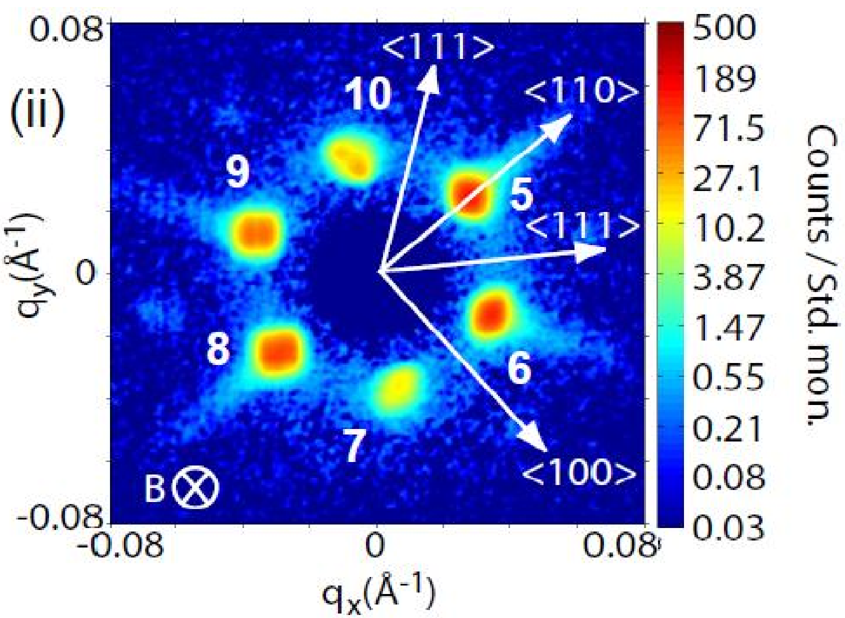
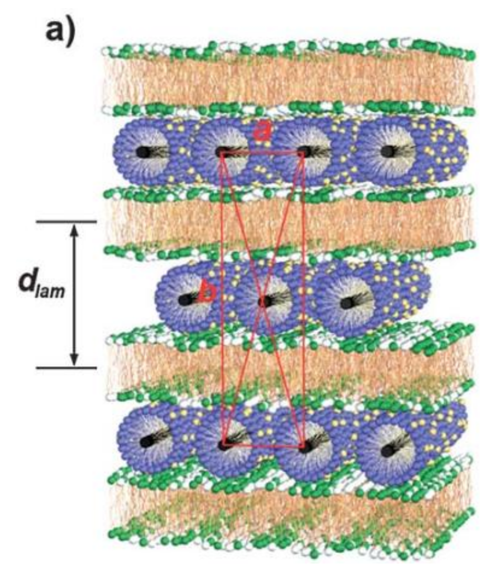
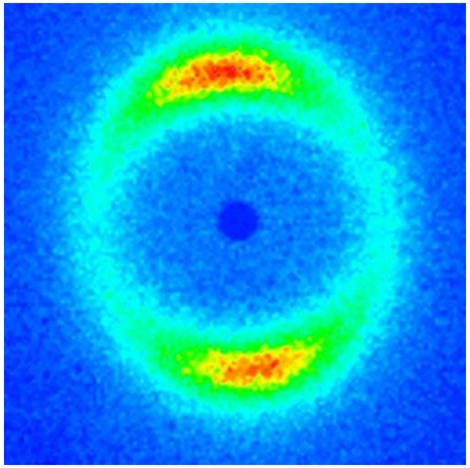
Physics with Neutrons II, SS 2016







Lecture 3, 2.5.2016

SANS – Reminder

Reminder SANS

Starting point: coherent elastic cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \int_{\infty}^{\infty} \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'} \mathrm{d}(\hbar\omega) = \sum_{j,j'} b_j b_{j'} \left\langle e^{-iqr_{j'}} e^{-iqr_j} \right\rangle$$

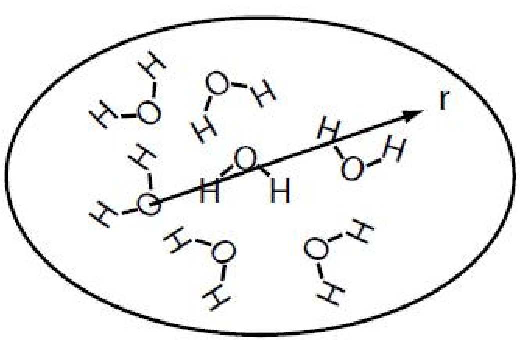
Sum over identical atoms $\displaystyle \frac{d\sigma}{d\Omega}(\mathbf{q}) = \frac{1}{N} \left| \sum_i^N b_i e^{i\mathbf{q}\cdot\mathbf{r}} \right|^2$

SANS: low q averages over large r

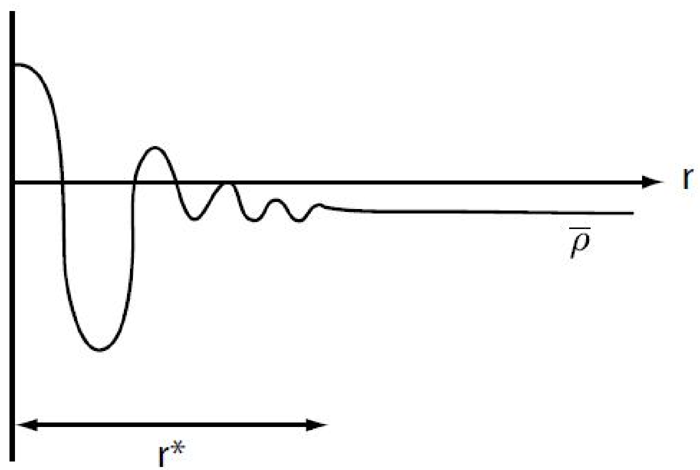
Scattering length b → Scattering length density $\displaystyle \rho = \frac{\sum_i^n b_i}{V}$

