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Off-specular Scattering, GISANS, Near-surface SANS

Adrian R. Rennie

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SANS and GISANS

- Transmission geometry SANS is usually a simpler experiment
- In principle, calculations are identical

BUT

Geometry and Multiple Scattering are important

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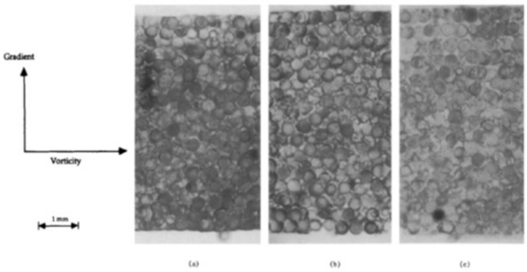
Interfaces are 3-dimensional



Understanding rheology – shear flow

Brown et al. *Progress in Colloid and Polymer Science* **98**, (1995) 99-102.

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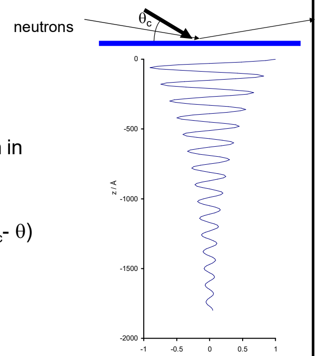
Evanescent Wave



Below k_c no travelling wave enters the sample

Amplitude decays with depth in sample

Decay length depends on $(\theta_c - \theta)$

Evanescent wave can cause scattering

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Looking at Materials

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Looking at Materials

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Off-specular & Reflection

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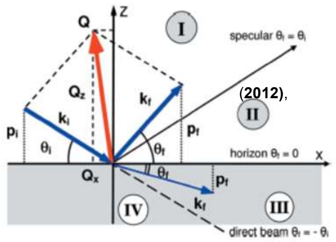

$Q_z \approx (2\pi/\lambda)\,(\theta_i + \theta_f)$

$Q_x \approx (2\pi/\lambda)\,(\theta_i + \theta_f)\,(\theta_i - \theta_f)$

Frédéric Ott, Sergey Kozhevnikov 'Off-specular data representations in neutron reflectivity', J. Appl. Cryst. 44, (2011), 359-369.

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What does background look like?

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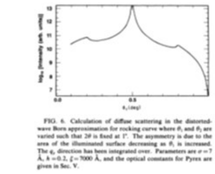
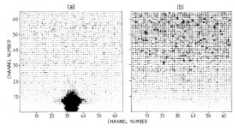
X-ray scattering – glass

Sinha et al., *Phys. Rev. B.* **38**, 2297, 1988.



Neutron scattering from D_2O and from null reflecting water

Rennie et al., *Macromolecules* **22**, 3466-3475 (1989).



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Scattering from Surface Structures

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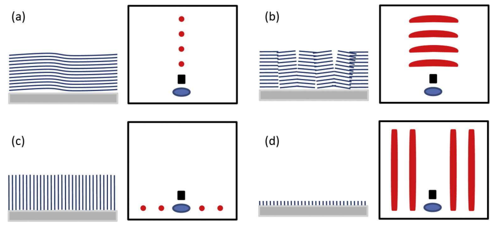

Peter Müller-Buschbaum 'GISAXS and GISANS as metrology technique for understanding the 3D morphology of block copolymer thin films' *European Polymer Journal* **81**, (2016), 470-493.

