

# Introduction to Neutron Reflectometry (NR)

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# Outline

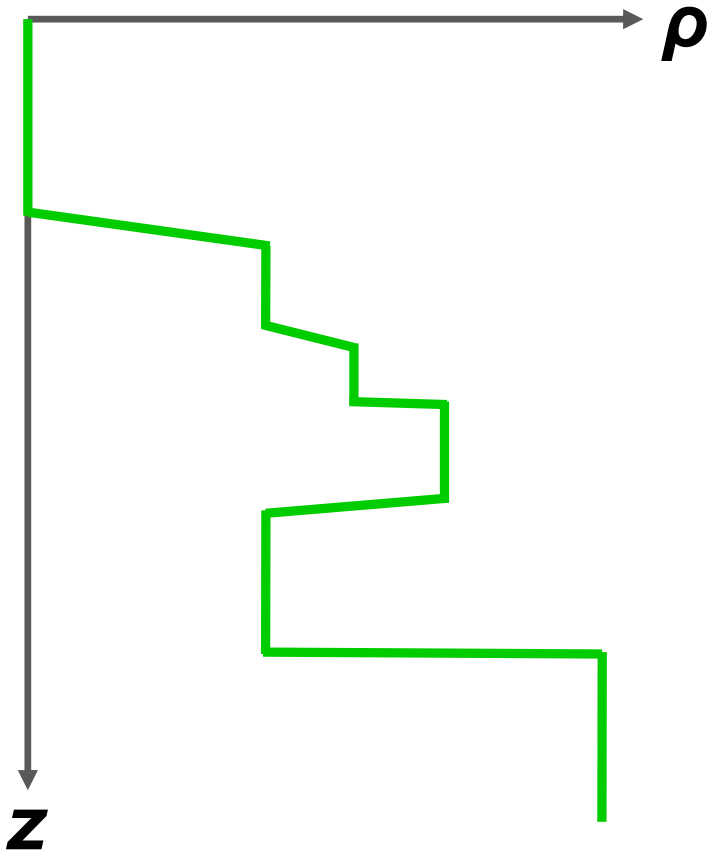
- Principles of Neutron Reflectometry
- Reflectometry of Non-Polarized and Polarized Neutrons from Solid Interfaces
- Neutron Reflectometry from Interfaces with Liquids
- Experimental Aspects of Neutron Reflectometry

## •Principles of Neutron Reflectometry

- Reflectometry of Non-Polarized and Polarized Neutrons from Solid Interfaces
- Neutron Reflectometry from Interfaces with Liquids
- Experimental Aspects of Neutron Reflectometry

