v_C}\right)V_A \frac{3j_1(QR_A)}{QR_A} + \left(\frac{b_B}{v_B} - \frac{b_C}{v_C}\right)\left(V_{A+B}\frac{3j_1(QR_B)}{QR_B} - V_A \frac{3j_1(QR_A)}{QR_A}\right)\right]^2 S_I(Q)$$

10% P85 Pluronic/D_2O, 40 °C



2. POLYMER BLENDS THERMODYNAMICS

SANS Intensity:

$$I(Q) = \frac{d\Sigma(Q)}{d\Omega} = \left(\frac{b_1}{v_1} - \frac{b_2}{v_2}\right)^2 S(Q)$$

Thermodynamics:

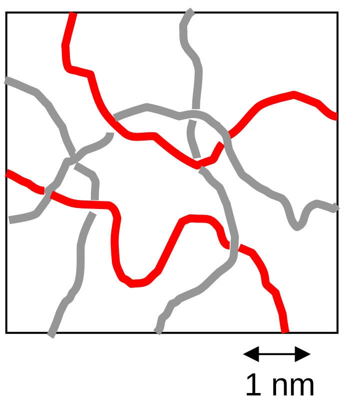
$$S^{-1}(Q=0) = \frac{1}{k_B T} \frac{\partial^2 G}{d\phi_1^{\,2}}$$

Gibbs Free Energy

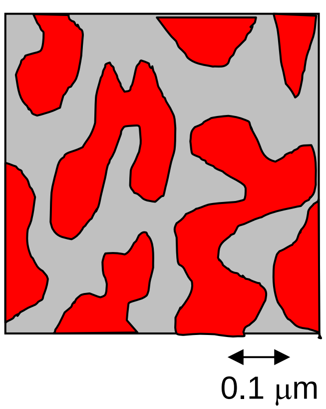
The Random Phase Approximation:

$$S^{-1}(Q) = \frac{1}{n_1\phi_1 v_1 P_1(Q)} + \frac{1}{n_2\phi_2 v_2 P_2(Q)} - 2\frac{\chi_{12}(T)}{v_0}$$