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Strong Off-specular Scattering

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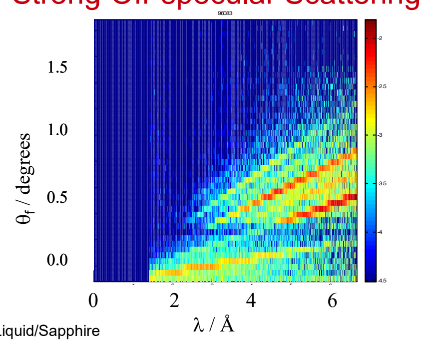

PS latex in D_2O Liquid/Sapphire

10% vol. dispersion, Radius ~350 Å. Sapphire substrate, θ_i = 0.35 deg

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PS latex in D_2O Liquid/Sapphire

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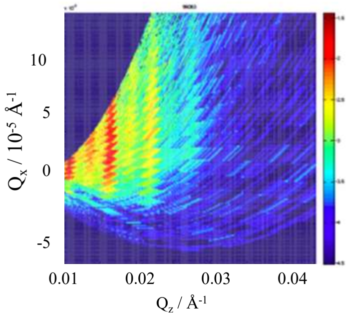
Transform to map of Q_zQ_x



10% vol. dispersion, Radius ~350 Å, sapphire substrate, θ_i = 0.35 deg

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Some Scattering at Interfaces

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X-ray scattering – glass

Sinha et al., *Phys. Rev. B.* **38**, 2297, 1988.

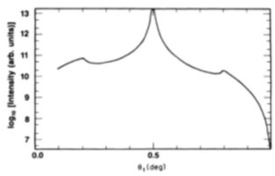

FIG. 6. Calculation of diffuse scattering in the distorted-wave Born approximation for rocking curve where θ_i and θ_f are varied such that 2θ is fixed at 1°. The asymmetry is due to the area of the illuminated surface decreasing as θ_i is increased. The q_y direction has been integrated over. Parameters are $\sigma = 7$ Å, $h = 0.2$, $\xi = 7000$ Å, and the optical constants for Pyrex are given in Sec. V.

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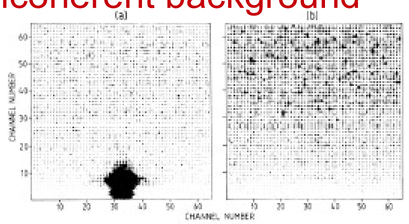
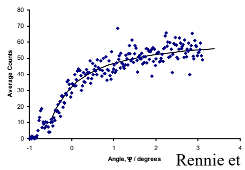
Incoherent background





Scattering from D_2O

and from null reflecting water

(8% D_2O)

Rennie et al., *Macromolecules* **22**, (1989), 3466-3475.

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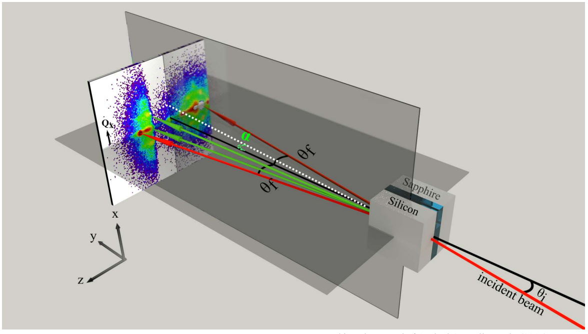
Interfacial structure: GISANS



Nouhi et al. *Journal of Applied Crystallography* (2017)

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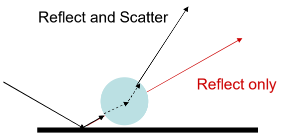
Calculating Scattering

Distorted Wave Born Approximation (DWBA)

Simply allow for sequential events e.g.

Reflection then Scattering
Refraction then Scattering
Scattering then Reflection



Reflection followed by weak scattering.

(a) Optical Matrix Calculation

(b) Weak Scattering (Born approximation)

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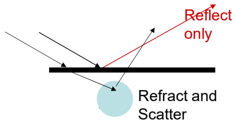
Calculating Scattering

Distorted Wave Born Approximation (DWBA)

Simply allow for sequential events e.g. for buried interface



Refraction followed by weak scattering.