$$\rho(\mathbf{r}) = b_i \delta(\mathbf{r} - \mathbf{r_i})$$

Example: water



$$\rho = \frac{\sum_i b_i}{\overline{v}}$$

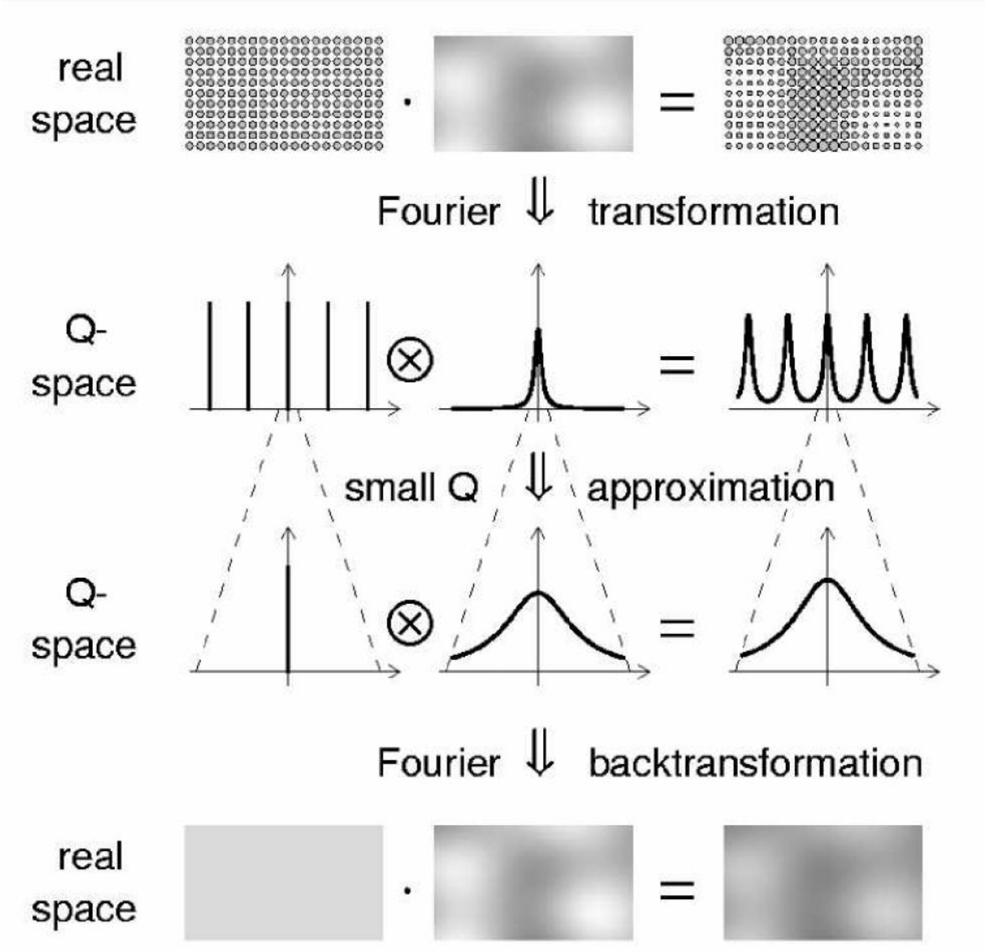


Reminder SANS

SANS measures inhomogeneities of scattering length density

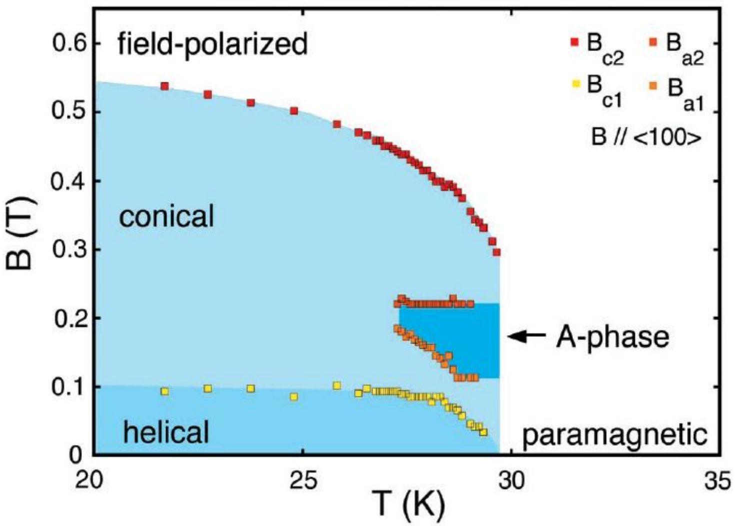
$$\Rightarrow \quad \frac{d\Sigma}{d\Omega}(\mathbf{q}) = \frac{1}{V}(\rho_1 - \rho_2)^2 \left| \int_{V_1} e^{i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r_1} \right|^2$$

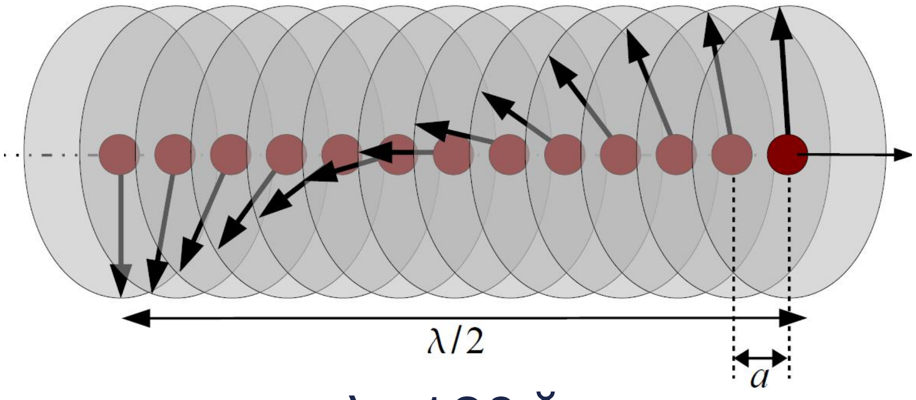
SANS measures mesoscopic information, independent of microscopic structure



SANS on Helical Magnets

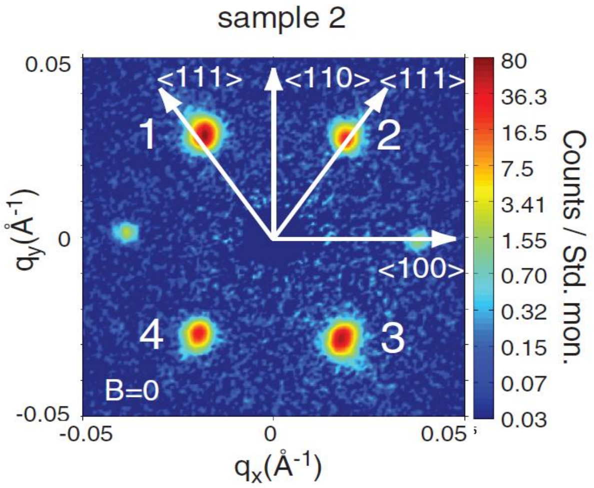
Archetypal Helimagnet MnSi



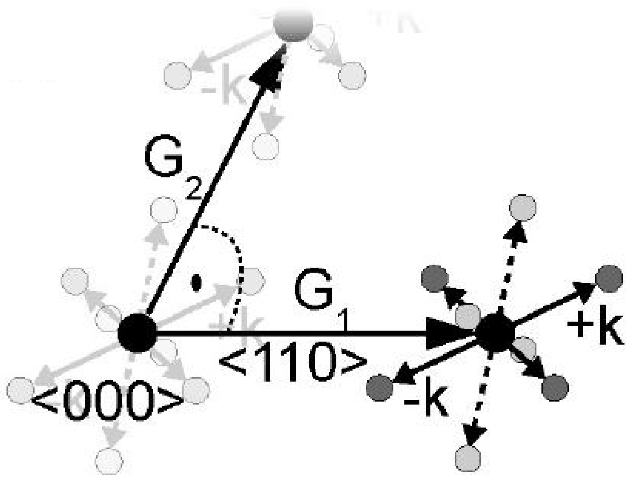


λ=180 Å.