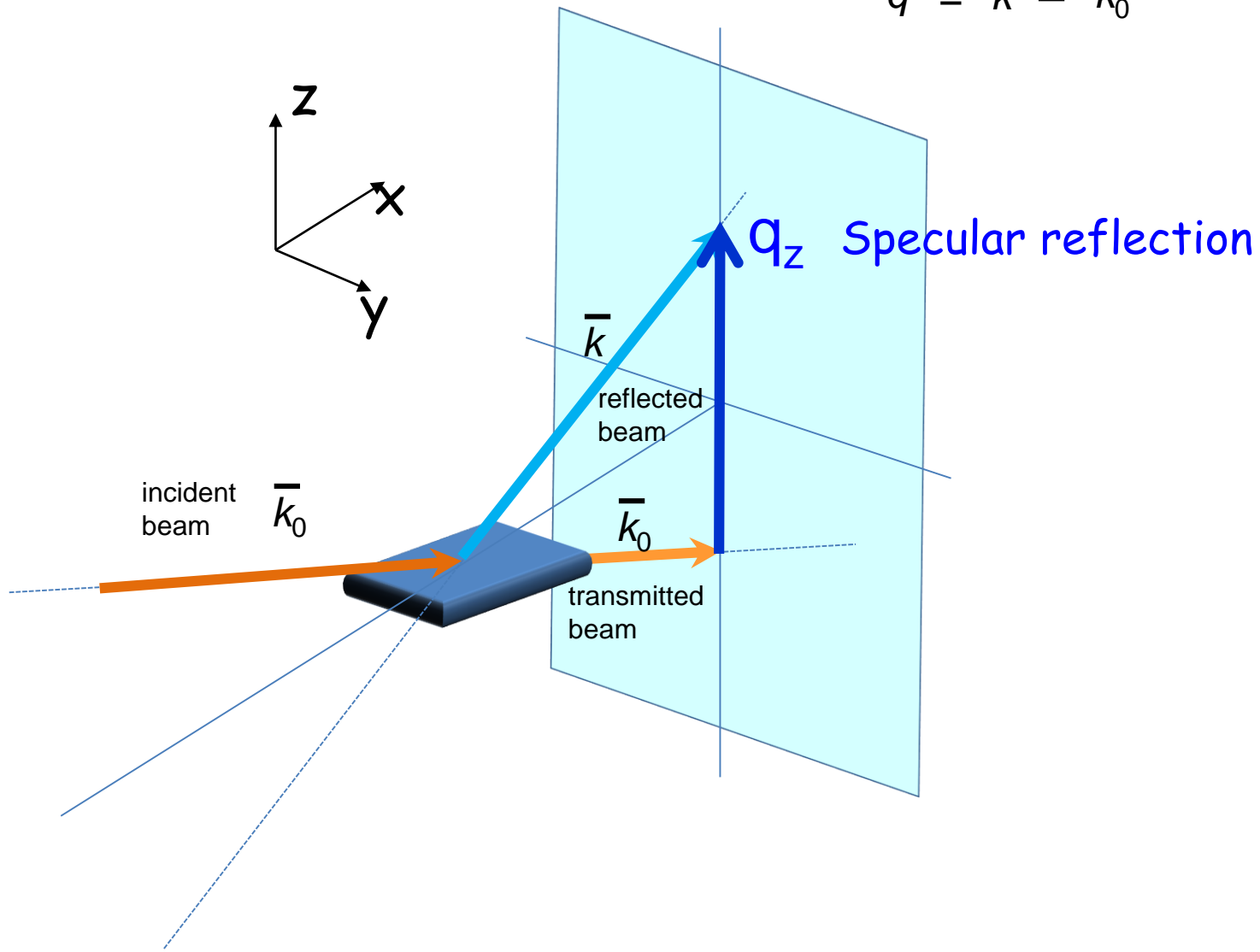
# Research Objects

sandwich-like structures



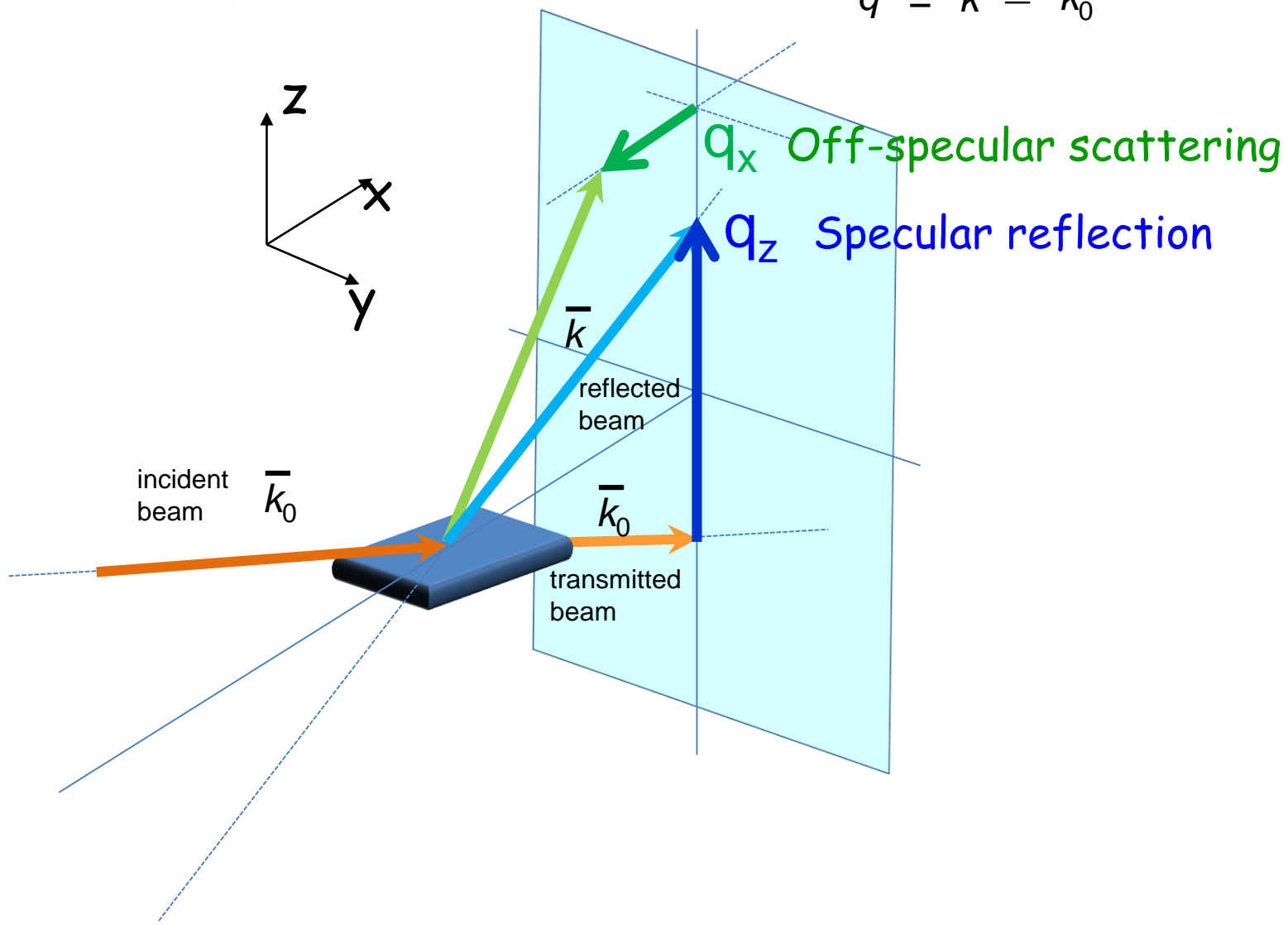
# NR modes

$$\bar{q} = \bar{k} - \bar{k}_0$$



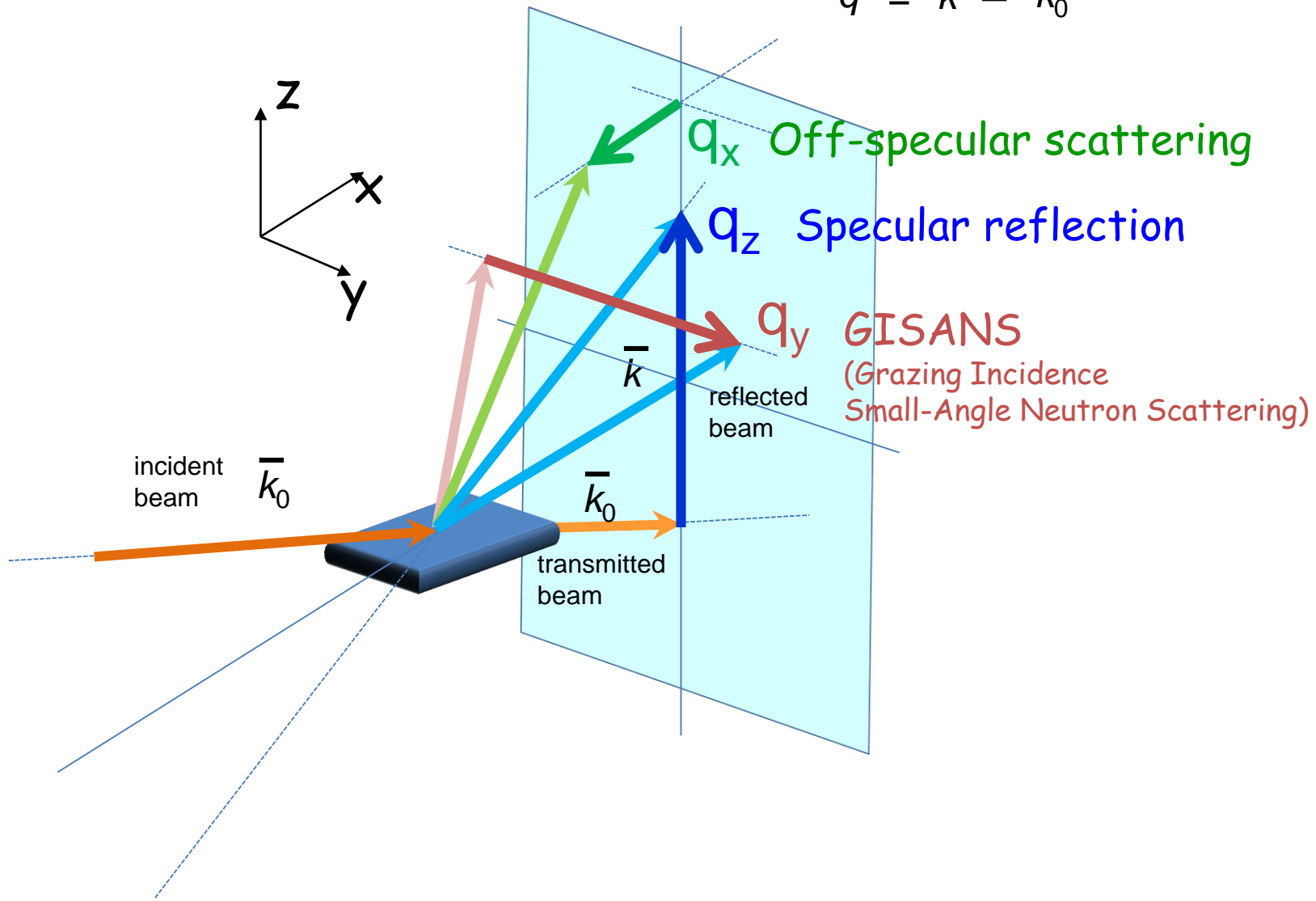
# NR modes

$$\bar{q} = \bar{k} - \bar{k}_0$$



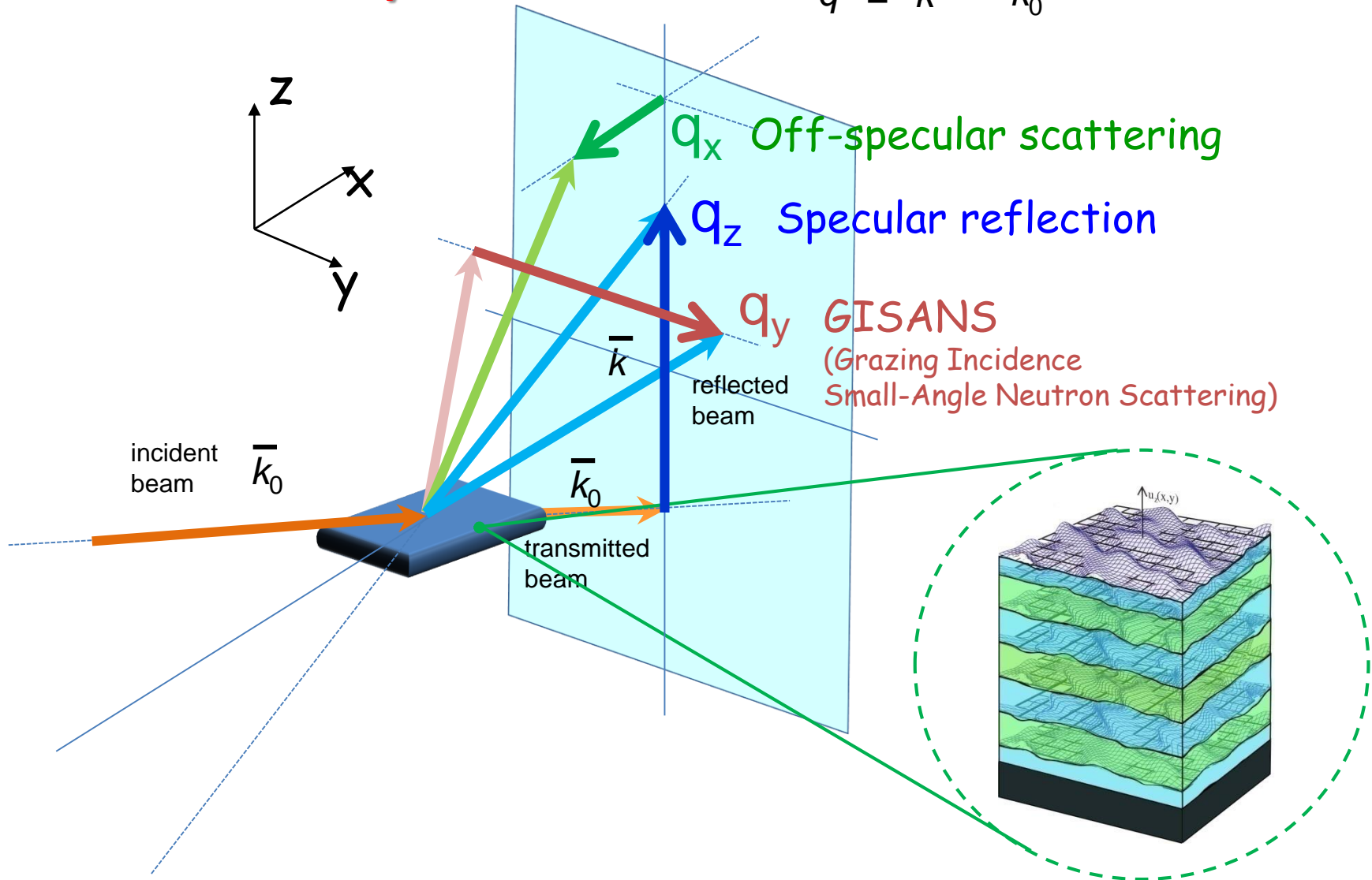
# NR modes

$$\bar{q} = \bar{k} - \bar{k}_0$$



# 3D Reflectometry

$$\bar{q} = \bar{k} - \bar{k}_0$$



Complete reflectometry

$q_x q_y q_z$



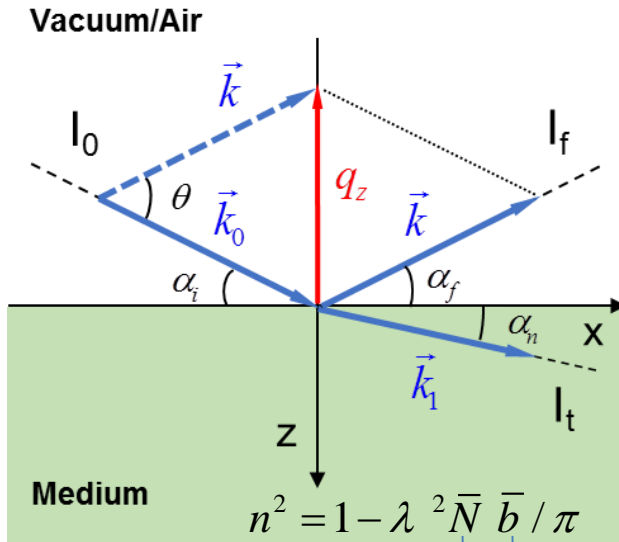
$u_z(x,y)$  - vertical surface displacement  
 $\xi_x, \xi_y$  - correlation lengths



# Specular reflection

## Tight collimation of incident beam over Z-direction

### Optical approach



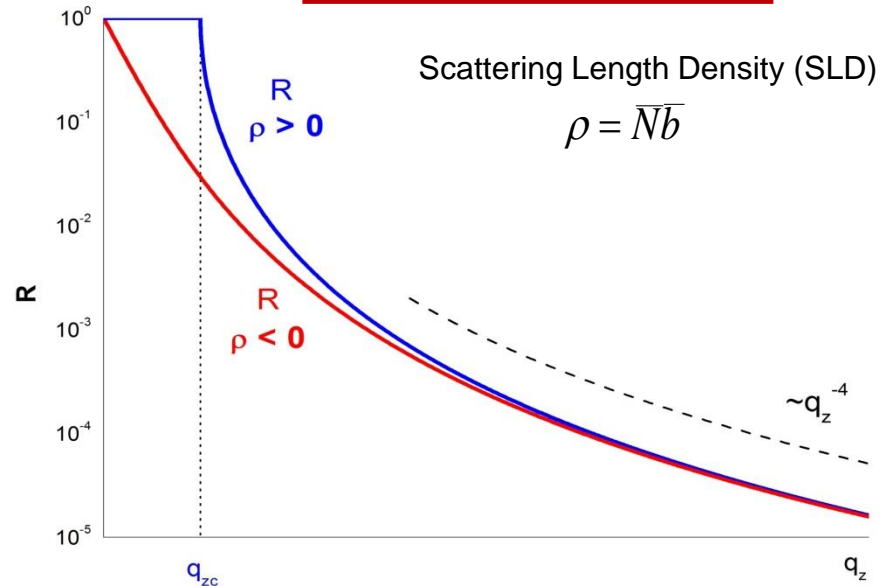
mean atomic density      mean scattering length

$$q_z = \frac{4\pi}{\lambda} \sin \frac{\theta}{2}$$

$$\theta = 2\alpha_i$$

$$\alpha_i \sim 1-10 \text{ mrad}$$

$Reflectivity R(q_z) = I_f/I_0$



### Fresnel law

#### Total external reflection

$$R = 1 \quad \text{at} \quad \alpha_i < \alpha_c \quad \cos \alpha_c = n$$

$$\alpha_c^2 \approx 1 - n^2 \quad \rightarrow \quad \alpha_c = \lambda \sqrt{\frac{\bar{N} \bar{b}}{\pi}}$$