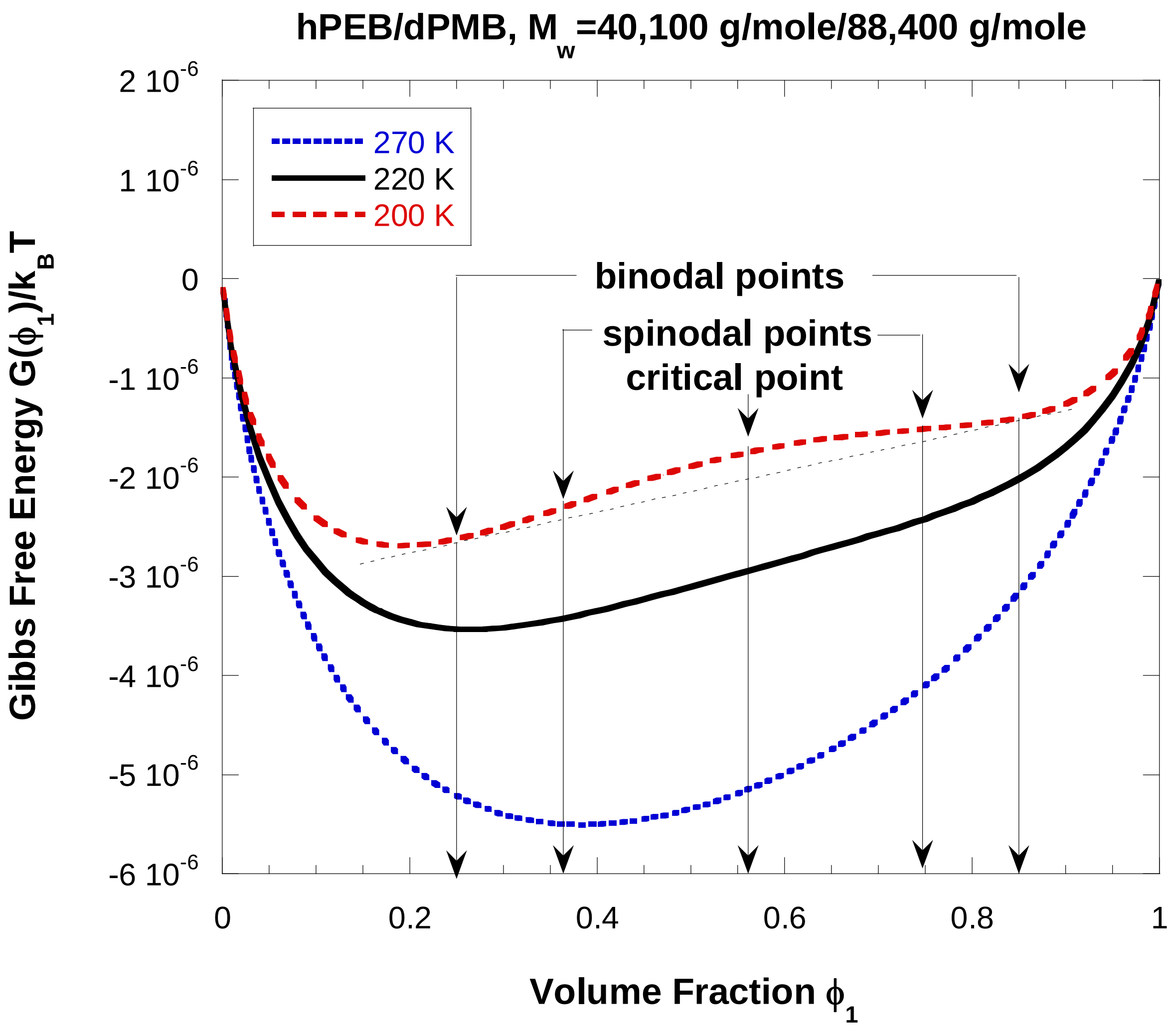
Mixed polymer blend



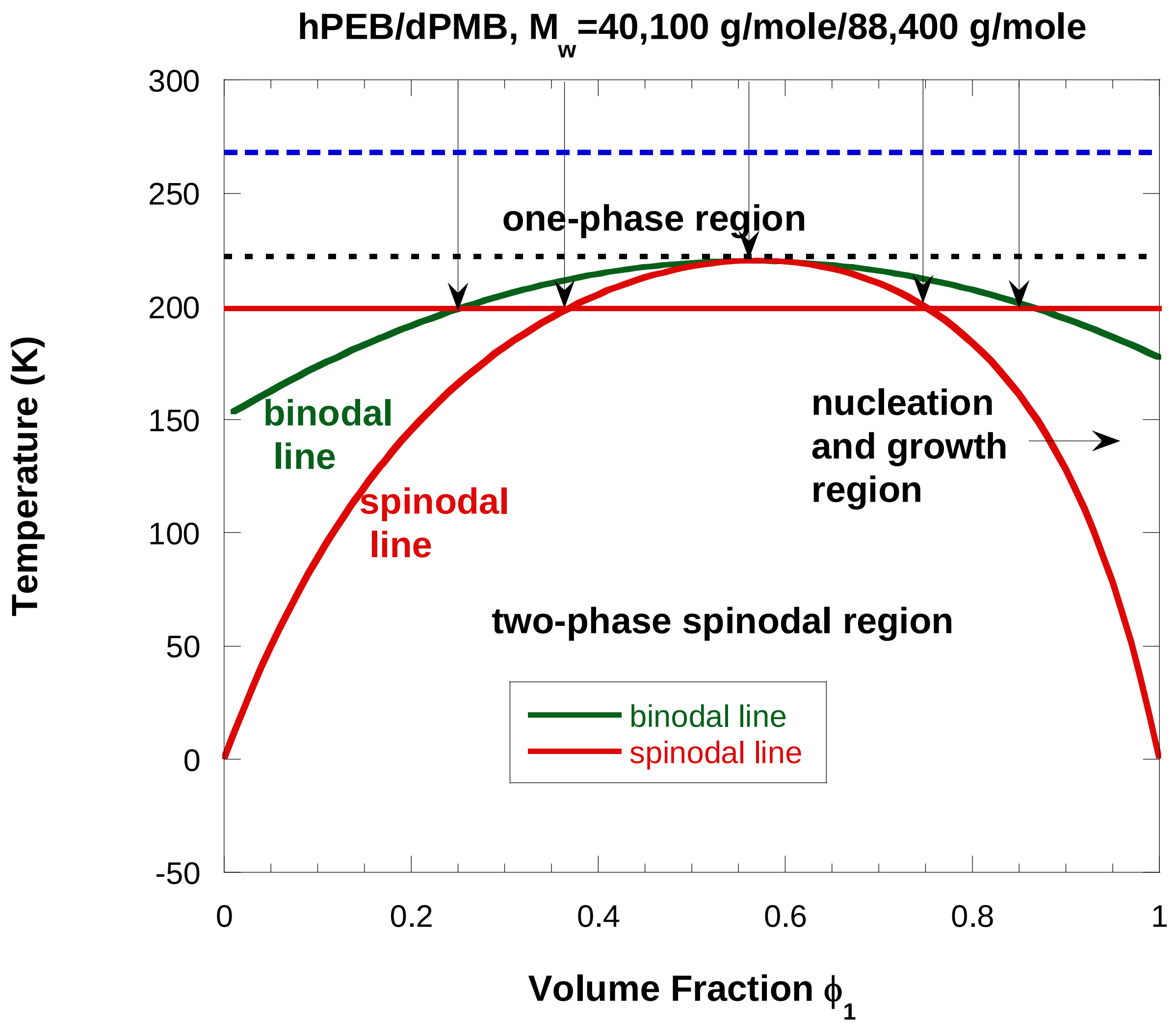
Phase separated blend



Gibbs Free Energy



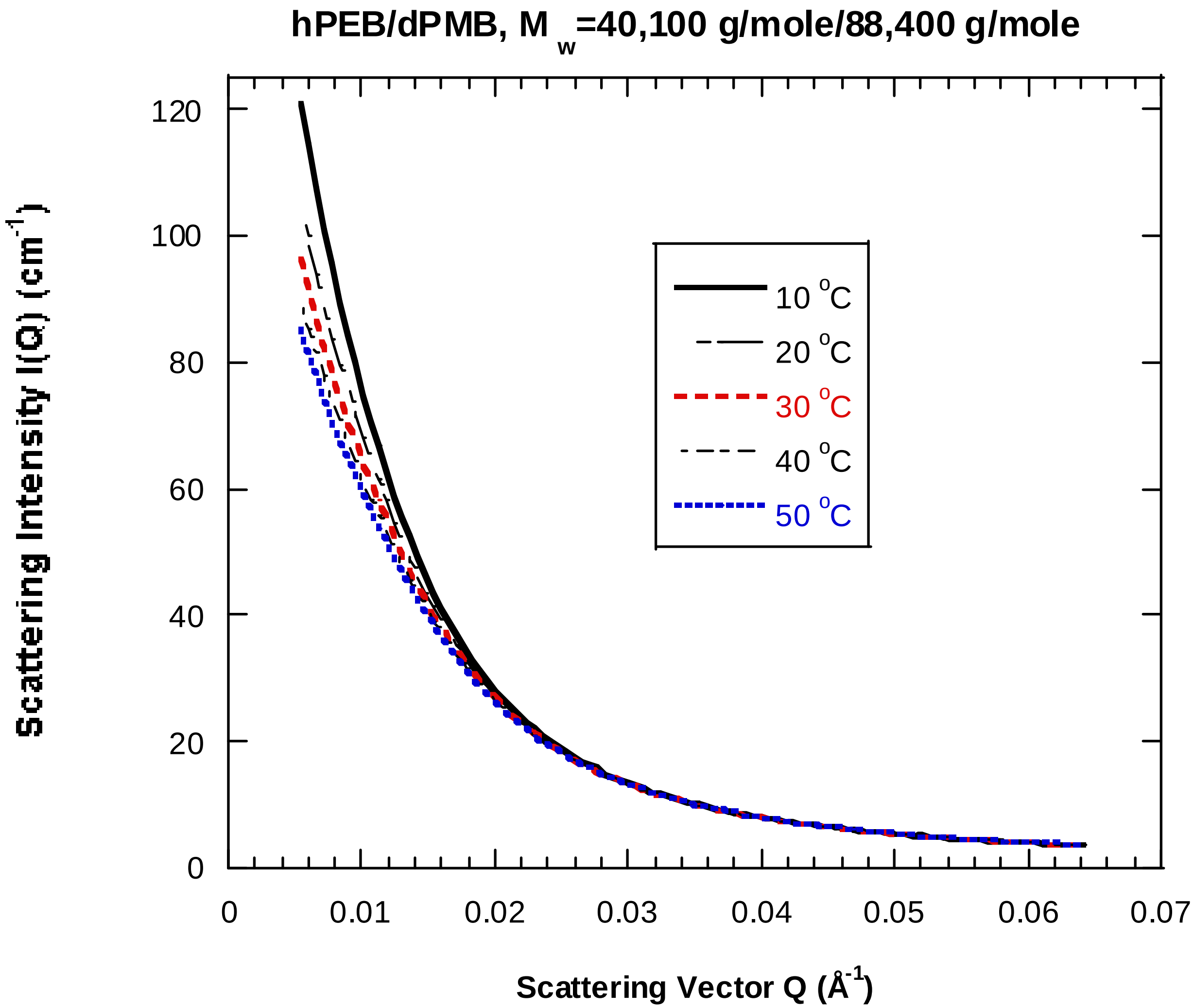
Phase Diagram



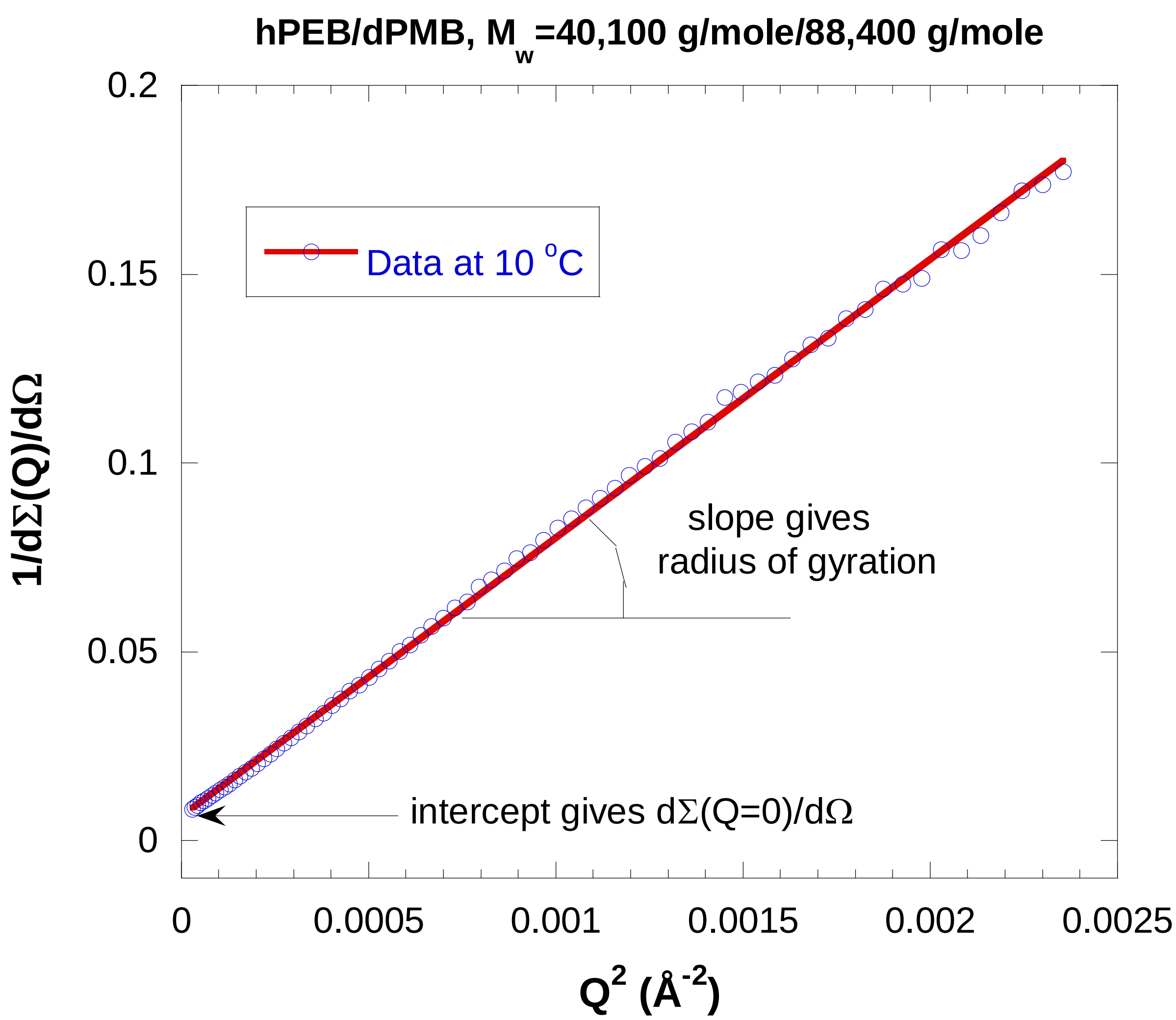
SANS From Polymer Blend Mixtures

Polymers:	Polyethylbutylene	/	Polymethylbutylene
	hPEB -(C_6H_{12})-	/	dPMB -($C_5H_5D_5$)-