(a) Optical Matrix Calculation

(b) Weak Scattering (Born approximation)

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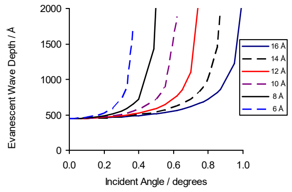
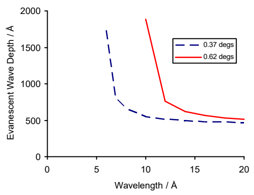
How deep is the evanescent wave?





Silicon/D_2O Interface

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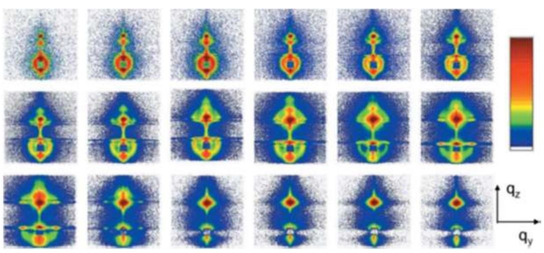
Copolymer films



P. Müller Buschbaum *et al. J. Appl. Cryst.* **47**, (2014), 1228–1237

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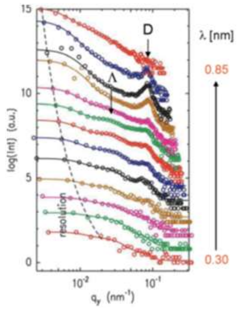
Changes with Depth

Horizontal cuts

- Used wavelength to probe different depths
- Longer wavelength looks neare the surface



J. Appl. Cryst. **47**, (2014), 1228–1237

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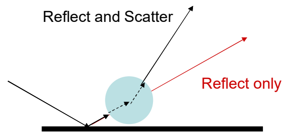
Calculating Scattering

Distorted Wave Born Approximation (DWBA)

Simply allow for sequential events e.g.

Reflection then Scattering
Refraction then Scattering
Scattering then Reflection



Reflection followed by weak scattering.

(a) Optical Matrix Calculation
(b) Weak Scattering (Born approximation)

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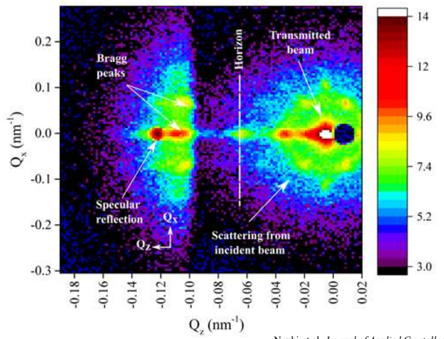
Diffraction from Surface Layers



Nouhi et al. *Journal of Applied Crystallography* (2017)

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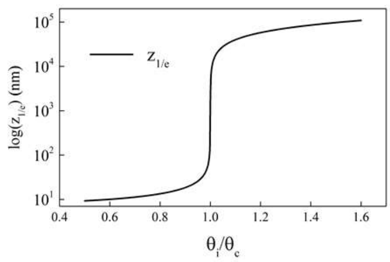
Penetration depth

$$z_{1/e} = \sqrt{2}\lambda \Big/ 4\pi\left[\sqrt{(\theta_i^2-\theta_c^2)^2+(\frac{\lambda}{2\pi}\mu)^2}-(\theta_i^2-\theta_c^2)\right]^{1/2}$$

A depth sensitive technique:

Wavelength
Incident angle



Nouhi et al. *Journal of Applied Crystallography* (2017)

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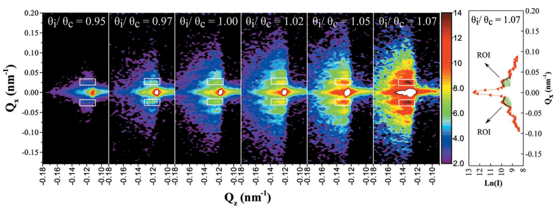
Data at different angles