$$\text{for } ^{58}\text{Ni} \quad (\alpha_c/\lambda) \approx 0,0017 \text{ rad/\AA}$$

$$R(q_z) = \left| \frac{\sin \alpha_i - n \sin \alpha_n}{\sin \alpha_i + n \sin \alpha_n} \right|^2 = \left| \frac{1 - \sqrt{1 - q_{zc}^2 / q_z^2}}{1 + \sqrt{1 - q_{zc}^2 / q_z^2}} \right|^2$$

$$q_{zc} \approx 4(\pi\rho)^{1/2}$$

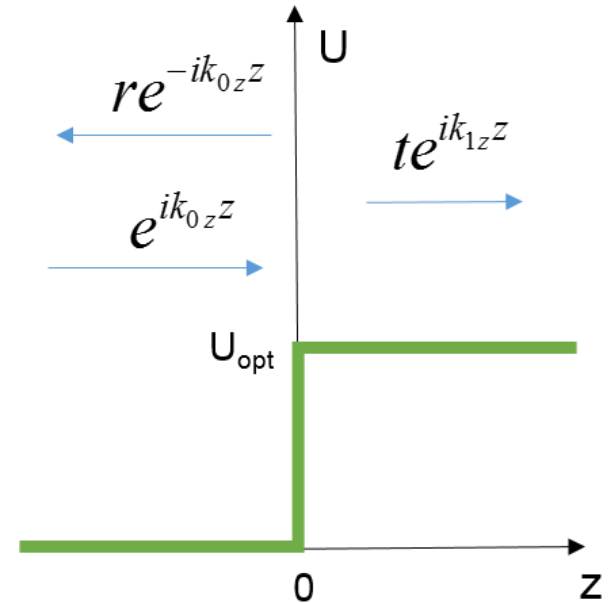
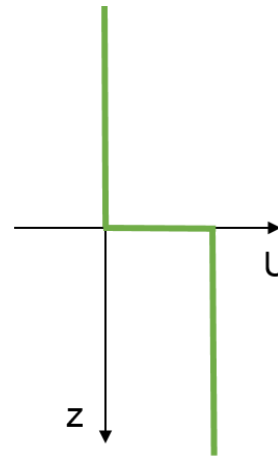
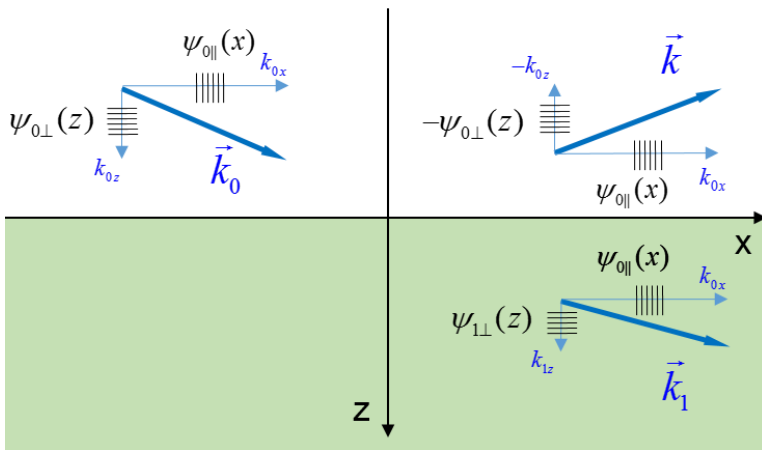
At  $q_z \rightarrow \infty$

$$R(q_z) \approx (1/16)(q_{zc}^4 / q_z^4)$$

# Specular reflection

## Tight collimation of incident beam over Z-direction

### Quantum-mechanical approach



$$r = (k_{0z} - k_{1z}) / (k_{0z} + k_{1z}),$$

$$t = 1 + r = 2k_{0z} / (k_{0z} + k_{1z}).$$

$$q_{zc} = 2\sqrt{2mU_{opt} / \hbar^2}$$



$$U_{opt} = 2\pi\hbar^2\rho/m$$

$$k_0 \cos \alpha_i = k_1 \cos \alpha_n$$



$$n = k_1/k_0 = v_1/v_0.$$

$$k_{0z} = \sqrt{2mE_{\perp} / \hbar^2},$$

$$k_{1z} = \sqrt{2m(E_{\perp} - U_{opt}) / \hbar^2}$$

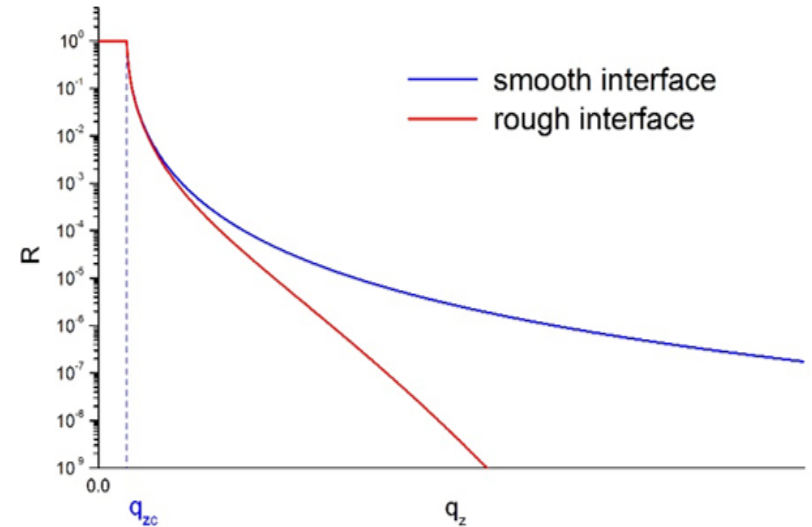
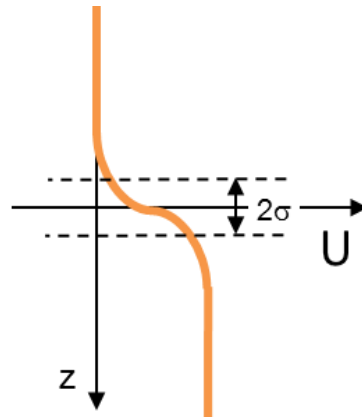
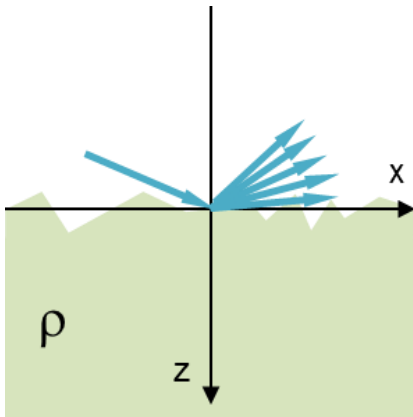
$$R = |r|^2 = \left| \frac{k_{0z} - k_{1z}}{k_{0z} + k_{1z}} \right|^2 = \left| \frac{1 - \sqrt{1 - U_{opt} / E_{\perp}}}{1 + \sqrt{1 - U_{opt} / E_{\perp}}} \right|^2 \quad E_{\perp} > U_{opt}, \text{ or } q_z > q_{zc}$$

# Off-specular scattering

Rough interface

$$G(z) = (1 / \sqrt{2\pi}\sigma) \exp[-z^2 / (2\sigma^2)]$$

$$R(q_z) = \exp(-4z^2 k_{0z}^2 k_{1z}^2 / \sigma^2) R_F(q_z)$$



Roughness should be as minimal as possible!

## Off-specular scattering

Correlated roughness  $\langle U_j(x, y)U_j(x', y') \rangle = \sigma^2 e^{-\frac{\tau}{\xi} 2H}$ ,  $\tau = [(x - x')^2 + (y - y')^2]^{\frac{1}{2}}$

- The Hurst parameter,  $H = 3 - D$  ( $D$  is the surface fractal dimension) is varied between 0 and 1.
- The lateral correlation length  $\xi$  acts as a cut-off for the lateral length scale on which an interface begins to look smooth. If  $\xi \gg \tau$  the surface is smooth.

### Distorted-wave Born approximation (DWBA)

non-distorted

$$[\mathbf{D}_0 - 4\pi\hat{v}(\mathbf{r})]\Psi(\mathbf{r}) = 0 \quad \mathbf{D}_0 := \nabla^2 + K^2 \quad v(\mathbf{r}) := \frac{m}{2\pi\hbar^2} V(\mathbf{r}) = \sum_j \langle b_j \delta[\mathbf{r} - \mathbf{r}_j(t)] \rangle$$

distorted

$\hat{v}(\mathbf{r}) = \bar{v}(z) + \hat{u}(\mathbf{r})$

$$\mathbf{D} := \mathbf{D}_0 - 4\pi\bar{v}(z) \quad \mathbf{D}(z)\Psi(\mathbf{r}) = 4\pi\hat{u}(\mathbf{r})$$

In-plane function

$$\frac{d\sigma}{d\Omega} = \left| \int d^3r \Psi_i(\mathbf{r}) \hat{u}(\mathbf{r}) \Psi_f^*(\mathbf{r}) \right|^2 \quad \mathbf{D}(z)\Psi(\mathbf{r}) = 0$$

### BornAgain program software

G. Pospelov, et al. J. Appl. Cryst. 53 (2020) 262–276

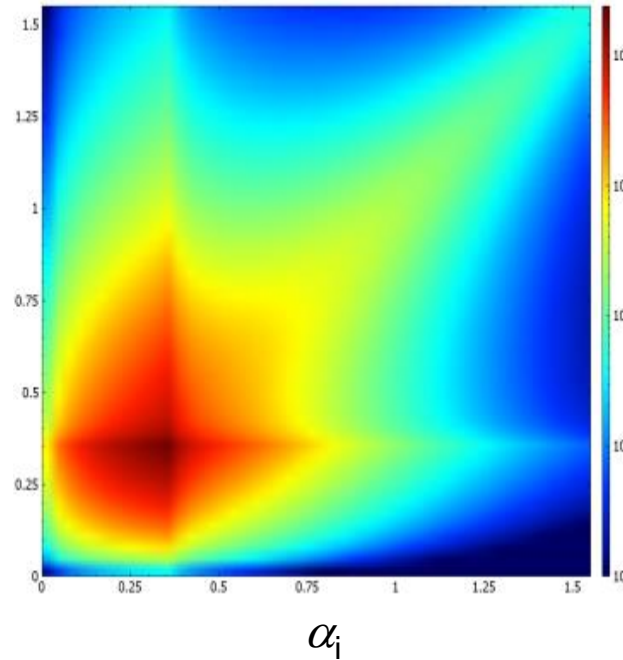
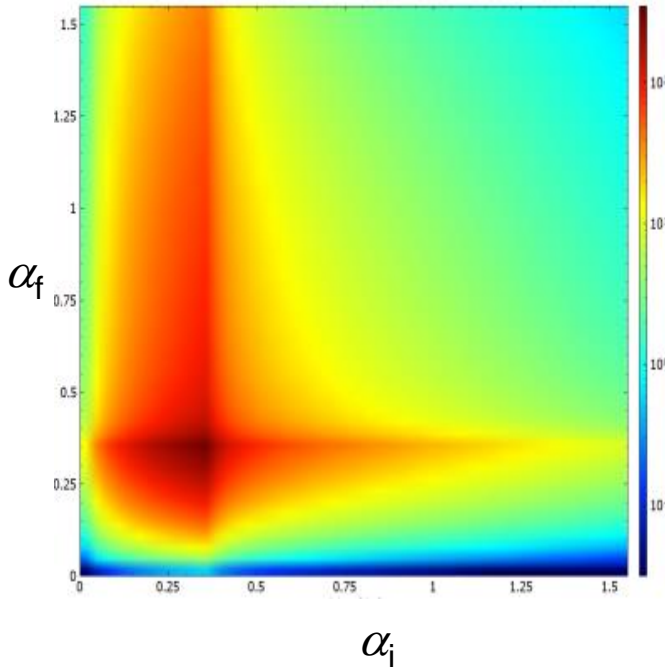
# Off-specular scattering