SANS: Incommensurate satellites around (0,0,0)

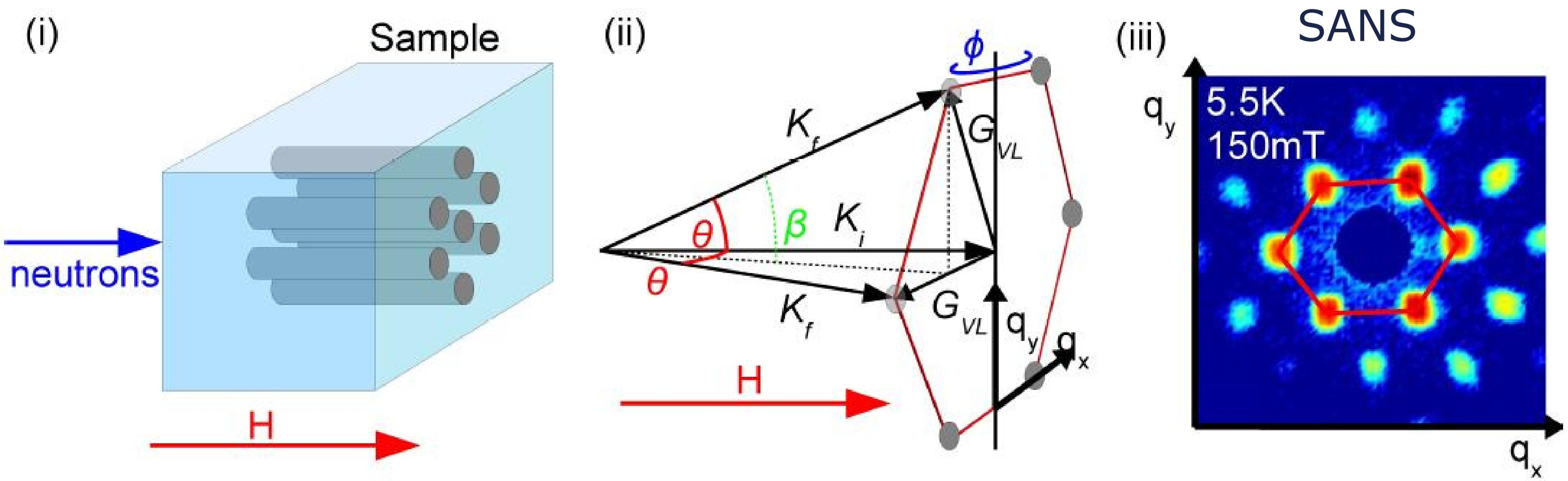


Diffraction: Incommensurate satellites around (h,k,l)



SANS on Vortex Lattices

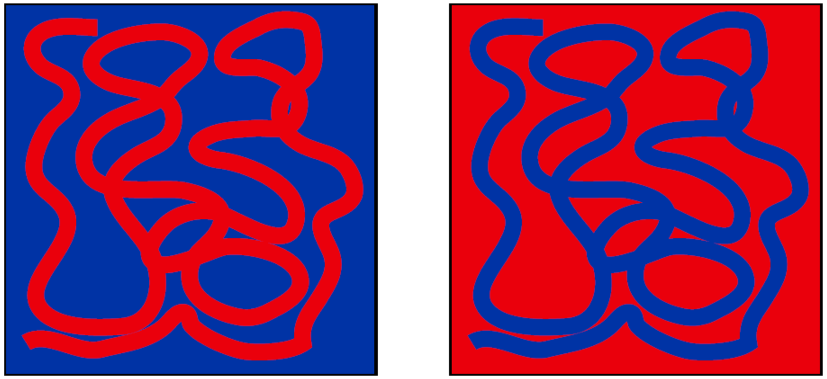
Vortex lattice: Long range magnetic diffraction grating for neutrons



Vortex lattice: Bragg peaks also around nuclear positions?

Structure & Form Factor

$$\frac{d\Sigma}{d\Omega}(\mathbf{q}) = \frac{1}{V}(\rho_1 - \rho_2)^2 \left| \int_{V_1} e^{i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r_1} \right|^2$$



Split up the integral over the sample

$$\frac{d\Sigma}{d\Omega}(q) = \frac{N}{V}(\rho_1 - \rho_2)^2 V_p^2 P(q) S(q)$$

Form factor P(Q)

Interference of neutrons scattered at the same object

Shape, surface and densitiy distribution of objects

Structure factor S(Q)

Interference of neutrons scattered from different objects

Arrangement or superstructure of objects

Form Factor

Form factor P(Q)

Interference of neutrons scattered at the same object

Patterson function

$$P(\mathbf{r}) = \int \rho(\mathbf{r}_1)\rho(\mathbf{r}_2)\, d\mathbf{V}, \qquad \text{with } \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

Convolution of an object with itself

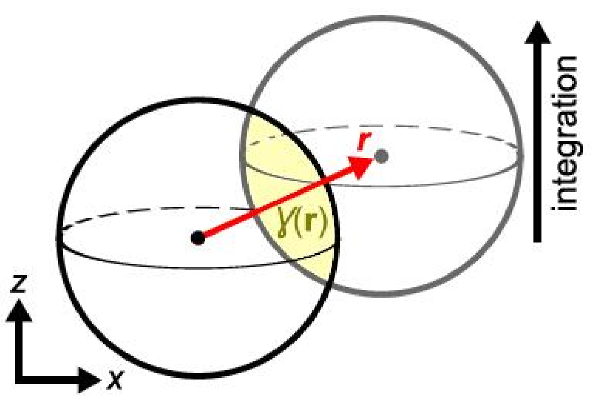
Correlation function (2D): Orientational average of P(r)

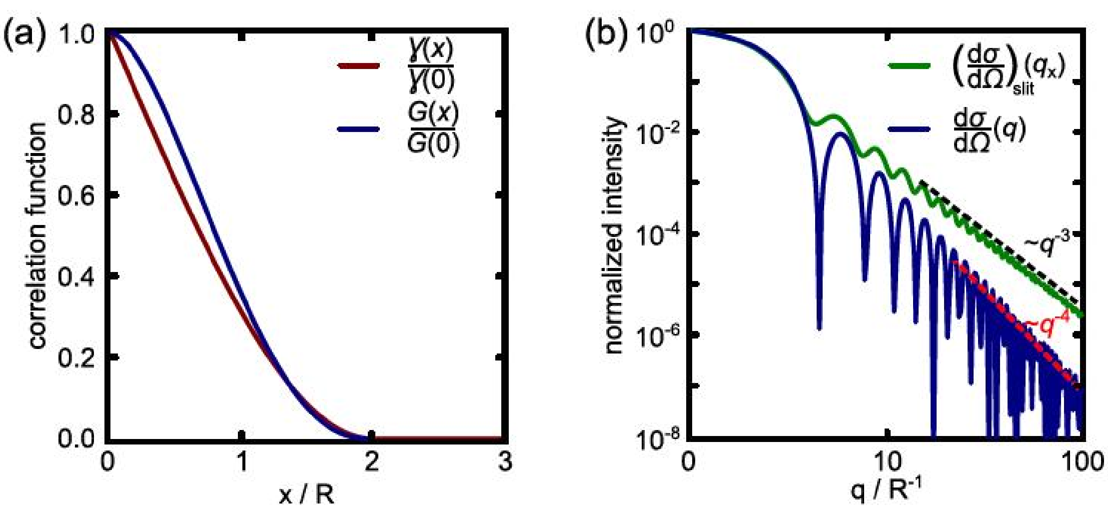
$$\gamma(r) = \frac{1}{2\pi}\int_0^{2\pi} P(\mathbf{r})\,\mathrm{d}\varphi$$