Molecular Weights:	M_w=44,100 g/mole		M_w=88,400 g/mole
Volume Fractions:	ϕ_{hPEB}=0.57		ϕ_{dPMB}=0.43

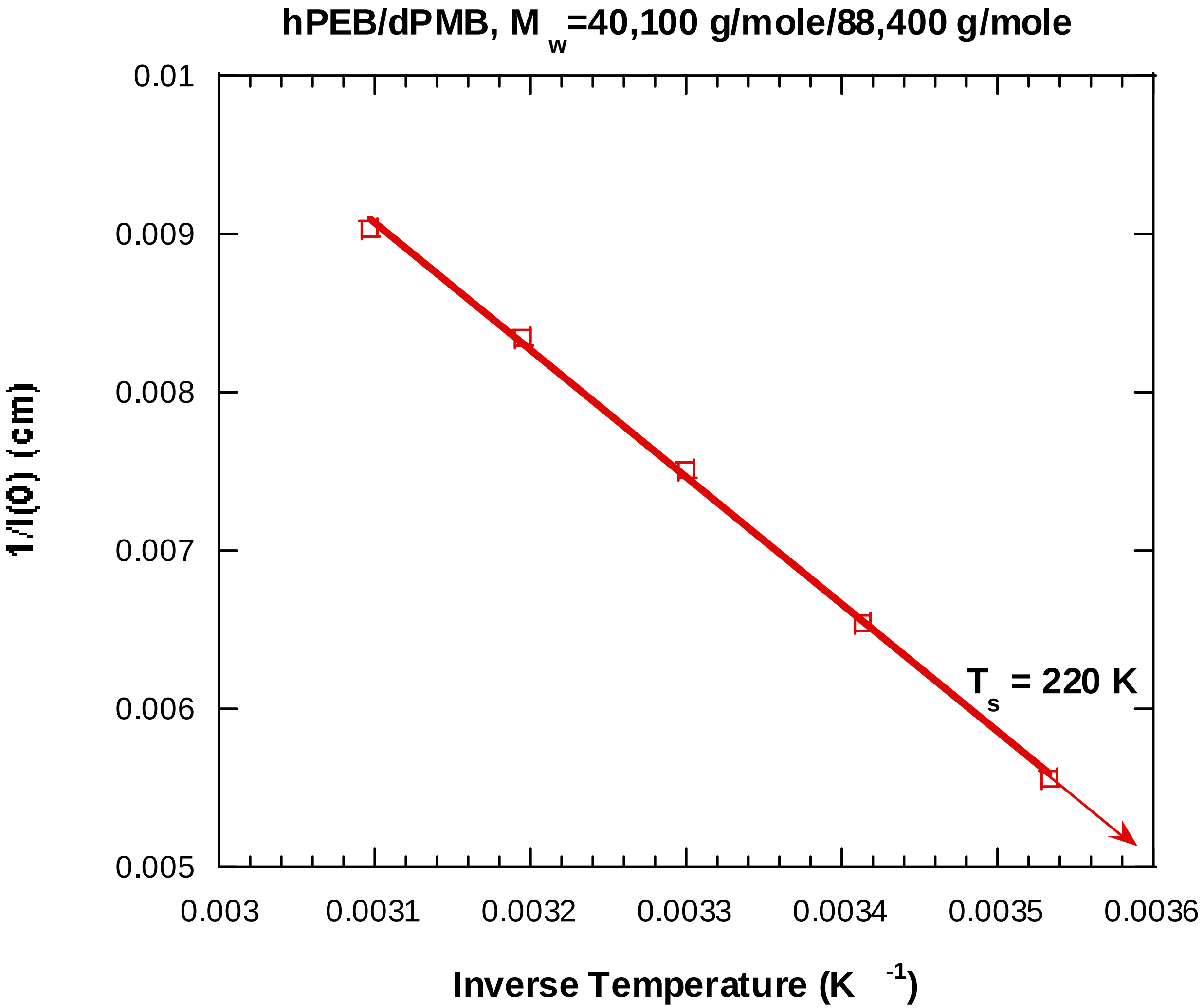
SANS Data


hPEB/dPMB, Mw=40,100 g/mole/88,400 g/mole
Scattering Intensity I(Q) (cm-1)
Scattering Vector Q (Å-1)
0
20
40
60
80
100
120
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
10 oC
20 oC
30 oC
40 oC
50 oC