(a)

(b)

Specular reflection line

$$\alpha_i = \alpha_f$$



Yoneda wings  
(evanescent wave)

$$\alpha_i = \alpha_{iC}$$

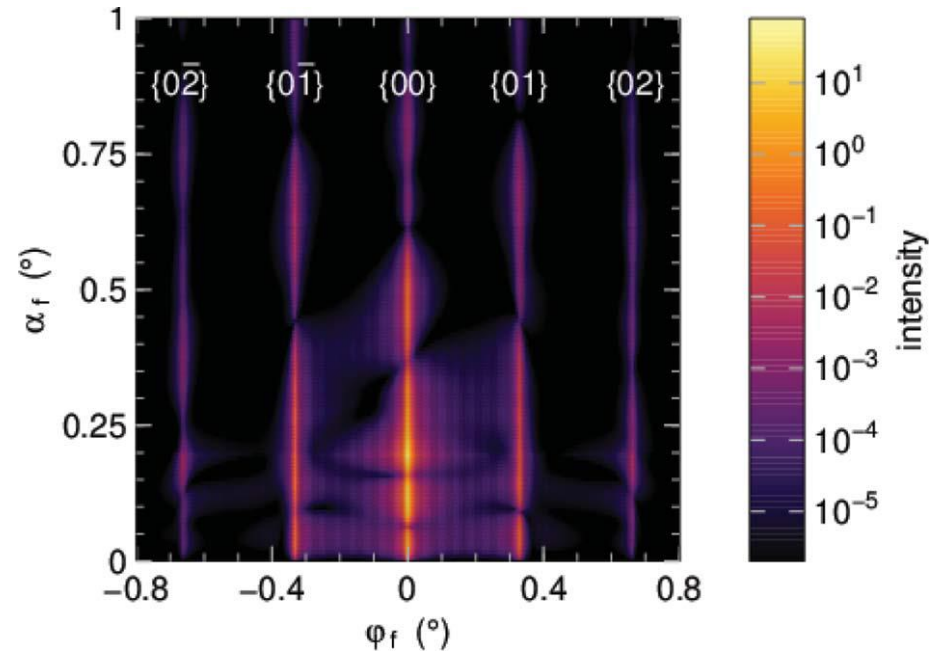
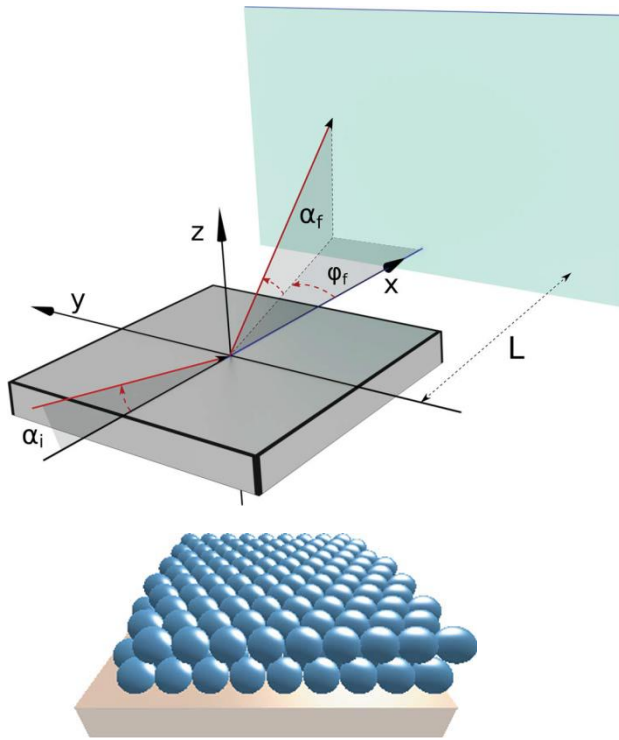
$$\alpha_f = \alpha_{iC}$$

Calculated 2D patterns of NR diffuse scattering from semi-infinite medium of Cu, interface roughness  $\sigma = 2$  nm, in-plane roughness correlation length  $\xi_{||} = 100$  nm (a),  $\xi_{||} = 1000$  nm (b).

Calculations have been made in the Distorted Wave Born approximation (DWBA) using Program BornAgain; <https://www.bornagainproject.org/>

# Grazing incidence small-angle scattering

Tight collimation of incident beam over Z- and Y- directions



$R = 10$  nm, hexagonal lattice (orientation  $\{11\}$ , along  $x$ ).  
 $\xi_{||} = 400$  nm;  $n = 1 - \delta$ ;  $\delta = 6 \times 10^{-4}$ ; substrate  $\delta = 6 \times 10^{-6}$ ;  
 $\lambda = 1$  Å,  $\alpha_i = 0.2^\circ$ .

Calculations have been made in the Distorted Wave Born approximation (DWBA) using Program BornAgain;

<https://www.bornagainproject.org/>

G. Pospelov, et al. J. Appl. Cryst. 53 (2020) 262–276

# Steady-state and TOF modes

## Steady-state (SS) mode

$\lambda$  is fixed (monochromatization)

$\theta$ -scan (grazing angle)

$$q = \frac{4\pi}{\lambda} \sin \theta$$

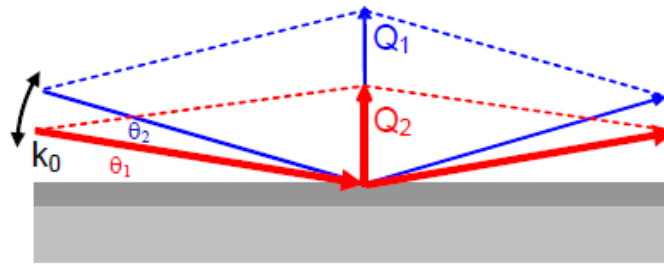
## Time-of-flight (TOF) mode

$\theta$  is fixed

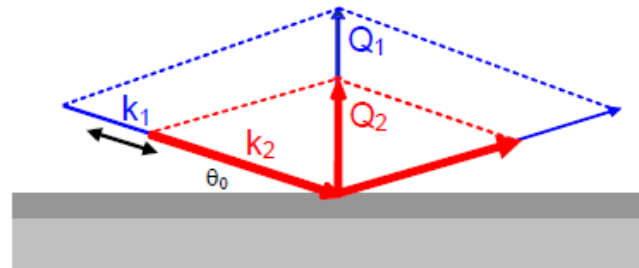
$\lambda$ -scan

$$q = \frac{4\pi}{\lambda} \sin \theta$$

monochromatic  
beam



TOF



$$\lambda = \frac{h \text{ TOF}}{mL}$$

time-of-flight  
flight path

## Summary to 'Principles of Neutron Reflectometry'

- ***Neutron reflectometry experiment is aimed at determining the scattering length density distribution at planar interfaces.***
- ***Two equivalent approaches to treat specular neutron reflectivity from planar interfaces exist. Optical approach is an extension of the laws of the geometrical optics of light to the case of neutrons. In quantum mechanical approach, the reflectivity is derived by considering neutron wave functions meeting barriers of the optical potential.***
- ***Off-specular scattering occurs for rough interfaces. It reduces the specular reflectivity. The distribution of off-specular scattering is sensitive to in-plane (lateral) correlations.***
- ***Lateral ordering of nanoscaled objects at interfaces produces 2D diffraction patterns (widened Bragg rods) in GISANS plane***



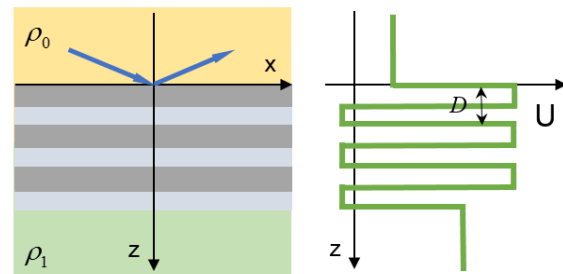
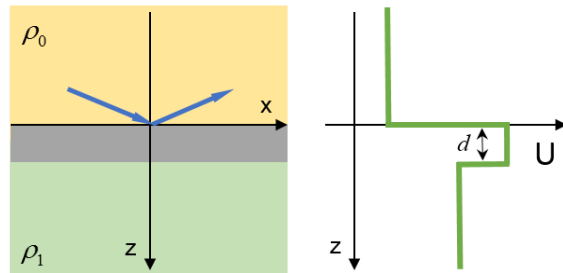
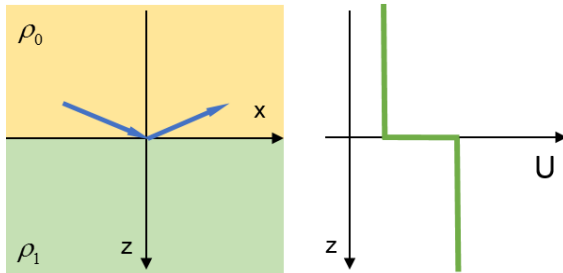
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# Reflectivity of arbitrary interface