FT of Patterson function: Scattering signal

$$I(Q) = 4\pi \int_0^D \gamma(r)\frac{\sin(Qr)}{Q} r\,\mathrm{d}r$$

$$|\mathcal{F}(\rho)|^2 = |\mathcal{F}(P)|$$





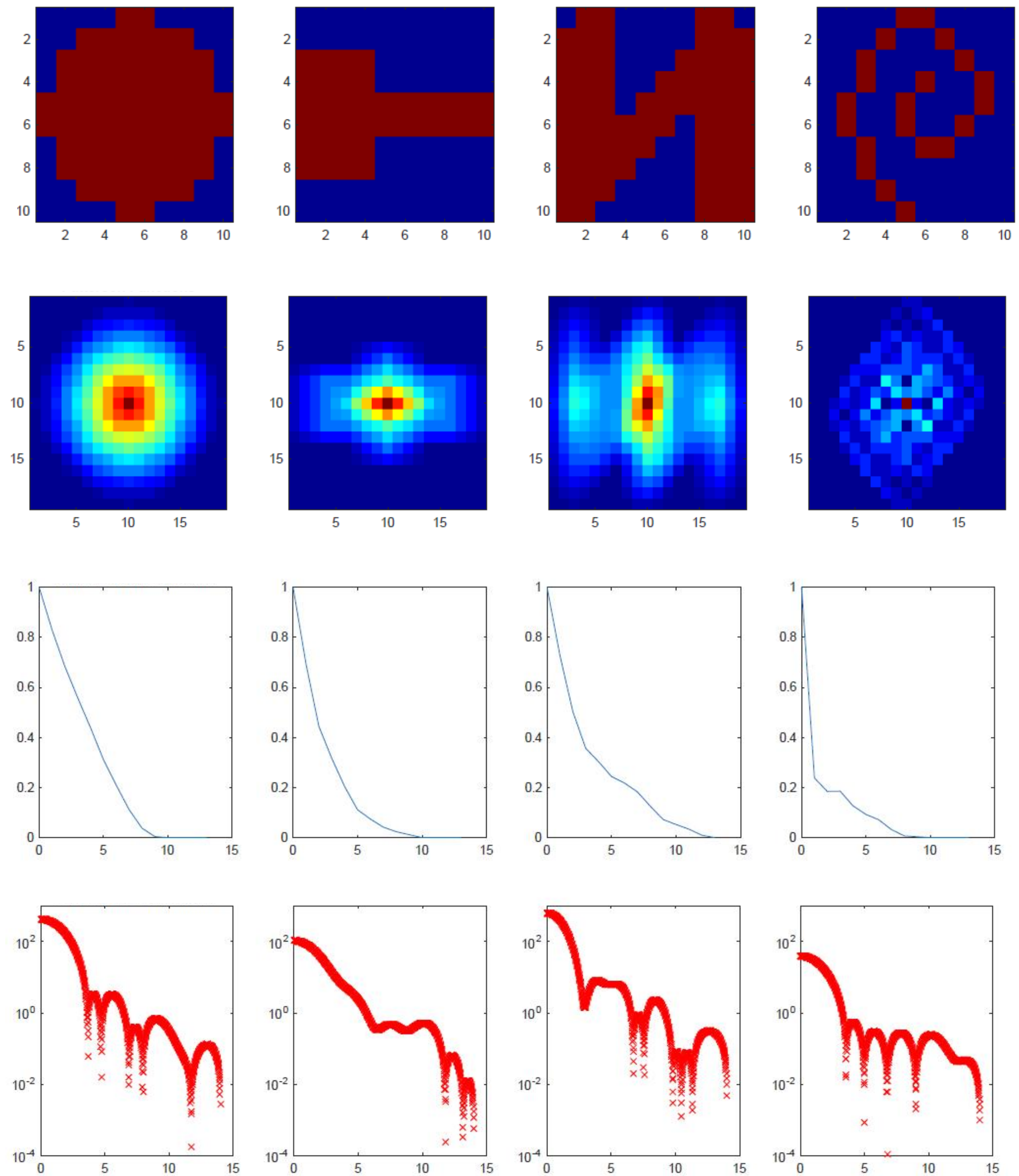
Form Factor

Particle shape

Patterson function

Characteristic function

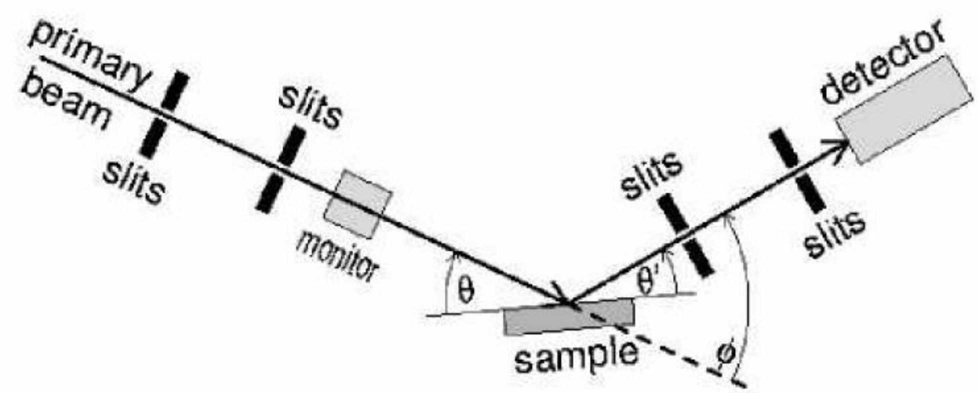
Fourier transform

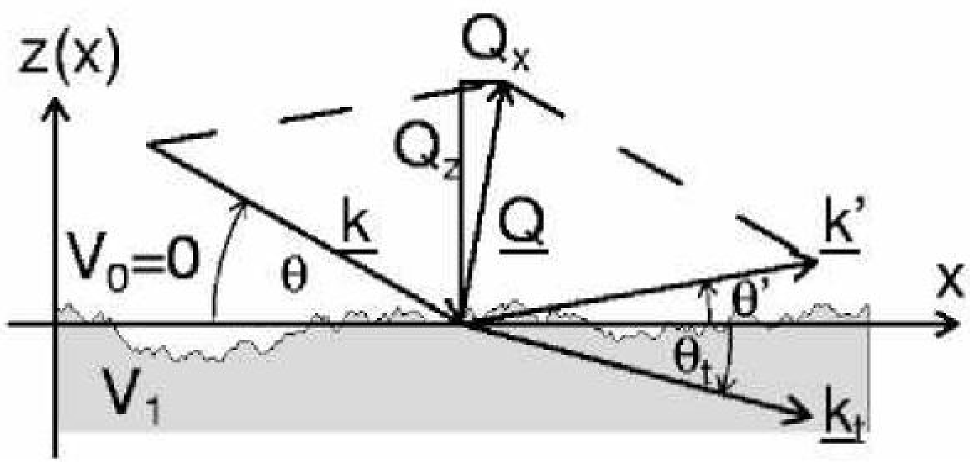


Neutron Reflectometry & GISANS

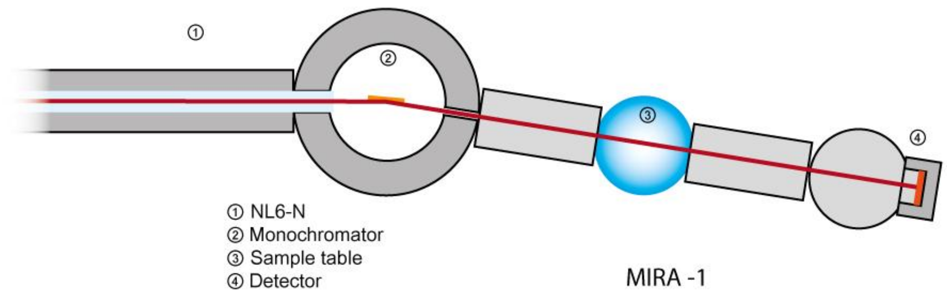
Reflectometry

Basic geometry & layout





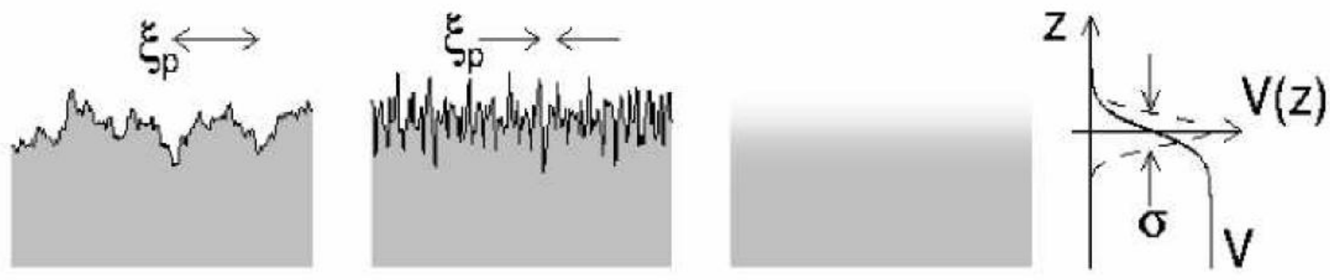
MIRA @ MLZ



Reflectometry

Specular reflectivity in Born approximation ϴ=ϴ`

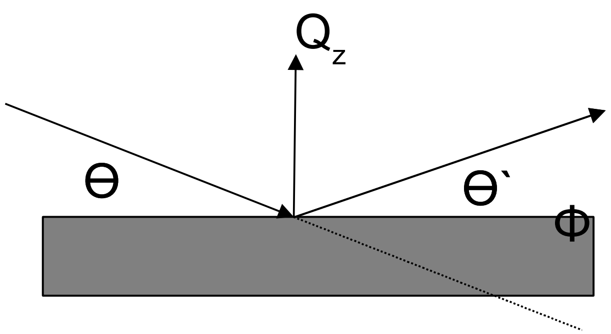
Effects of surface roughness