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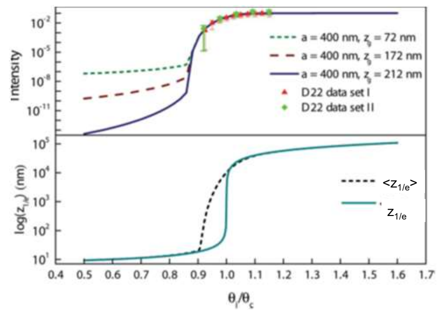
Data at different angles



Nouhi et al. *Journal of Applied Crystallography* (2017)

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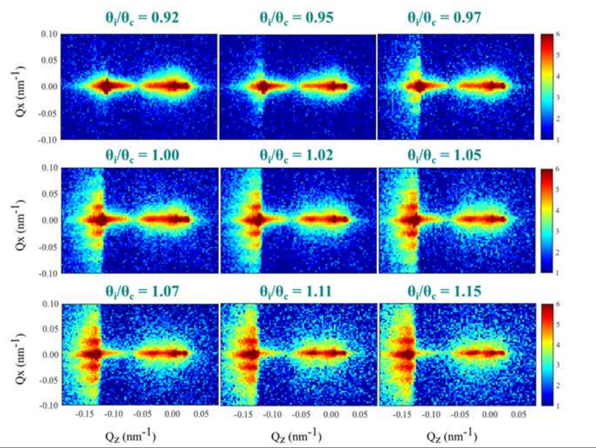

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Scattering at Interfaces

- Off-specular scattering
- Near Surface SANS
- GISANS

What is the difference?

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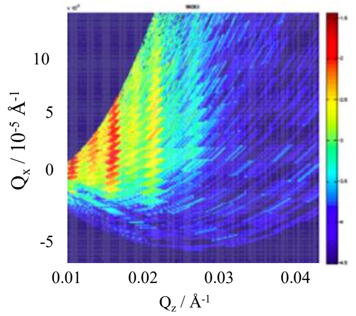
PS latex in D_2O Liquid/Sapphire

Transform to map of Q_zQ_x



10% vol. dispersion, Radius ~350 Å, sapphire substrate, θ_i = 0.35 deg

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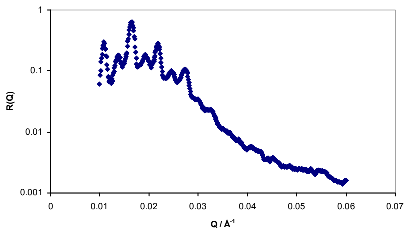
PS latex in D_2O – sapphire surface

Sum along Q_x



10% vol dispersion, 0.35

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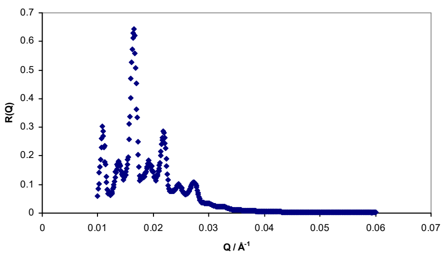
PS latex in D_2O – sapphire surface

Sum along Q_x



10% vol dispersion, 0.35

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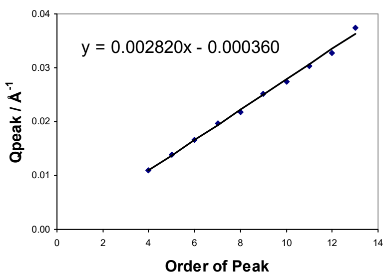
PS latex in D_2O – sapphire surface

Assign Bragg peaks (index)

Q_1 = 0.00282 Å^{-1}

d = 2230 Å

3 first peaks outside range



10% vol dispersion, 0.35, 0.8 and 1.5 deg

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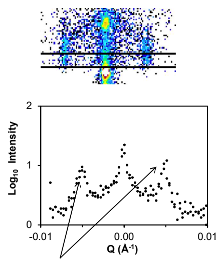
Compare Qx and Qz



M. S. Hellsing, et al. *Applied Physics Letters*, **100**, (2012), 221601.

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