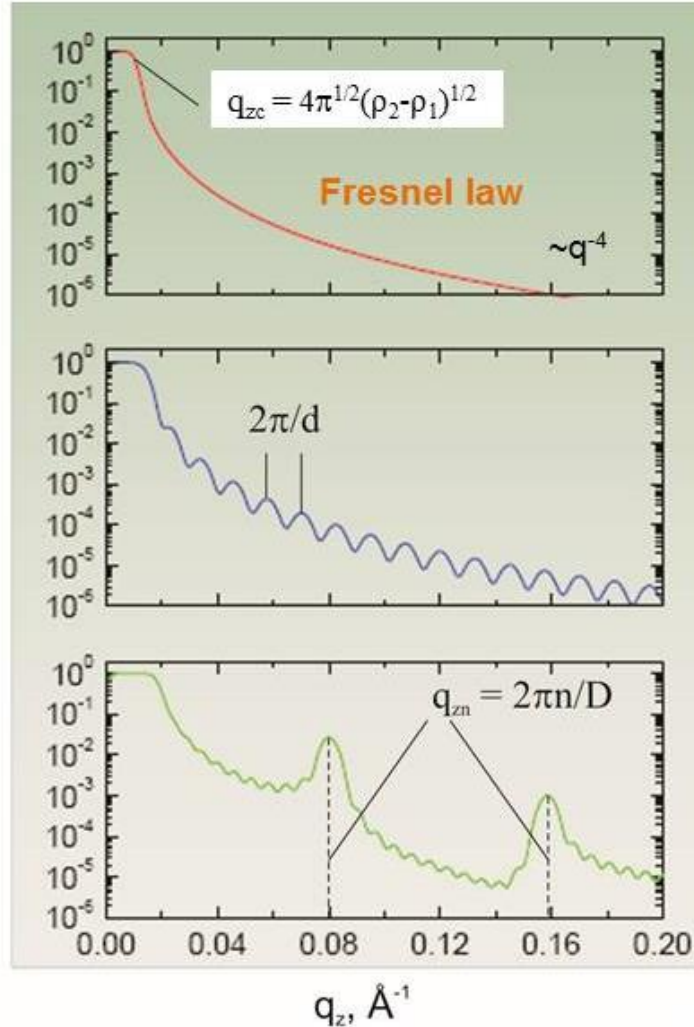
Born approximation

$$R(q_z) \approx \frac{16\pi^2}{q_z^4} \left| \int_{-\infty}^{+\infty} \left( \frac{d}{dz} \rho(z) \right) e^{-iq_z z} dz \right|^2$$

$q \gg q_{zc}$



Reflectivity



→ contrast  $\Delta\rho$

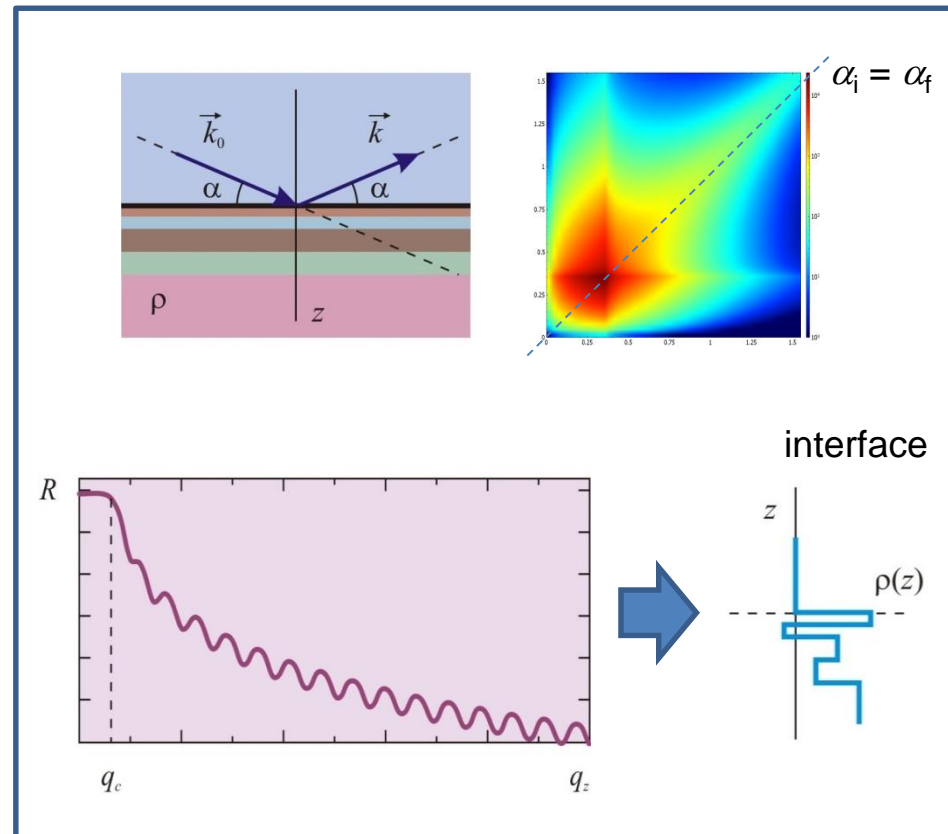
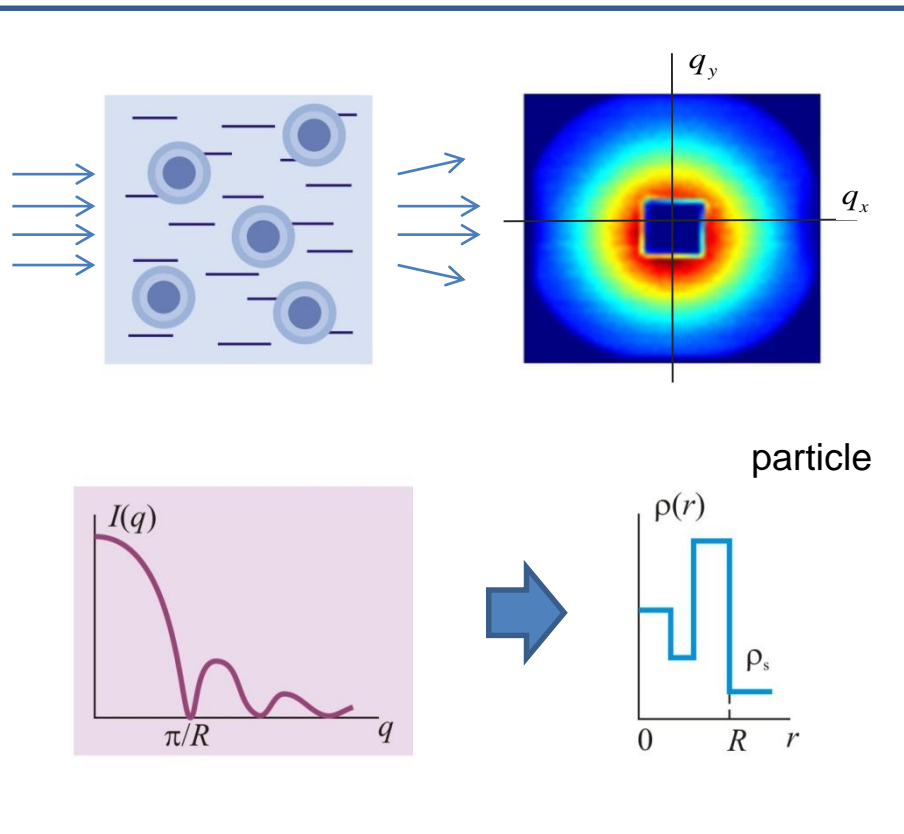
→ thickness of thin layer

→ period of superlattice

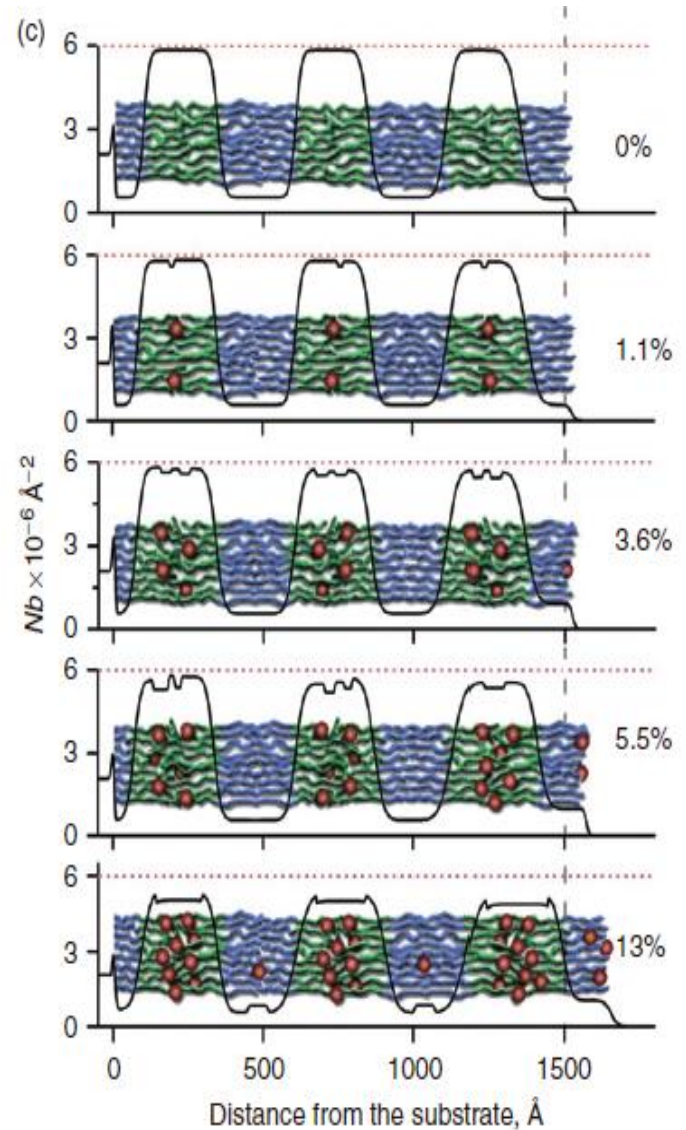
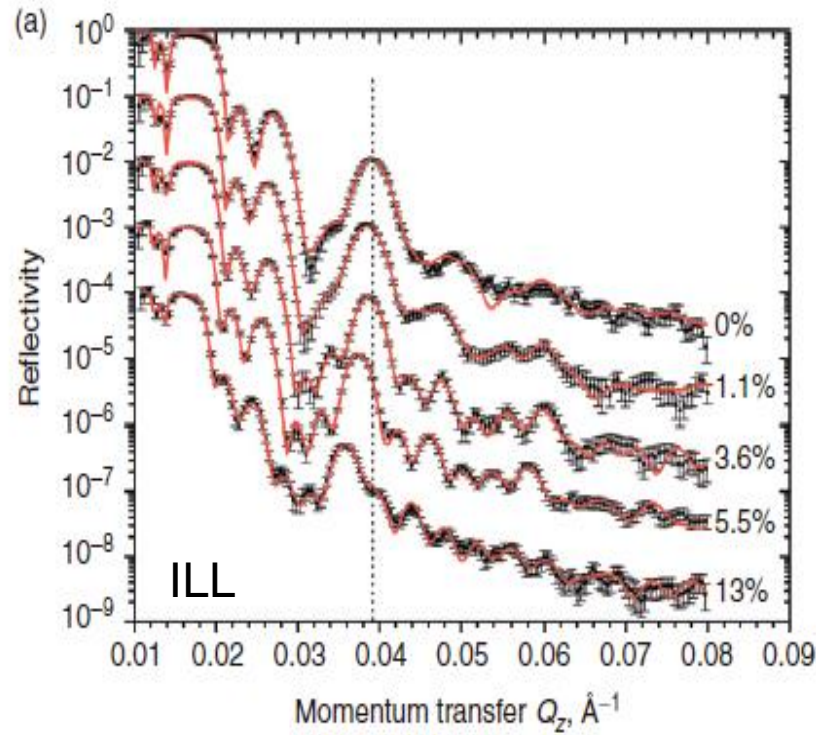
# Small-angle Scattering and Reflectometry