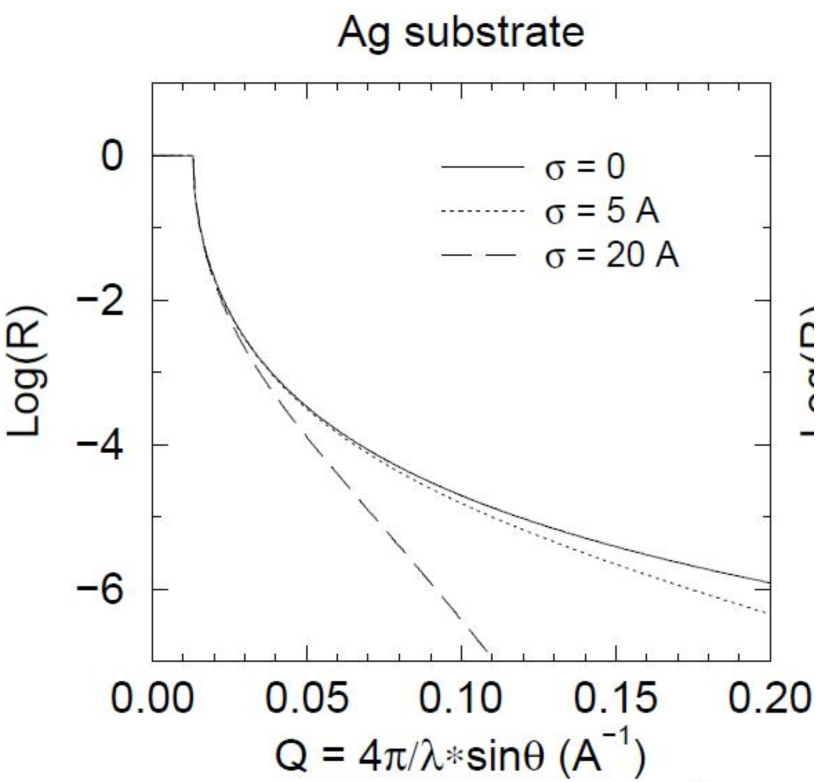


Reflectivity of a single, infinite layer

$$V(z) = \frac{2\pi\hbar^2 b\rho}{m_n}\left(\frac{1}{2} - \frac{1}{2}\Theta(z)\right) = \begin{cases} 0 & : \quad z > 0 \\ 2\pi\hbar^2 b\rho / m_n & : \quad z \le 0 \end{cases}$$

$$I(Q_z) \sim \frac{1}{Q_z^4}\left|\int \frac{\mathrm{d}V(z)}{\mathrm{d}z}\exp(-iQ_z z)\mathrm{d}z\right|^2$$



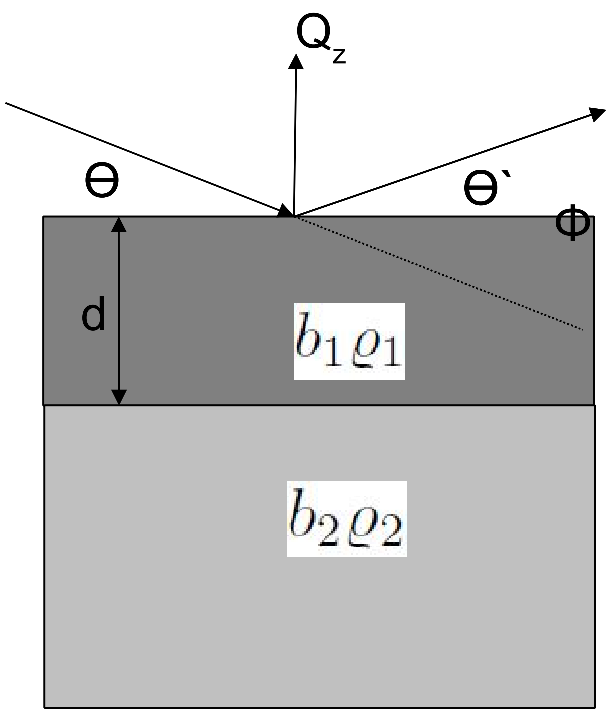


Reflectometry

Specular reflectivity in Born approximation ϴ=ϴ`

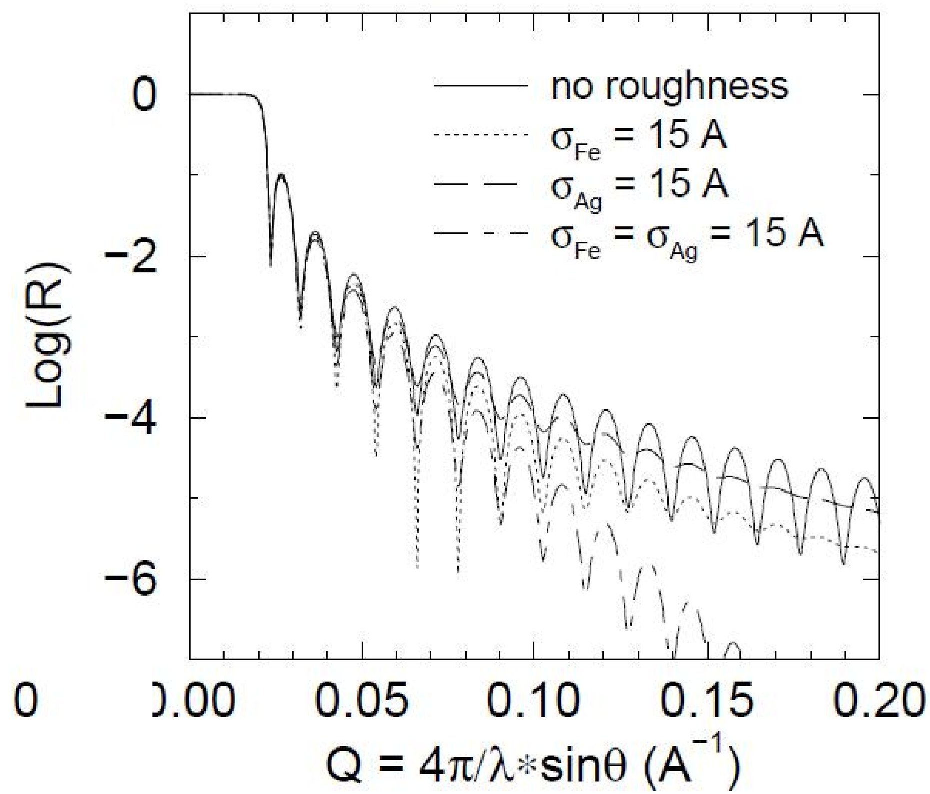
$$I(Q_z) \approx \frac{1}{Q_z^4}\left[(b_2\varrho_2 - b_1\varrho_1)^2 + (b_1\varrho_1)^2 + 2(b_2\varrho_2 - b_1\varrho_1)(b_1\varrho_1)\cos(Q_z d)\right]$$