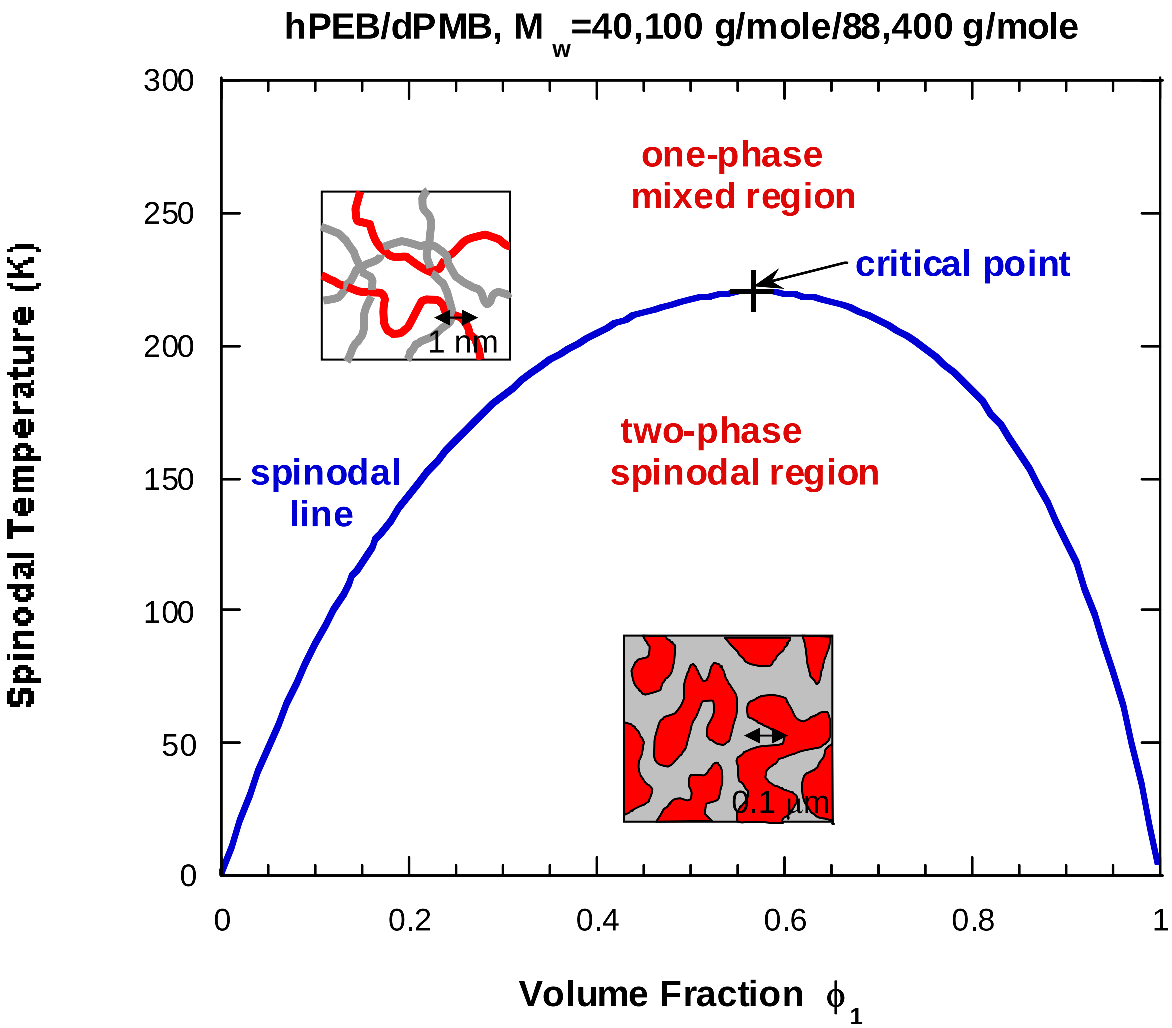
The Zimm Plot



Spinodal Temperature



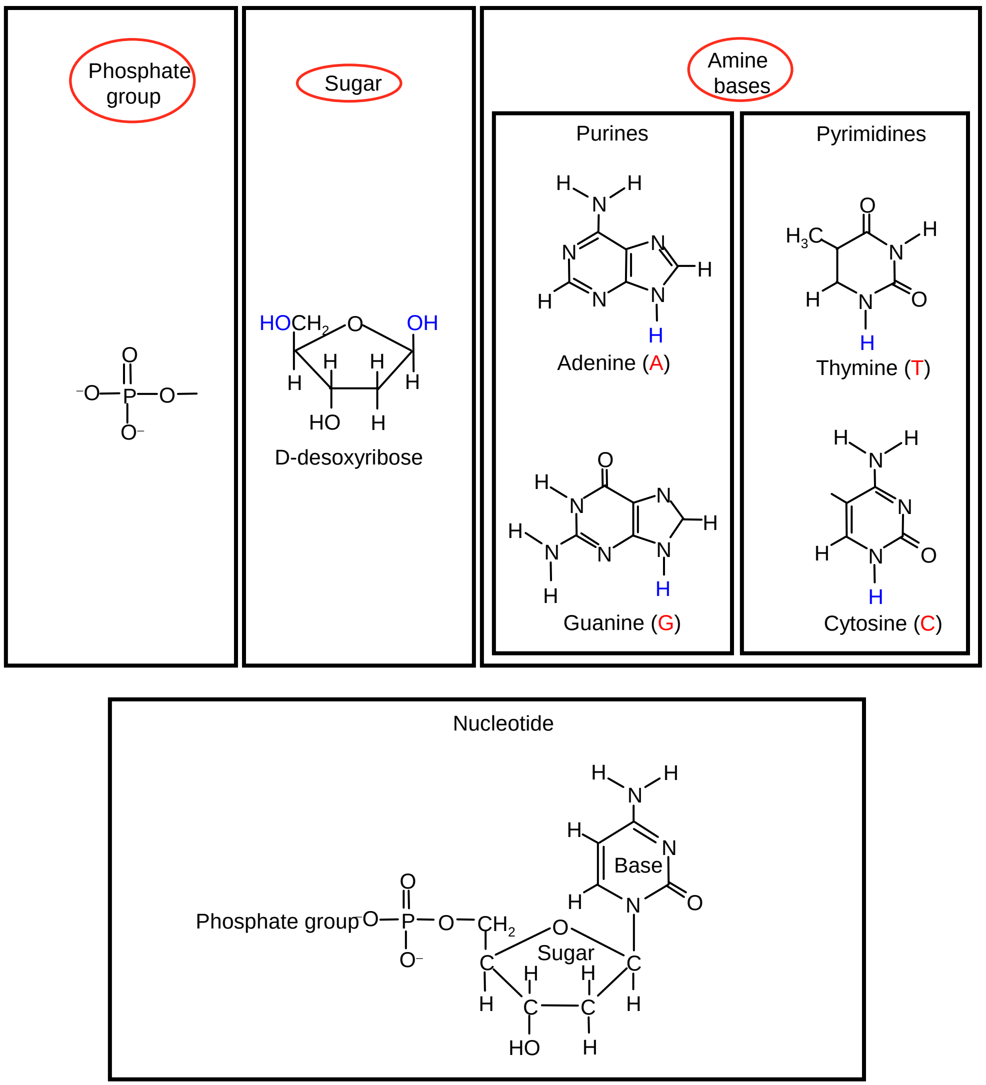
Spinodal Temperature



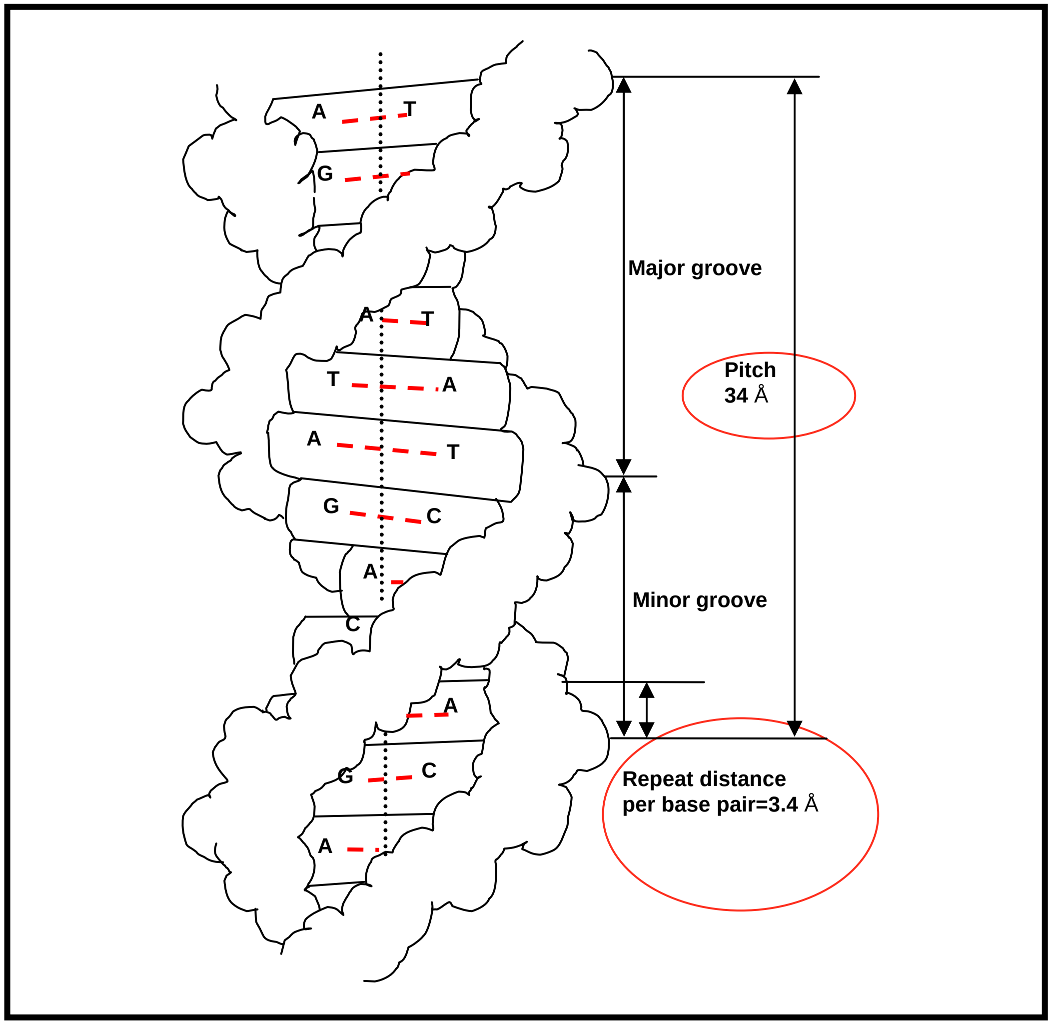
3. HELIX-TO-COIL TRANSITION IN DNA

DNA is the basic building block for life. It encodes for the synthesis of proteins.