Small-angle scattering (SAXS, SANS)  
- bulk structure

Reflectometry (XRR, NR)  
- structure at interface



# Reflectivity from composite films



**Block copolymer (PS-d-b-PBMA)  
multilayers mixed with nanoparticles  
( $\text{Fe}_3\text{O}_4$ ,  $D \sim 5 \text{ nm}$ ) on Si substrate.**

Lauter, H.J.C., Lauter, V., Toperverg, B.P.  
*Polymer Science: A Comprehensive Reference*  
(2012) 2, 411

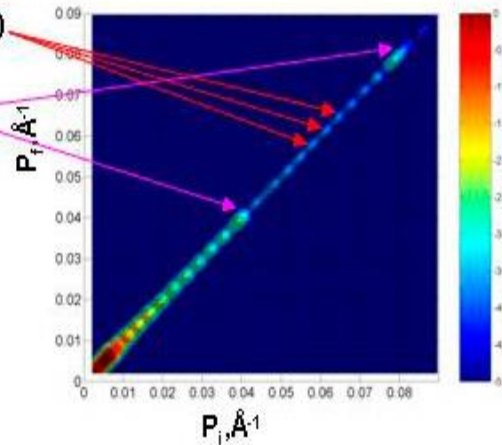
# Off-specular scattering from multilayers

## Ideal interfaces



$d = 80 \text{ \AA}$   
 $D = 960 \text{ \AA}$   
 $N = 12 \text{ layers}$

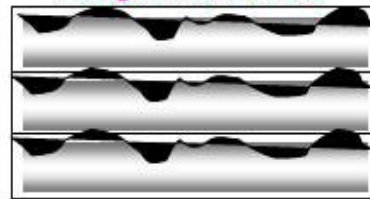
## Scattering from a non-magnetic multilayer



$2n\pi/D$   
 total thickness  
 oscillations

$2n\pi/d$   
 bilayer thickness  
 Bragg peaks

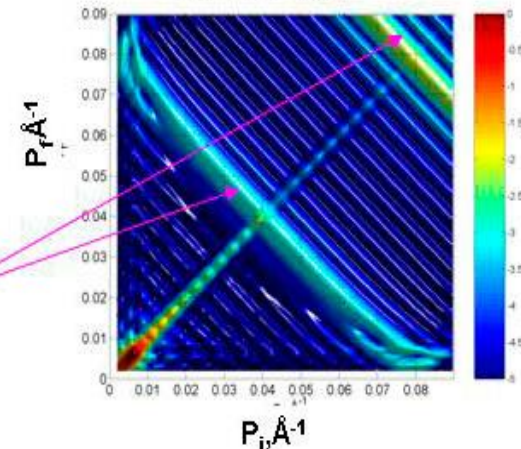
## Rough interfaces



$\sigma = 0.5 \text{ nm}$ ,  
 $\zeta_{\parallel} = 30 \text{ nm}$   
 $\zeta_{\perp} = \infty$

## Bragg-sheet scattering

Conf =  $\infty$

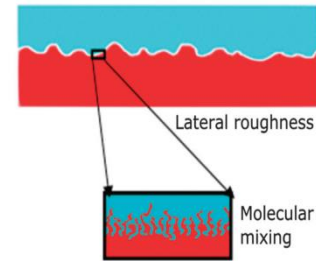




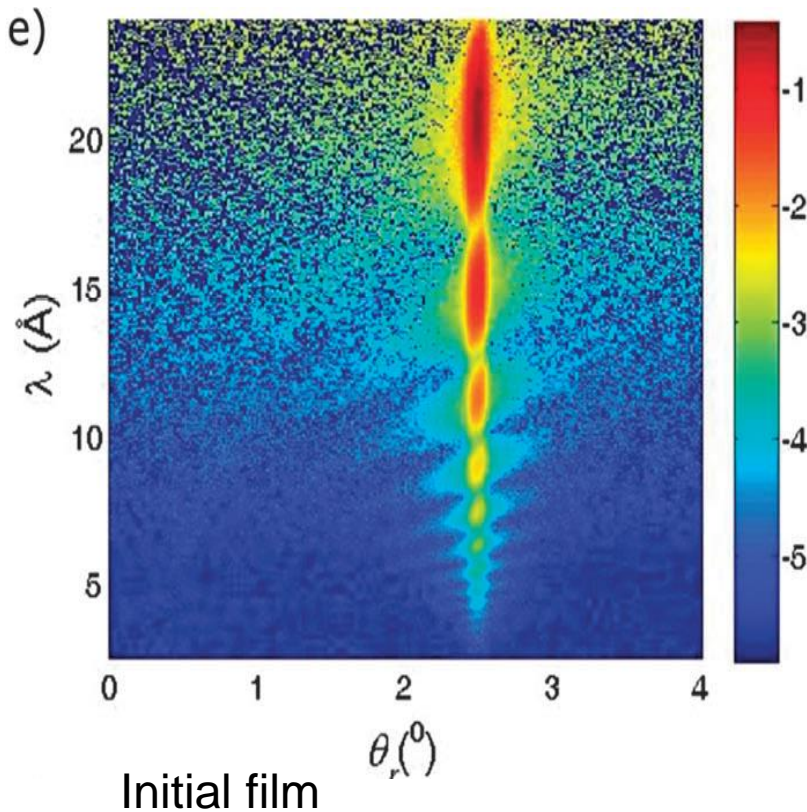
# Off-specular scattering in TOF mode

## Molecular mixing at a conjugated polymer interface

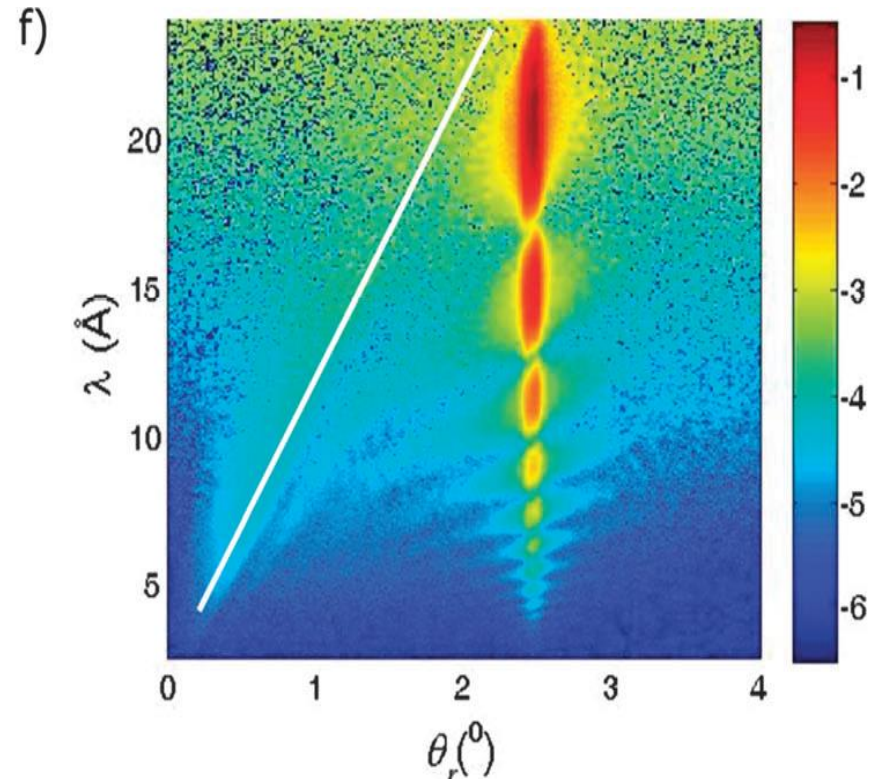
F8 [100 nm]/ d-PMMA [48 nm] / Si



D17, ILL



D.James, et al., *Soft Matter*  
**11**(48), 9393 (2015)



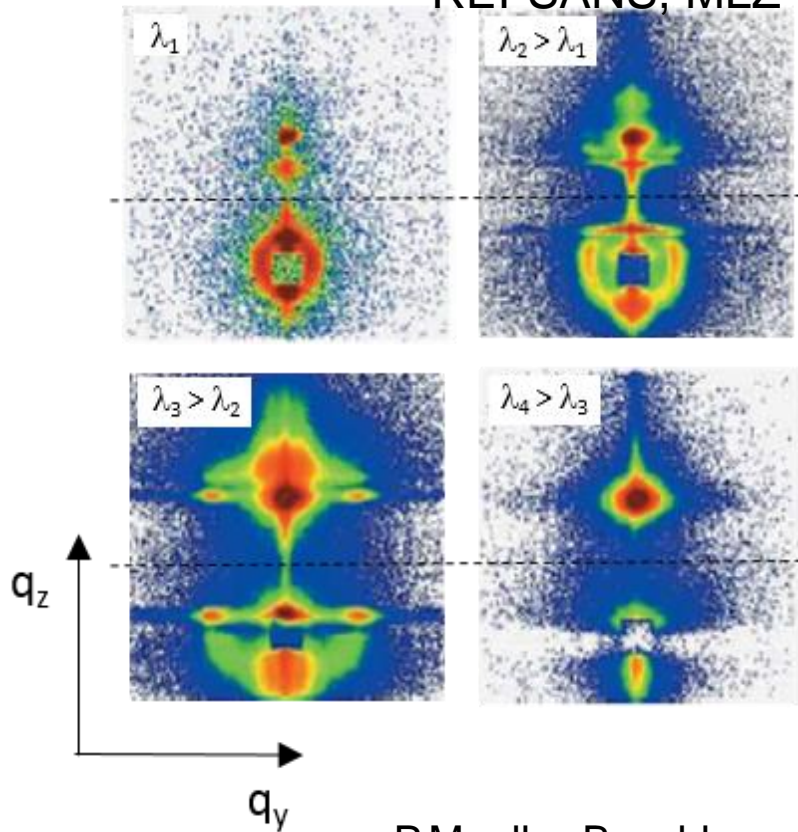
After annealing (Yoneda wing is  
marked by white line)

# GISANS

**Polymer P(S-b-MMA<sub>d</sub>) film  
(thickness 800 nm) on Si.**

Penetration depth depends on  
neutron wavelength

REFSANS, MLZ



$$z_{1/e} = \frac{\lambda}{2^{1/2} \pi (l_i + l_f)},$$

$$l_{i,f} = \left( (\alpha_c^2 - \alpha_{i,f}^2) + \sqrt{(\alpha_{i,f}^2 - \alpha_c^2)^2 + (\lambda \mu / 2\pi)^2} \right)^{1/2}$$