Reflectivity of a single, layer with thickness d



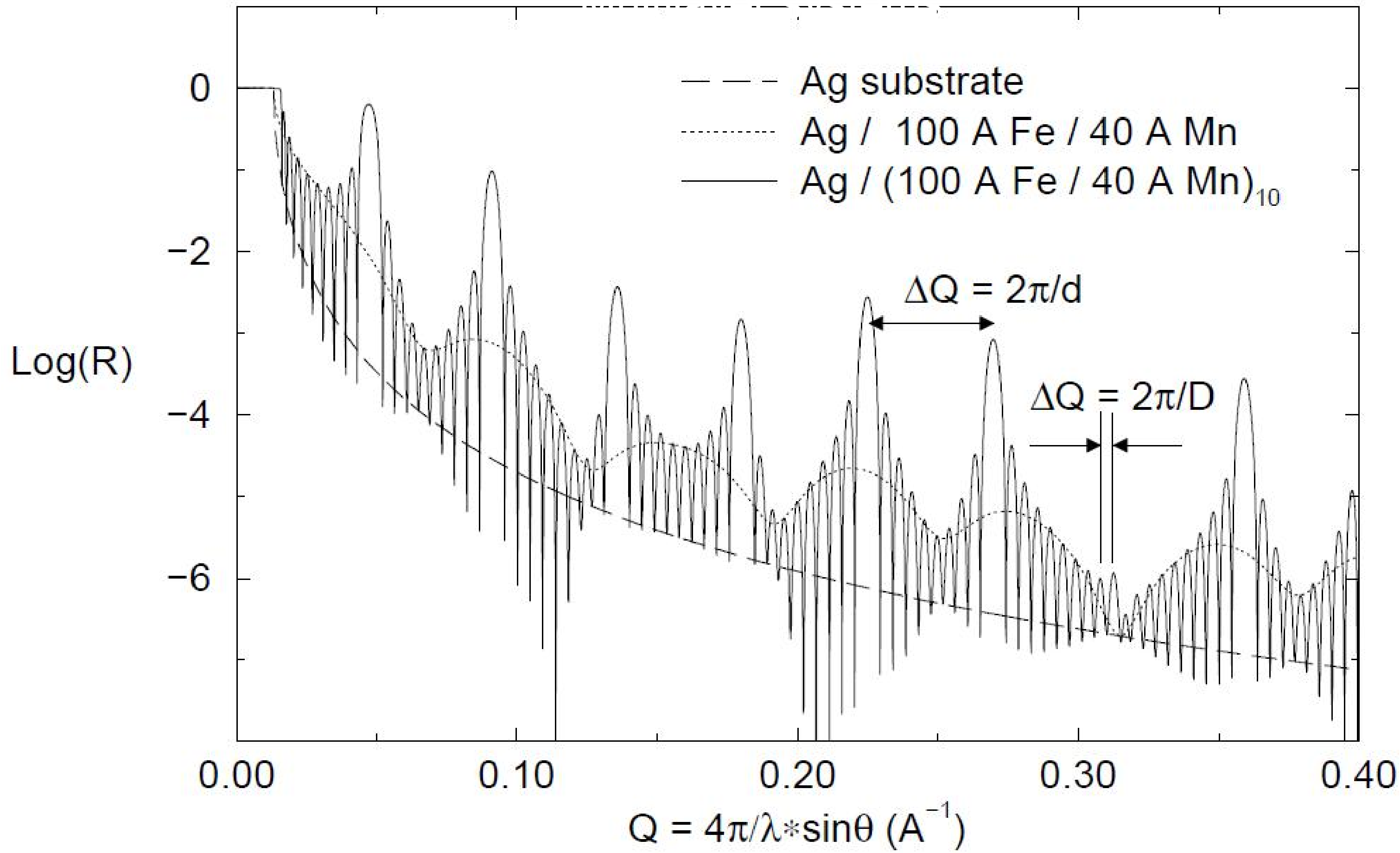
Effects of surface roughness and finite thickness

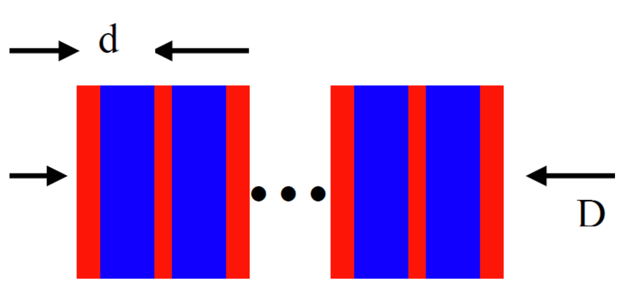
Ag / 500 A Fe



Reflectometry

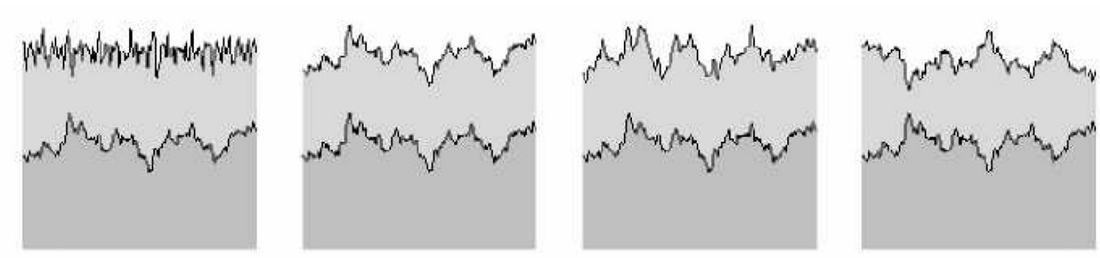
Multilayer systems





Reflectometry

Diffuse reflectivity in Born approximation $\Theta \neq \Theta'$



Surface correlation function

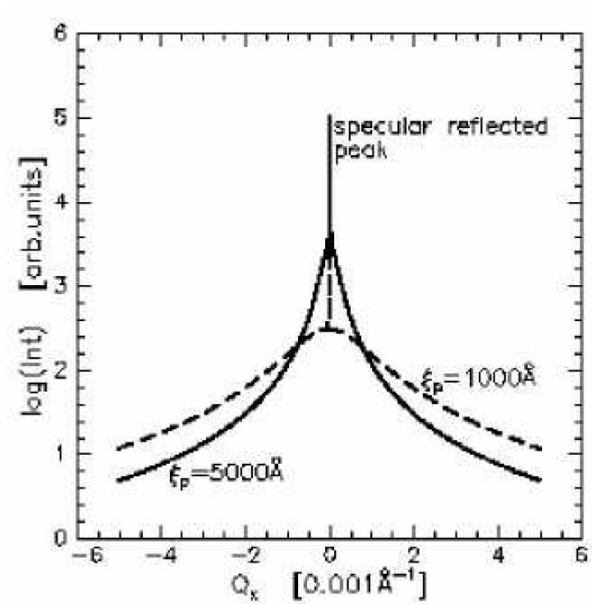
$$C_{jk}(R) = \int z_j(r) z_k(r+R) \mathrm{d}^2 r$$