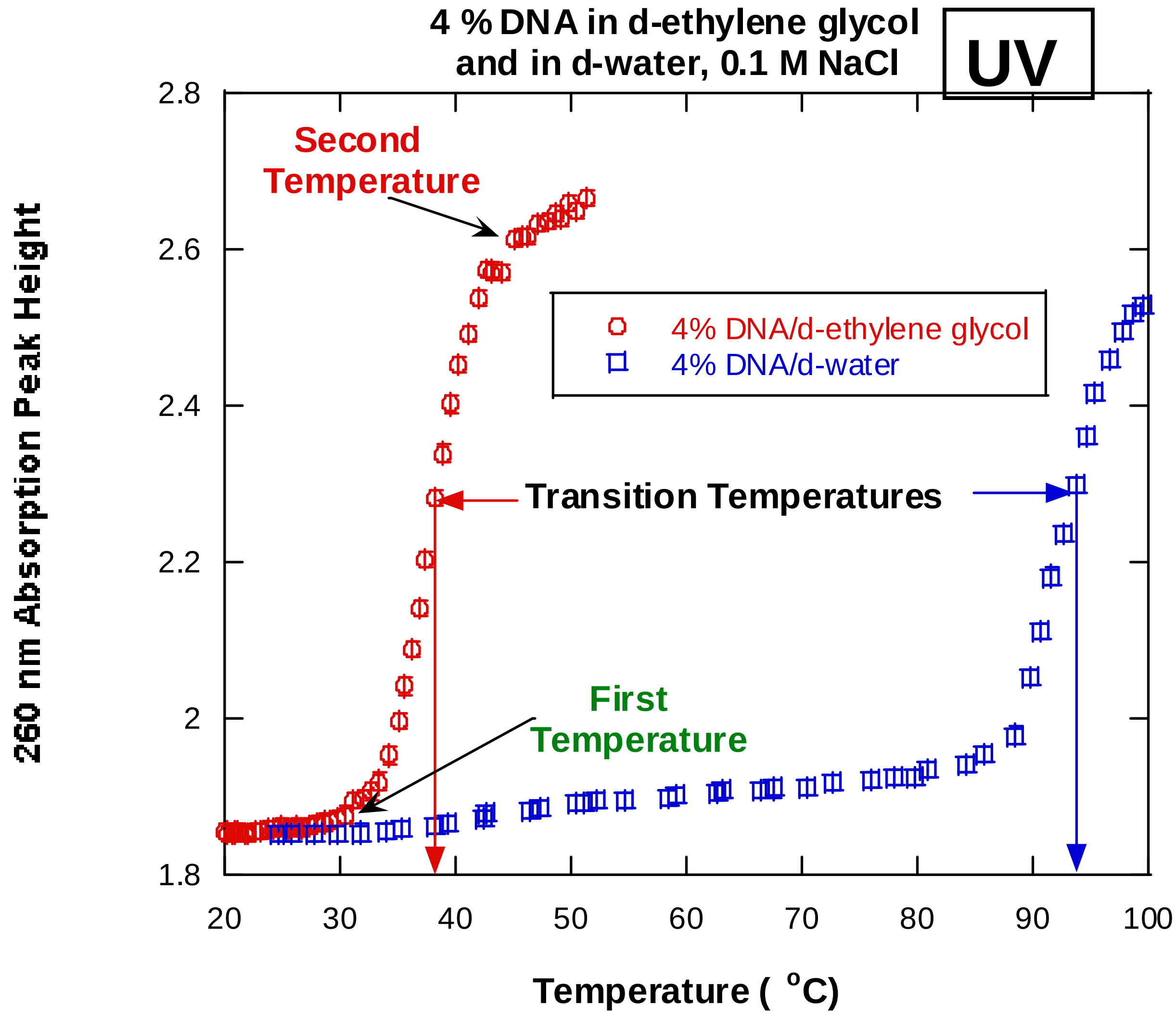
THE DNA MOLECULE



The DNA Helix

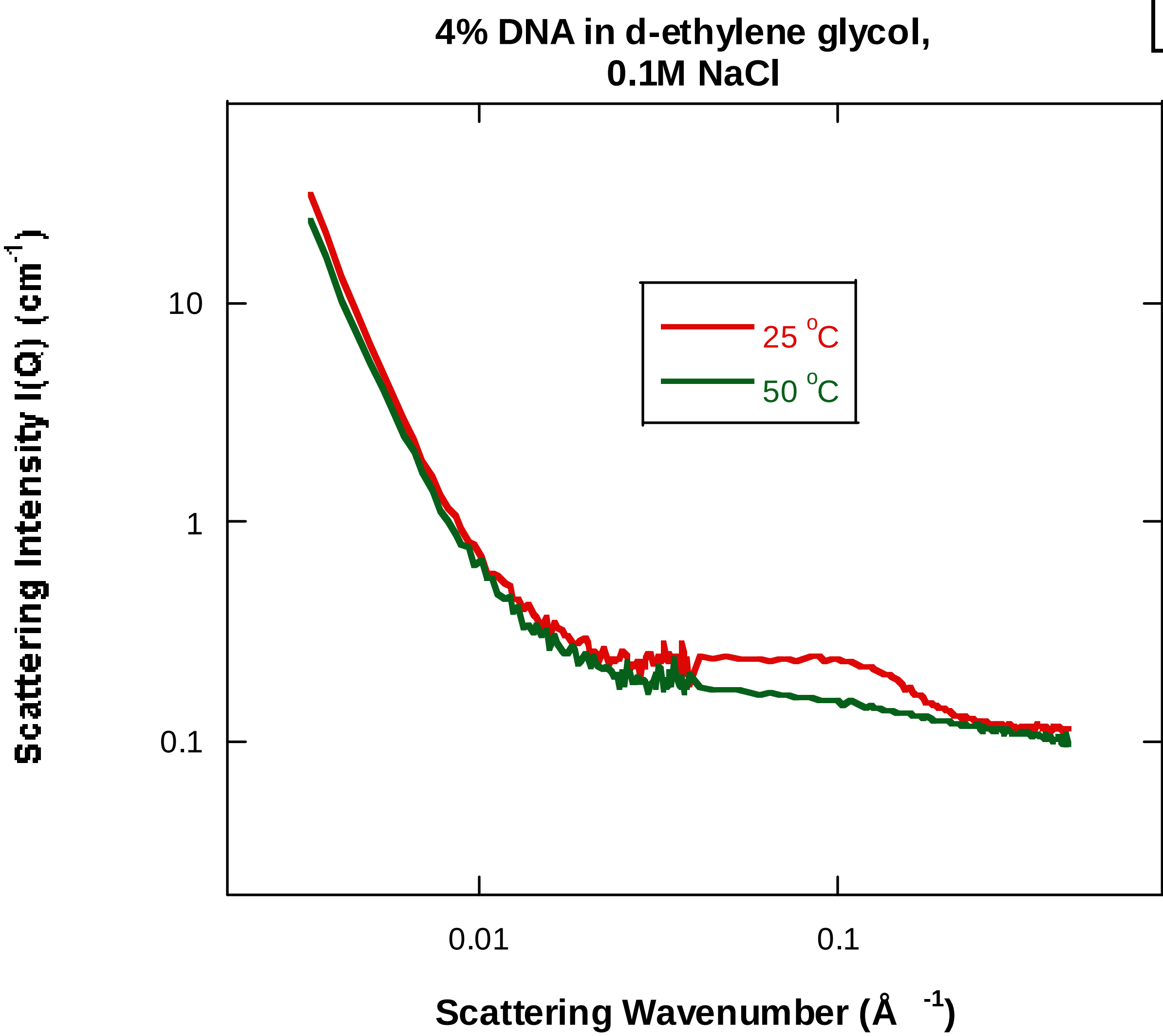


Helix-to-Coil Transition in DNA

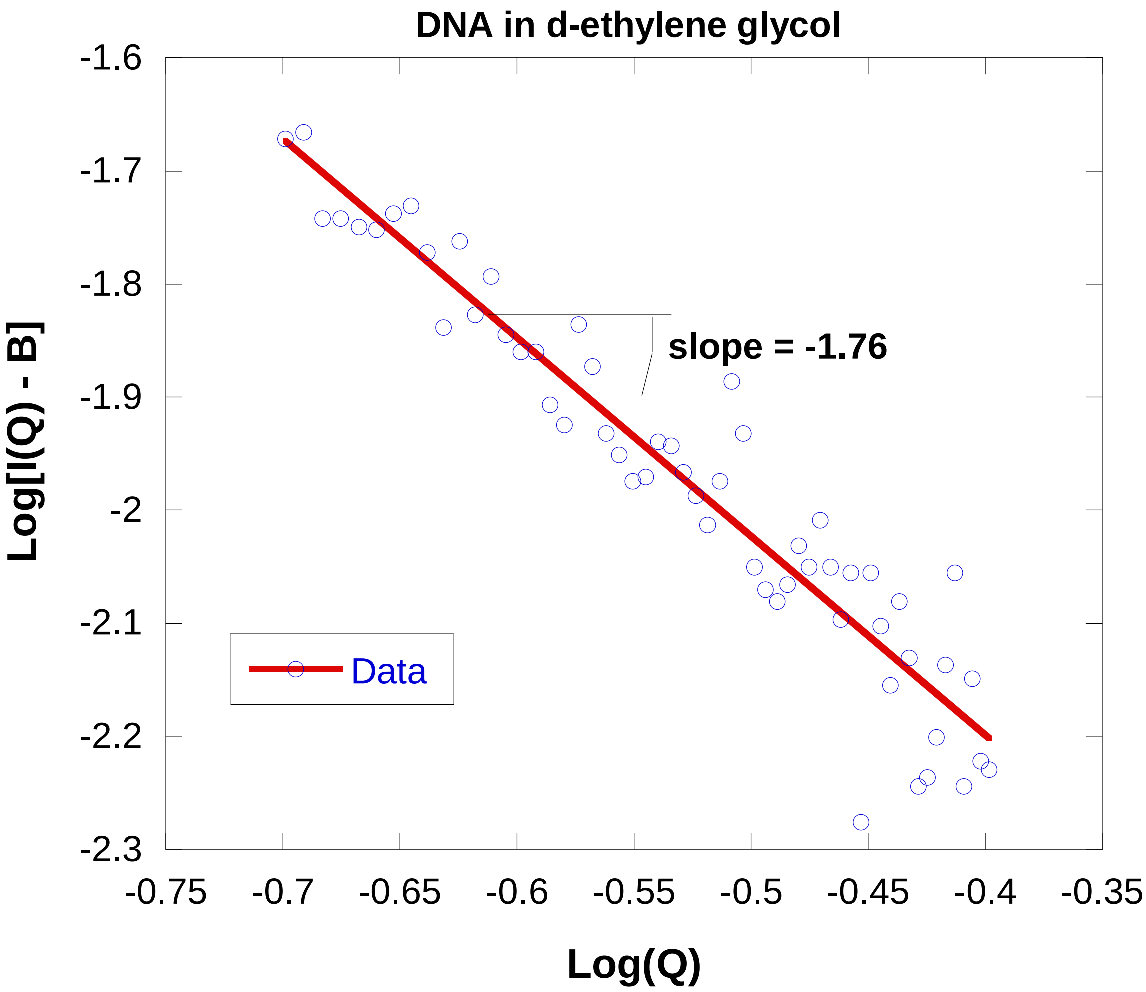