$\mu = \Sigma_{\text{tot}}$  - volume adsorption coefficient

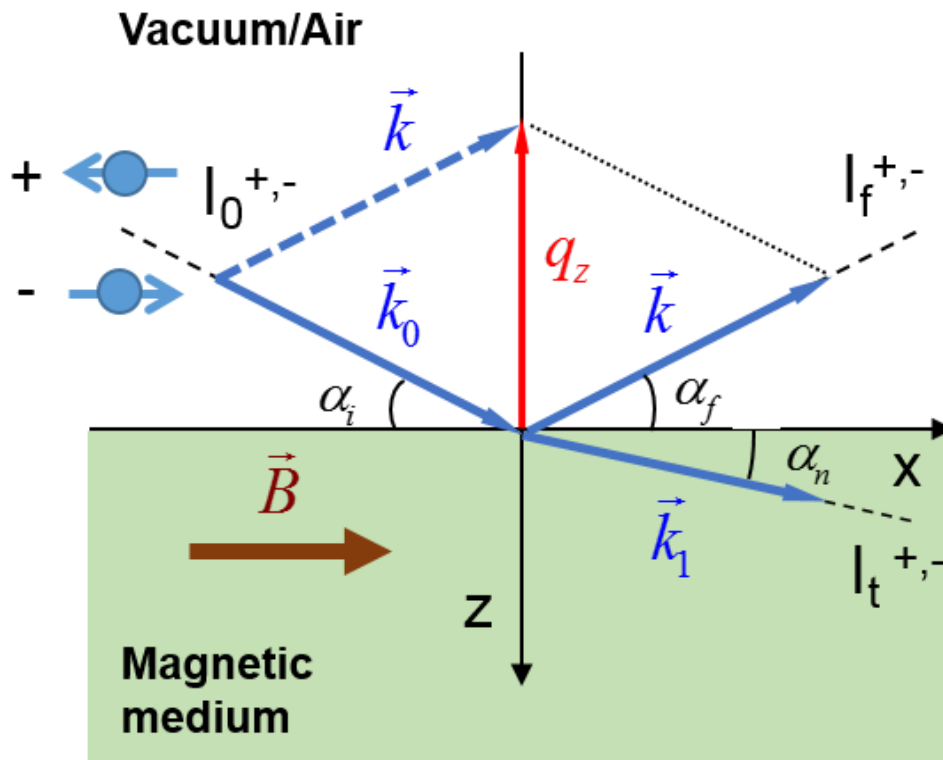
Both reflected and refracted beams  
are measured!

- Reflected beam
- Horizon
- Refracted beam

P.Mueller-Buschbaum, et al., Eur. Phys. J. 167, 107–112 (2009)

# Polarized neutrons

Specular reflection. Polarized beam.  
Tight z-collimation.



Refraction index

$$(n^\pm)^2 = 1 - [\lambda^2 Nb / \pi \pm (m / 2\pi\hbar^2) \mu B]$$

Nuclear SLD  $\rho_n = Nb$

Magnetic SLD  $\rho_m = (m\mu B / 2\pi\hbar^2)$

$$q_{zc}^\pm = (q_{zcn}^2 \pm q_{zcm}^2)^{1/2}$$

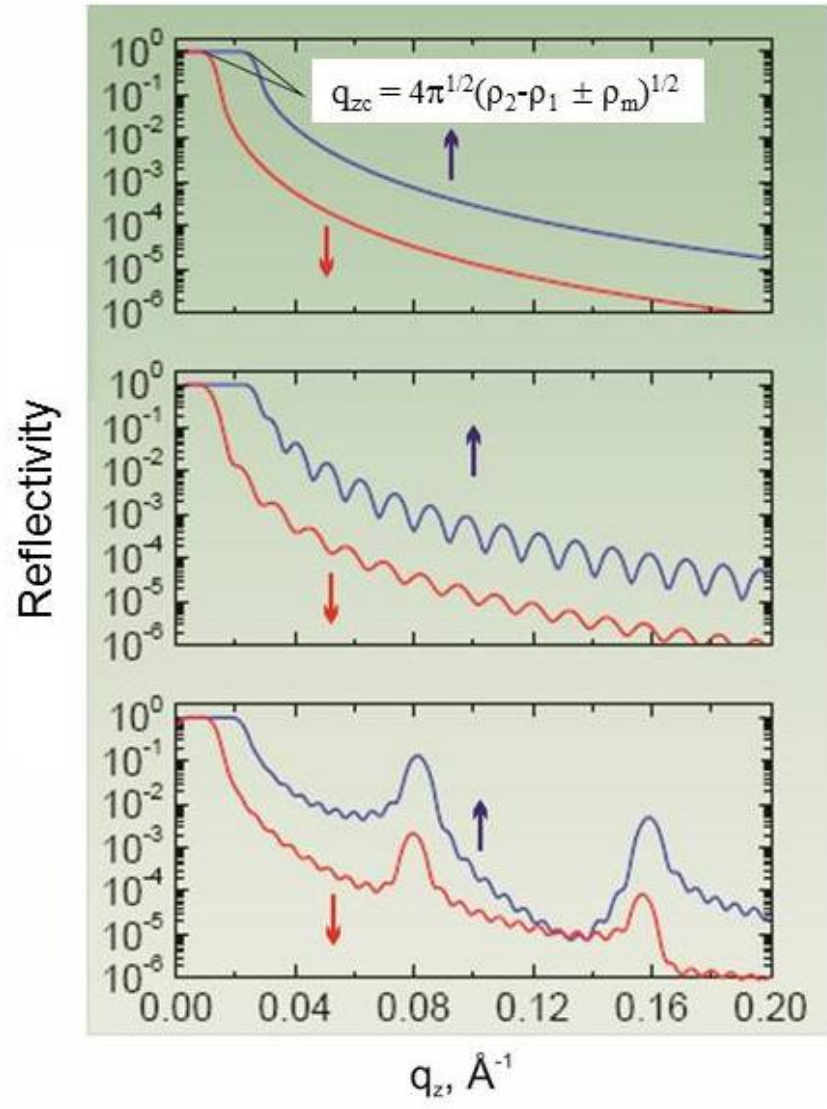
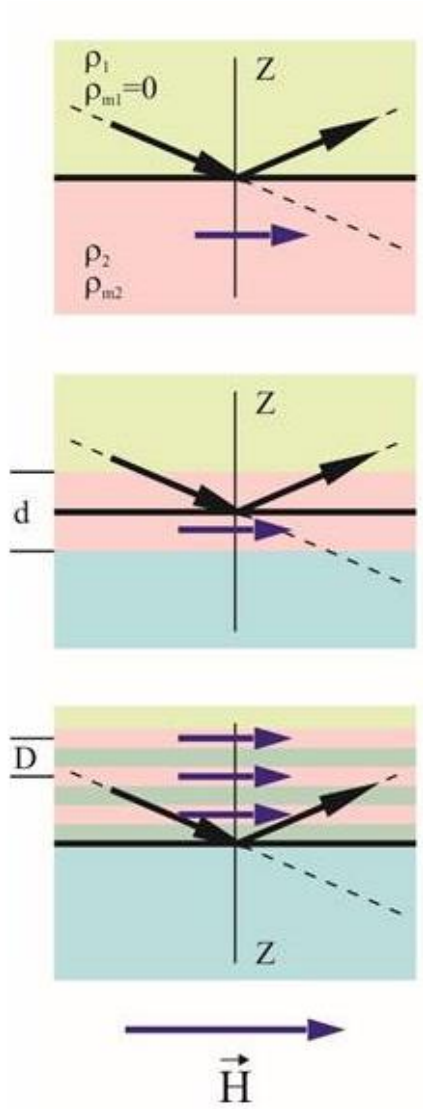
$$q_{zcn, zcm} = 4(\pi\rho_{n,m})^{1/2}$$

$$R^\pm(q_z) = \left| \frac{1 - \sqrt{1 - (q_{zc}^\pm)^2 / q_z^2}}{1 + \sqrt{1 - (q_{zc}^\pm)^2 / q_z^2}} \right|^2$$

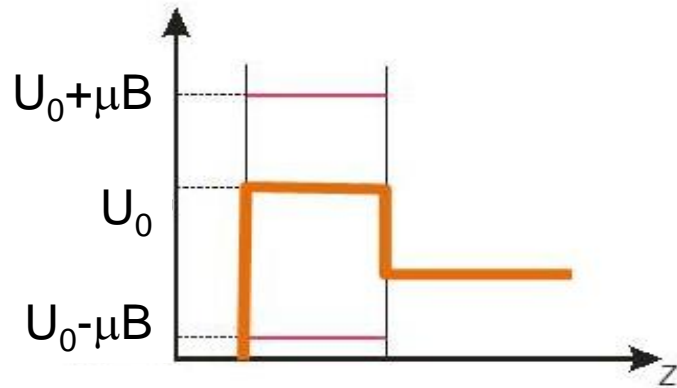


# Reflectivity of arbitrary interface. Polarized neutrons

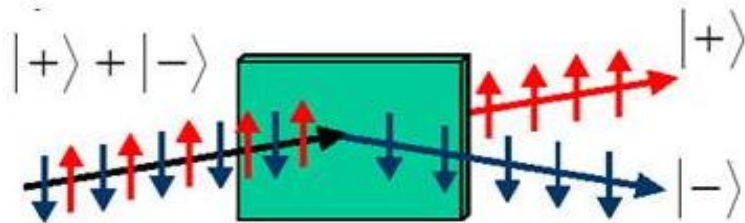
Born approximation  $R^\pm(q_z) = \frac{16\pi^2}{q_z^4} \left| \int_{-\infty}^{+\infty} \left( \frac{d}{dz} [\rho_n(z) \pm \rho_m(z)] \right) e^{-iq_z z} dz \right|^2 \quad q \gg q_{zc}$