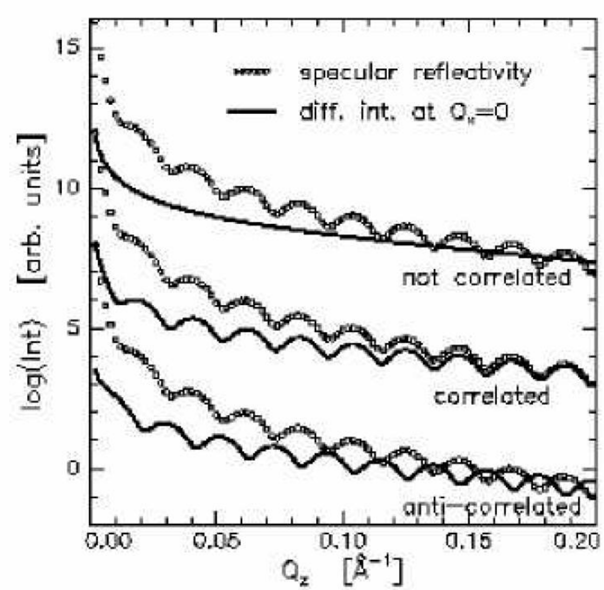
Diffuse offspecular intensity

$$I_{diff}(Q_x, Q_z) \approx \frac{1}{Q_z^2}[(b_2\varrho_2 - b_1\varrho_1)^2 e^{-Q_z^2\sigma_2^2} S_{22}(Q_x) + (b_1\varrho_1)^2 e^{-Q_z^2\sigma_1^2} S_{11}(Q_x) + 2(b_2\varrho_2 - b_1\varrho_1)(b_1\varrho_1) e^{\frac{-Q_z^2(\sigma_2^2+\sigma_1^2)}{2}} S_{12}(Q_x) \cos(Q_z d)$$

„Structure factor"

$$S_{jk}(Q_x) = \int (e^{Q_z^2 C_{jk}(x)} - 1) e^{-iQ_x x} \mathrm{d}x$$





Reflectometry

Born approximation: Intensity would diverge for Q->0

Multiple scattering occurs!

Regime of total reflection: Dynamical scattering theory

Single, smooth layer using QM

$$\left[-\frac{\hbar^2}{2m_n}\Delta + V(r)\right]\Psi(r) = E\Psi(r)$$

Refractive index for neutrons

$$n_t = 1 - \frac{\lambda^2}{2\pi}\sum_j b_j \varrho_j = 1 - \delta_t$$

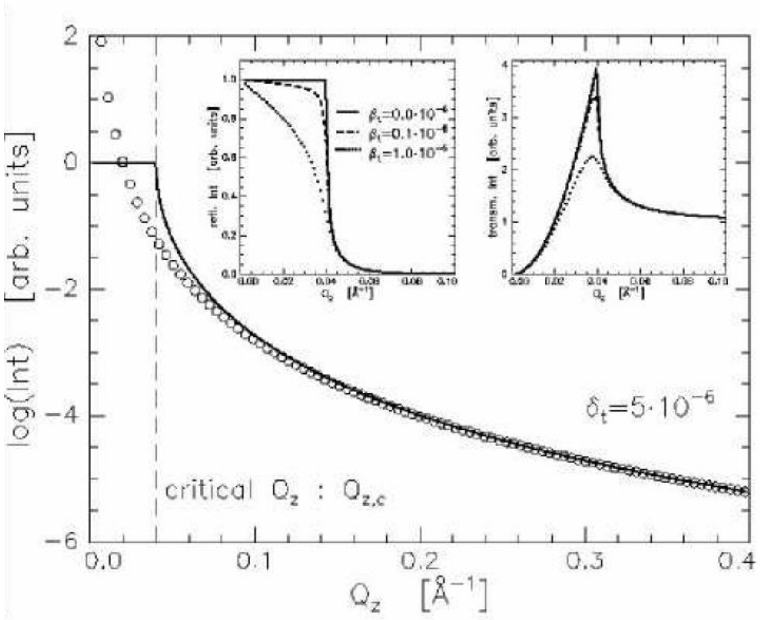
Transmitted and reflected wave

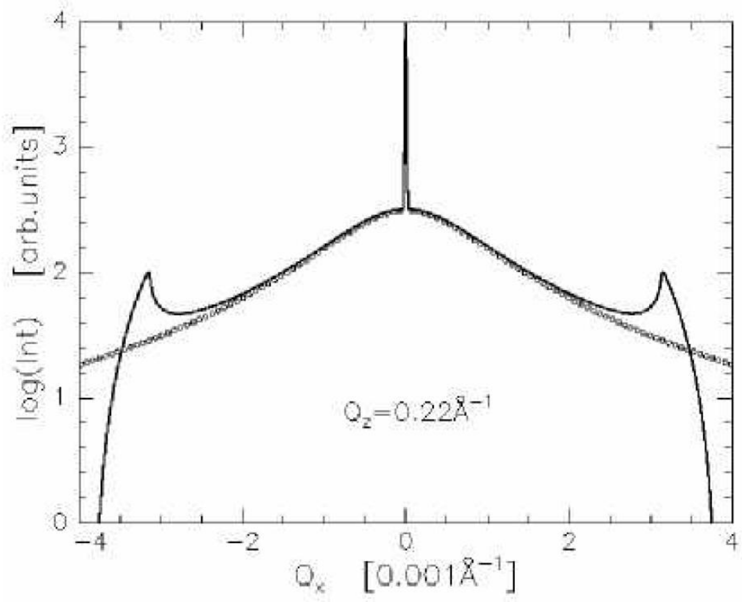
$$r_t = \frac{2k_z}{k_z + k_{t,z}} \qquad r_f = \frac{k_z - k_{t,z}}{k_z + k_{t,z}}$$

Absorption: Imaginary part

$$n_t = 1 - \delta_t + \mathrm{i}\beta_t$$

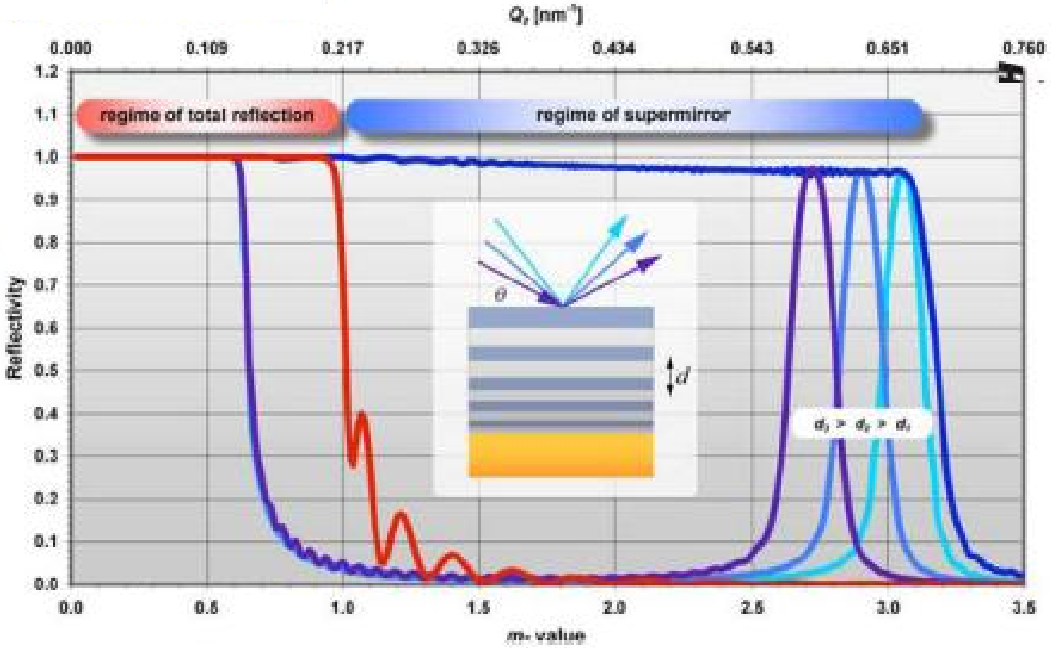
Evanescent wave for Θ=Θ` (Yoneda peak)