SANS Data

SANS



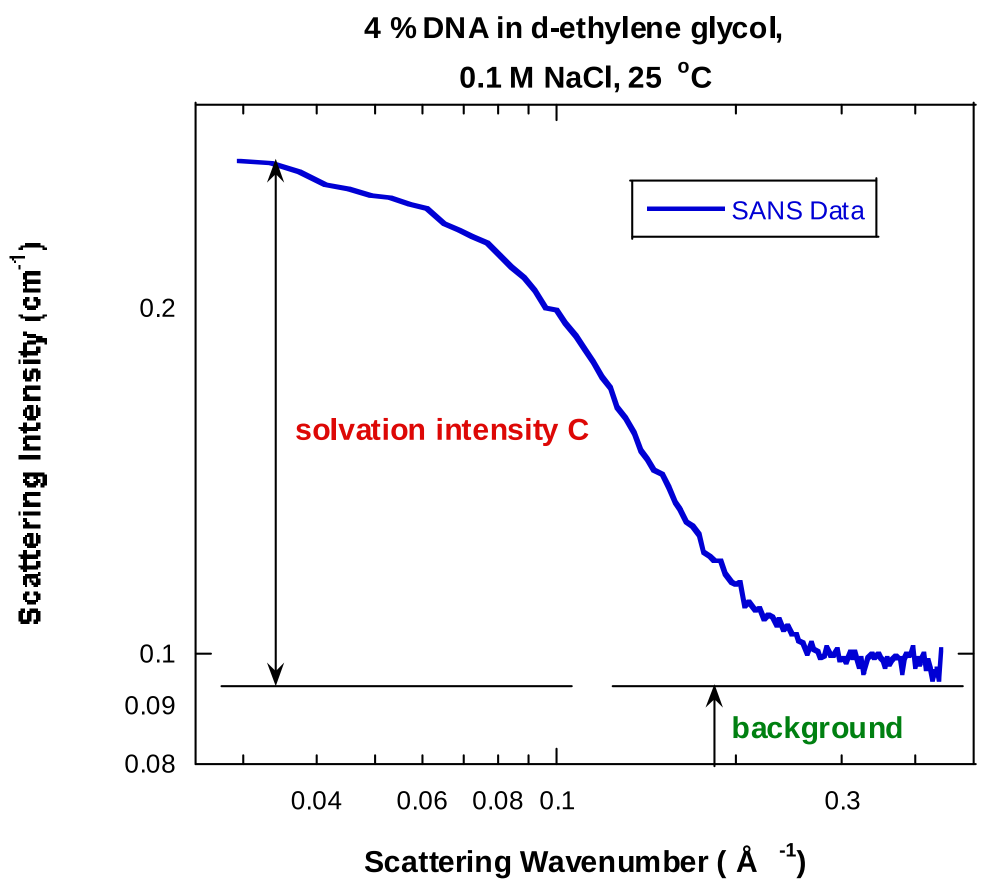
The Porod Plot $I(Q) \sim C/Q^m$



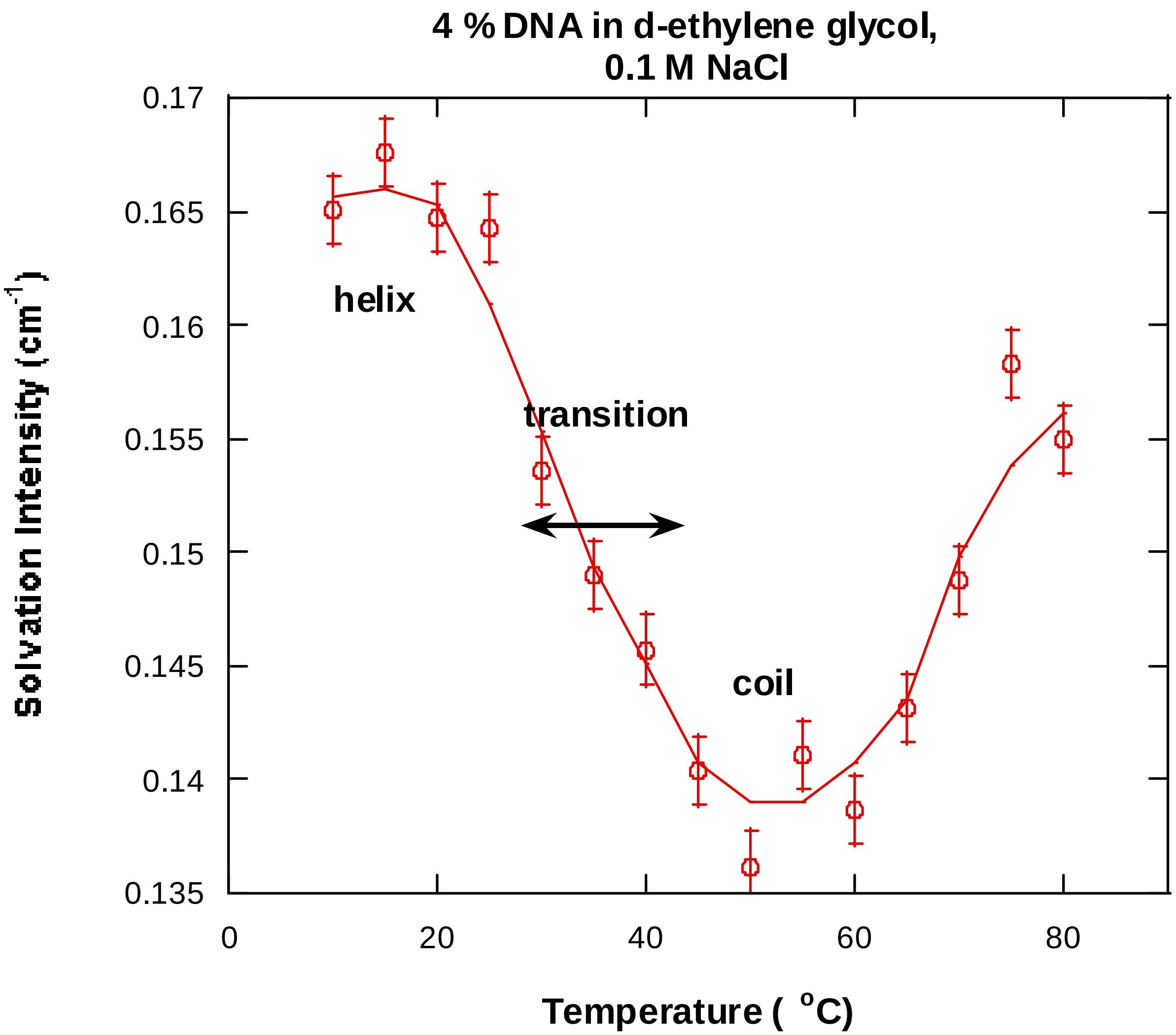
Nonlinear Least-Squares Fit

