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Modelling Data – Better Approaches
How to get useful information?

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Monolayers – Simple Interpretation

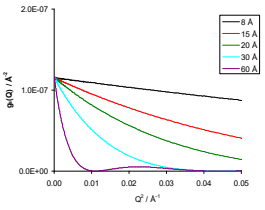
Define $g_s(Q_z)$ in terms of measured reflectivity and $R_F(Q_z)$ (the Fresnel reflectivity for perfectly sharp interface):

$g_s(Q) = Q^2 (R - R_F) / (1 - R)$

$\ln g_s(Q) \approx -t^2 Q^2 /12$

Roughly $\ln (Q^2 R) \approx -t^2Q^2/12$

Contrast match of two bulk phases $R_F(Q) = 0$



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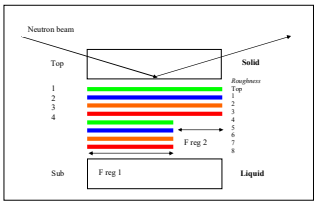
Real Interfaces are not just layers

Slab models are easy to calculate but people are not very interested in just thickness and scattering length density



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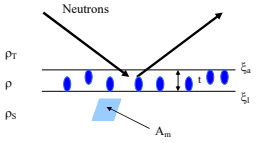
Surface Excess and Area per Molecule

Volume per molecule: V_m
Scattering length: b_m
Scattering length density:
$\rho = b_m / V_m$

Thickness of layer: t
Scattering length density ρ
Area per molecule: A_m
$V_m = t A_m$
Scattering length density:
$\rho = (b_m / V_m) = b_m/(t A_m)$

Area per molecule: $A_m = b_m / t \rho$



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Adsorption of Surfactant

Surface active molecules
Amphiphilic
Bind to surface – how?
What are properties?

Hexadecyl trimethyl ammonium bromide
$C_{16}H_{33}N(CH_3)_3^+ Br^-$

Tail Head

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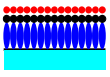
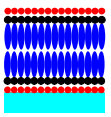
Some Possible Structures

- Monolayer



- Bilayer



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Cationic Surfactant

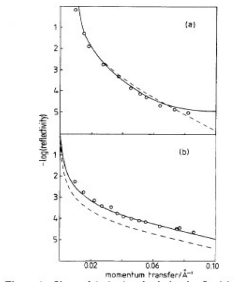
CTAB at 27° C on amorphous SiO_2

(a) D_2O (b) $cmSiO_2$ at 6 ×10^{-4} M

Models

Solid line – Bilayer

Dashed line - Monolayer



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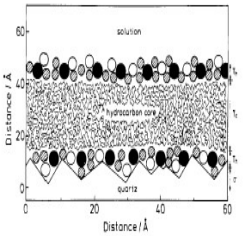
Cationic Surfactant

- **CTAB** 27 C on SiO_2
- Label heads & tails

Head 6 +/- 2 Å
Tail 28 +/- 4 Å
Roughness ~ 8 Å
Fractional Coverage
35% at 3 ×10^{-4} M
80% at 6 ×10^{-4} M



Langmuir **6**, 1031-1034 (1990).
J. Colloid Interf. Sci. **162**, 304-310 (1994).

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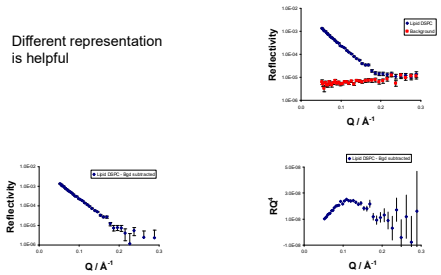
Plotting Data

Different representation is helpful



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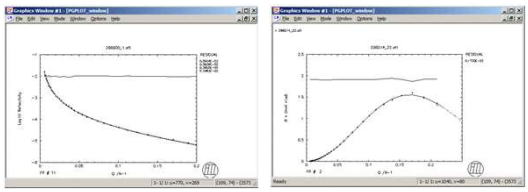
How to Look at Data?



Log_{10} R vs Q

RQ^4 vs Q

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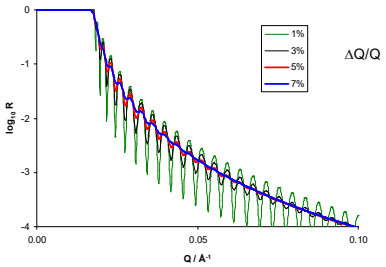
Effects of Resolution



Silicon substrate: film thickness 1500 Å
scattering length density 6.3 × 10^{-6} $Å^{-2}$

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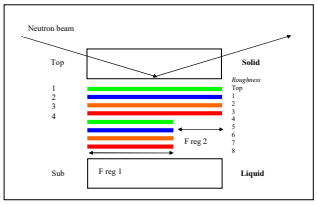
Non-Uniform Surfaces

If you have patches of different layers at an interface do you average the density or average the reflectivity?



What is the coherence length of a neutron?

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Describing Polymers

- Interdiffusion – is this roughness?
- Brushes – parabolic density profile

(E. P. K. Currie et al *Physica* B, **283** 17 – 21)

- Other scaling laws e.g. O. Guiselin *J. Phys.* **50**, 3407-3425 (1989).

We expect smooth profiles!

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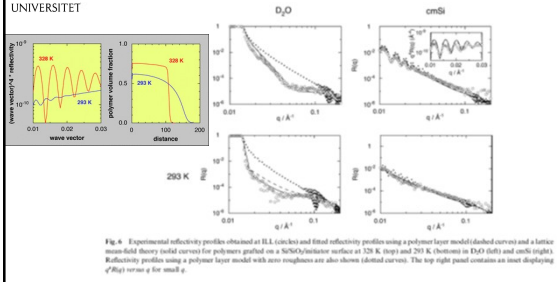
Thermoresponsive polymer brush



J. Zhang, et al., *Soft Matter*, 4, 500–509 (2008).

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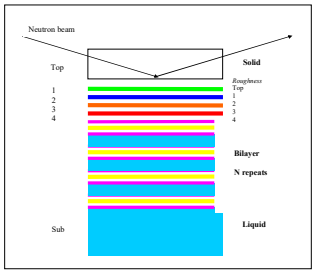
Repeating Layers

A one dimensional crystal

Bragg's law

Intensity of peaks may Depend on size and disorder



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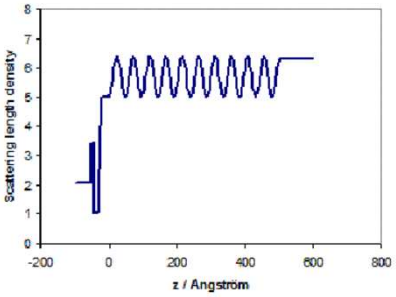
Calculate reflectivity for a profile



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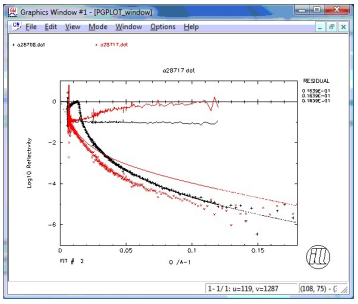
Using Multiple Contrasts



Simultaneous fits for multiple data sets

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More Ideas

www.reflectometry.net

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