Applications: Reflectometry & GISANS

Neutron guides & supermirrors

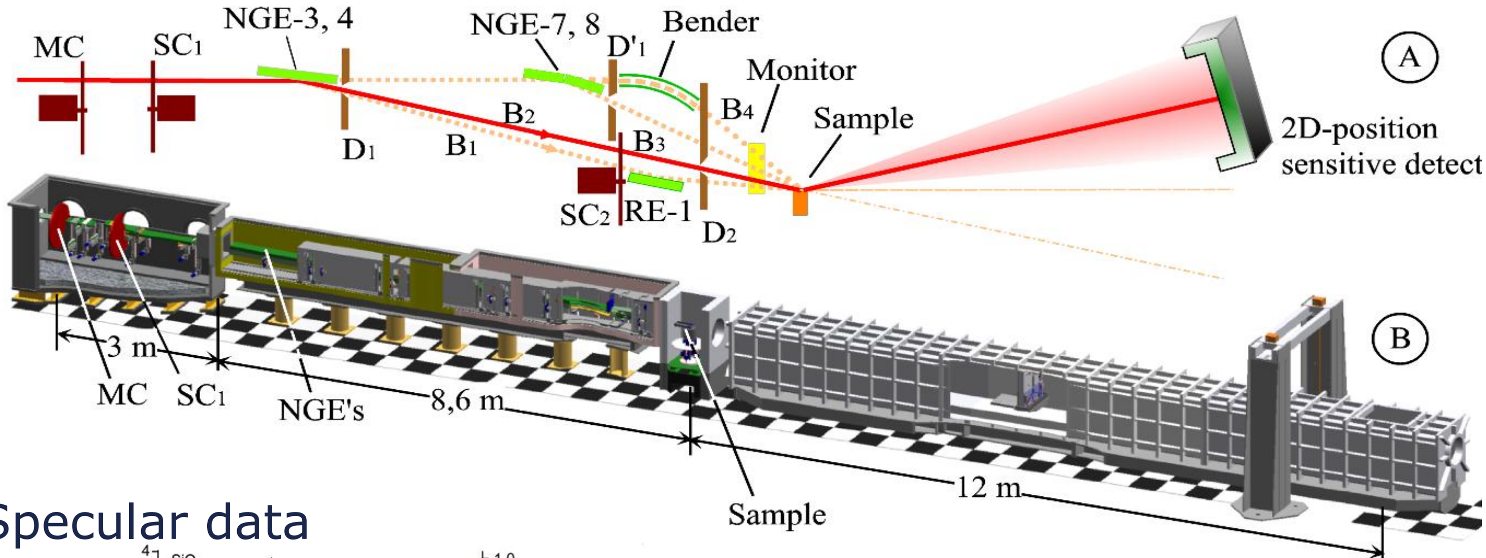


Regime of total reflection: $\Theta_c = \lambda \sqrt{\frac{\rho b}{\pi}}$

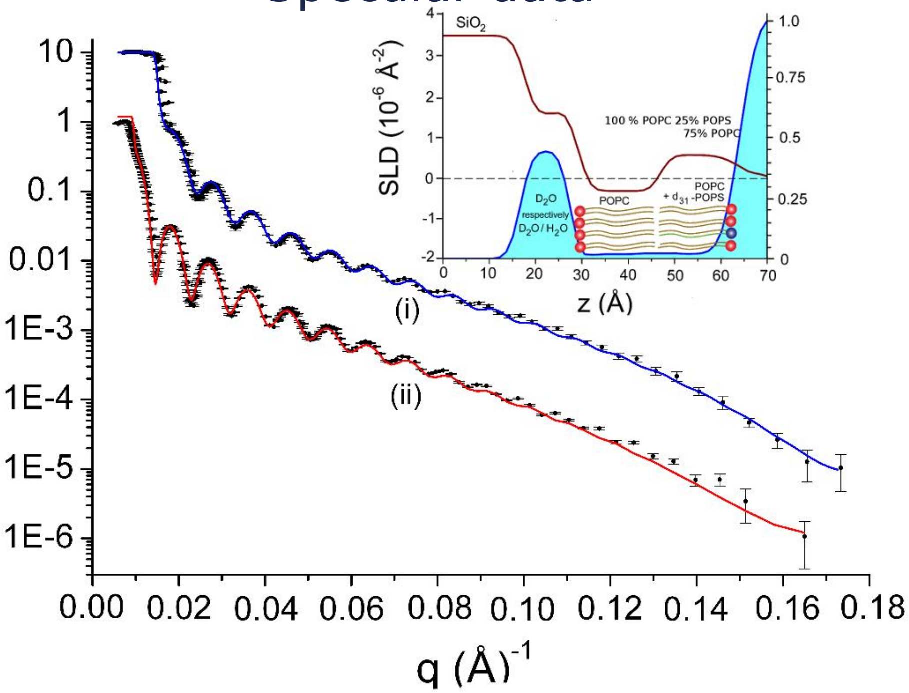
Regime of supermirror: $Q = \frac{4\pi}{\lambda}\sin(\Theta)$

Applications of Reflectometry

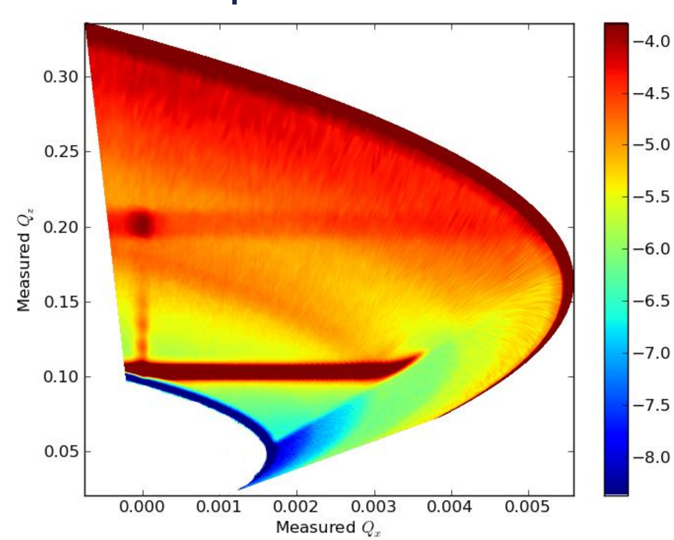
GISANS @ REFSANS



Specular data



Offspecular data



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Spatial correlation in dewetted polymer thin films