Functional form: $I(Q) = \mathbf{C}/[1+(Q\mathbf{L})^{\mathbf{m}}]$ + Background

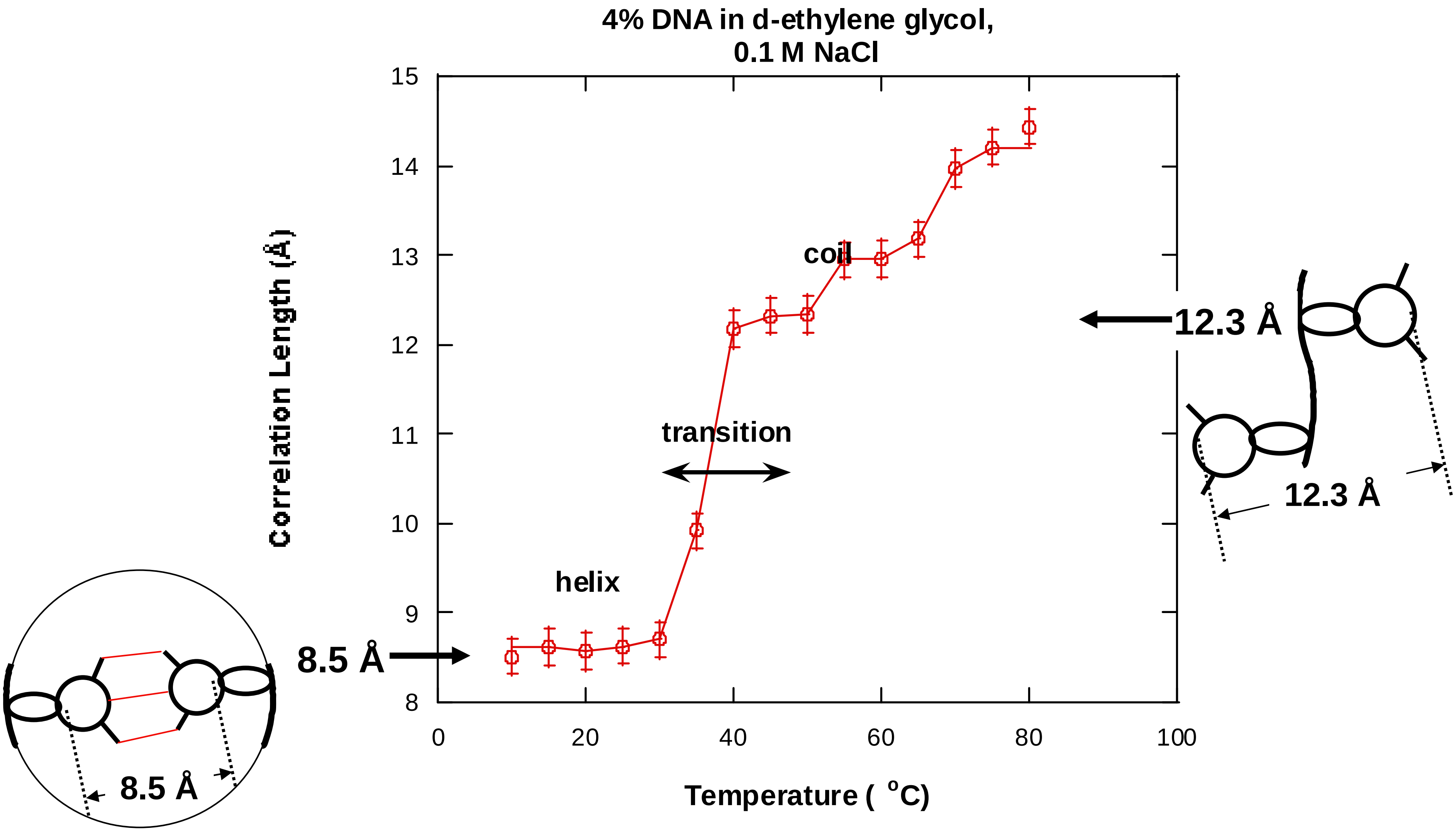
C: solvation intensity
L: correlation length
m: Porod exponent



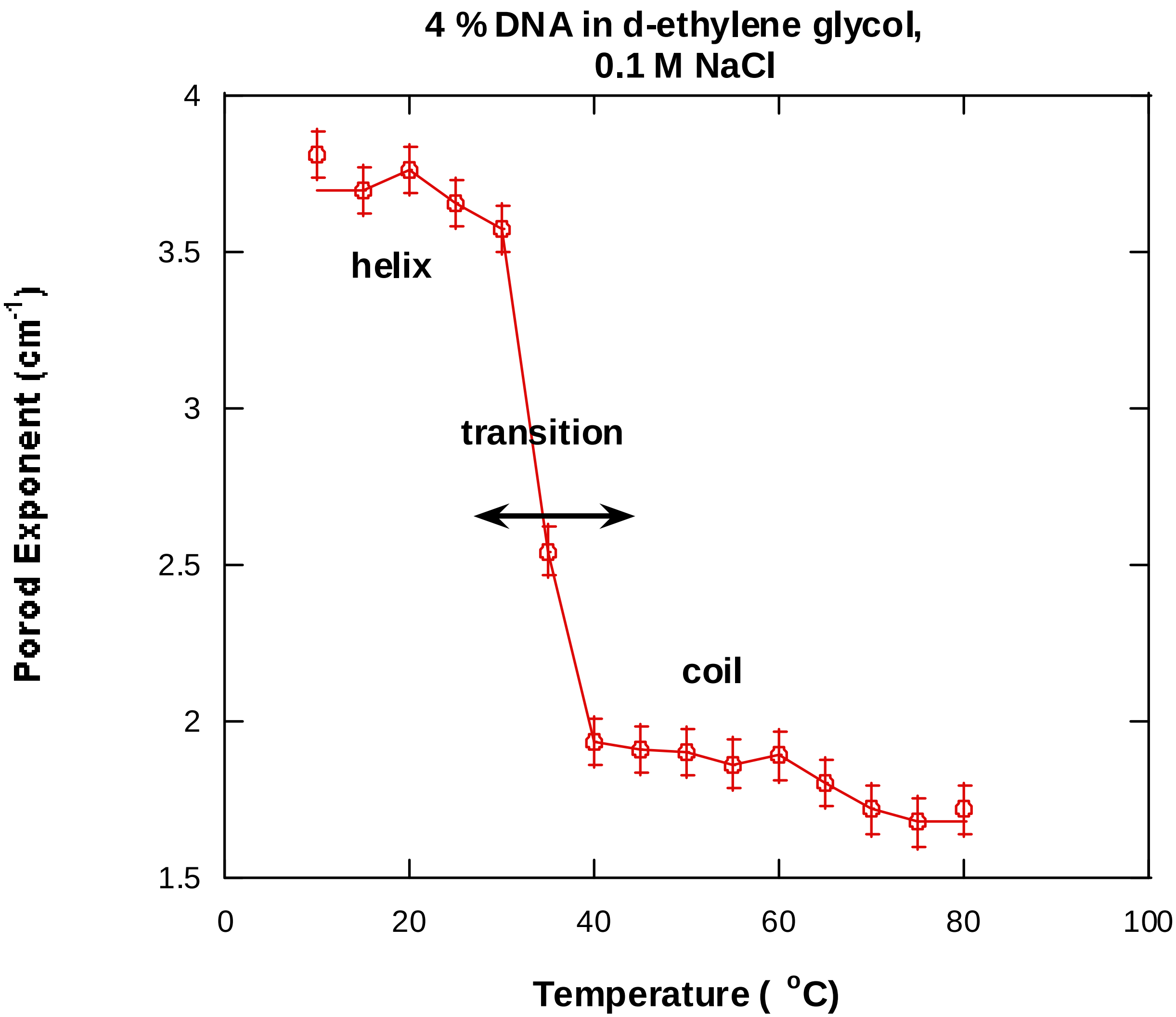
The Solvation Intensity



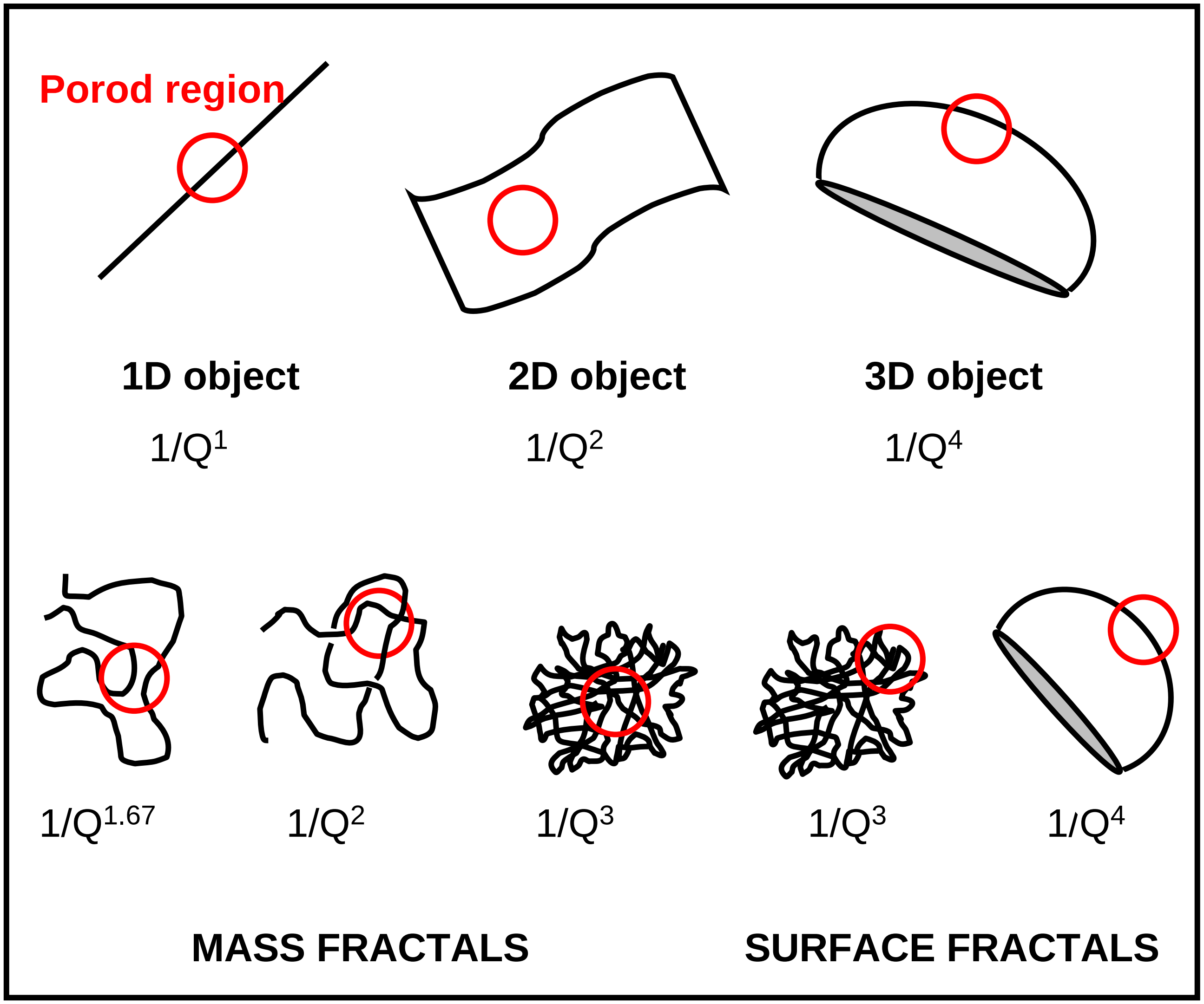
The Correlation Length



The Porod Exponent



POROD EXPONENTS



CONCLUSIONS

-- The SANS technique is a valuable characterization method.

-- SANS has been effective in complex fluids, polymers, biology, etc.

-- SANS can determine structures, phase transitions, and morphology.

-- The NIST SANS gets over 200 users per year, resulting in over 70 publications per year.

ACKNOWLEDGMENTS

NSF-DMR, Steve Kline, Nitash Balsara, David Worcester.

PROBING NANOSCALE STRUCTURES –THE SANS TOOLBOX

http://www.ncnr.nist.gov/staff/hammouda/the_SANS_toolbox.pdf