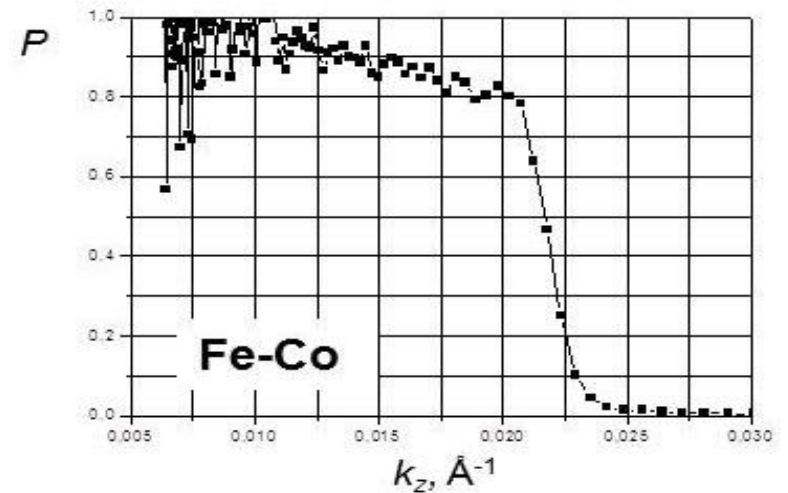
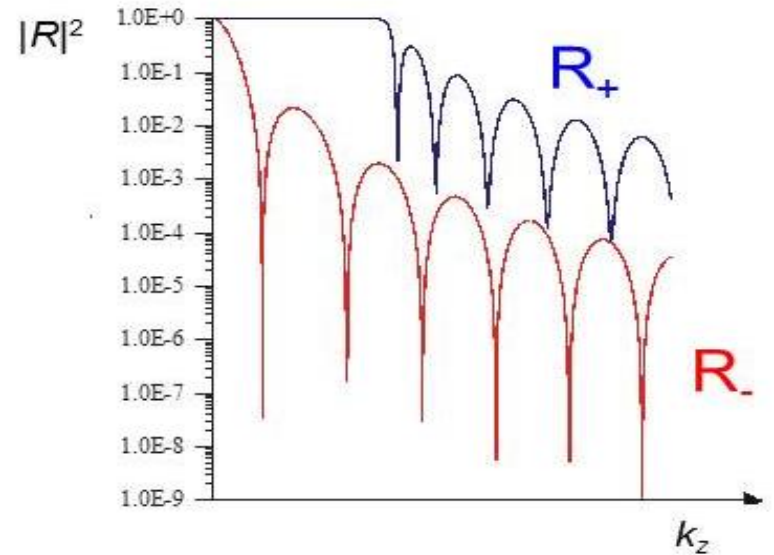
# Polarization of neutron beams



Polarization



$$P = \frac{N_+ - N_-}{N_+ + N_-} \quad P = \frac{R_+(k) - R_-(k)}{R_+(k) + R_-(k)}$$



# Off-specular scattering of polarized neutrons

Mixed states

$$\psi_{\perp i}(z) = \exp(ik_{0z}z) \begin{pmatrix} \psi_+^{(i)} \\ \psi_-^{(i)} \end{pmatrix}; \quad \text{- Incident beam}$$

$$\psi_{\perp f}(z) = \exp(-ik_{0z}z) \begin{pmatrix} \psi_+^{(f)} \\ \psi_-^{(f)} \end{pmatrix}. \quad \text{- Reflected beam}$$

Coefficient of reflection



$$\hat{r} = \begin{pmatrix} r_{++} & r_{+-} \\ r_{-+} & r_{--} \end{pmatrix} \quad \begin{pmatrix} \psi_+^{(f)} \\ \psi_-^{(f)} \end{pmatrix} = \hat{r} \begin{pmatrix} \psi_+^{(i)} \\ \psi_-^{(i)} \end{pmatrix}$$

Solutions of the system of Schrödinger equations!

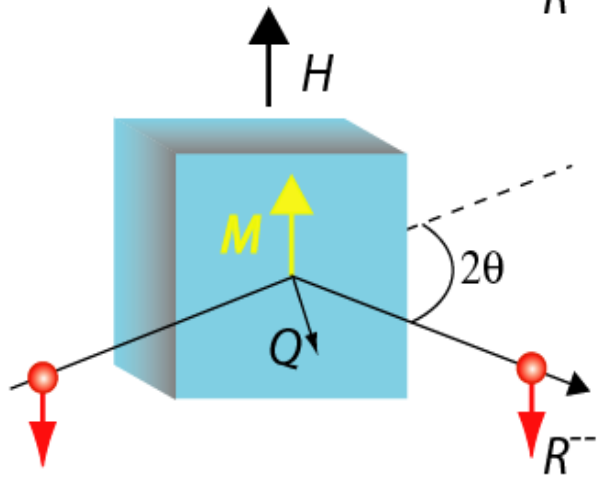
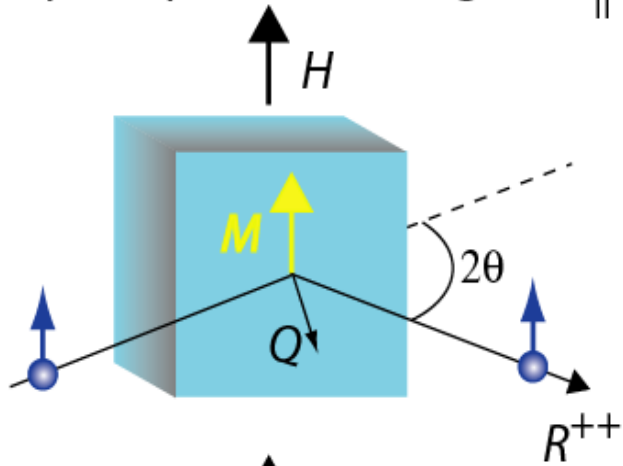
**Reflectivity matrix**

$$\left. \begin{array}{l} R_{++} = R_+ = |r_{++}|^2 \\ R_{--} = R_- = |r_{--}|^2 \end{array} \right\} \quad \underline{\text{reflection from in-plane } M\text{-component}}$$

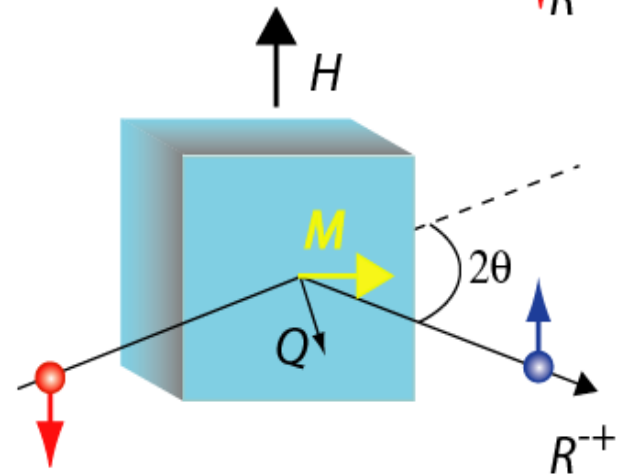
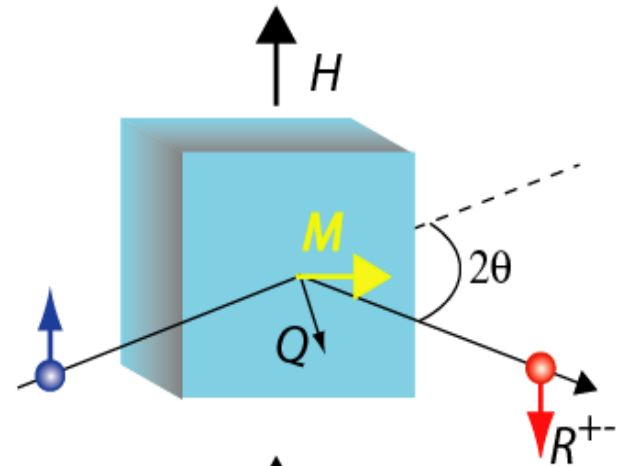
$$\left. \begin{array}{l} R_{+-} = |r_{+-}|^2 \\ R_{-+} = |r_{-+}|^2 \end{array} \right\} \quad \underline{\text{reflection from out-of-plane } M\text{-component}} \\ \underline{\text{(e.g. magnetic roughness)}}$$

# Full polarization analysis

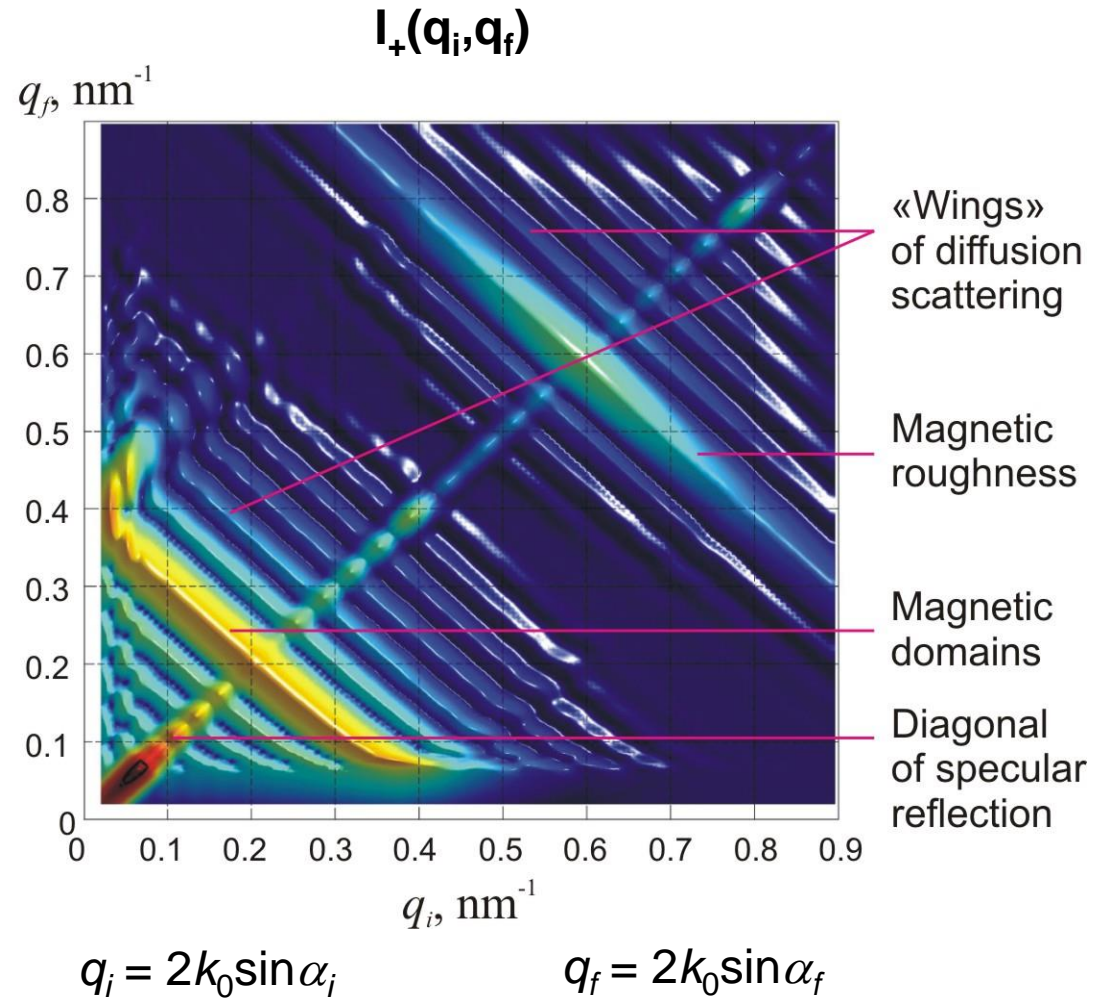
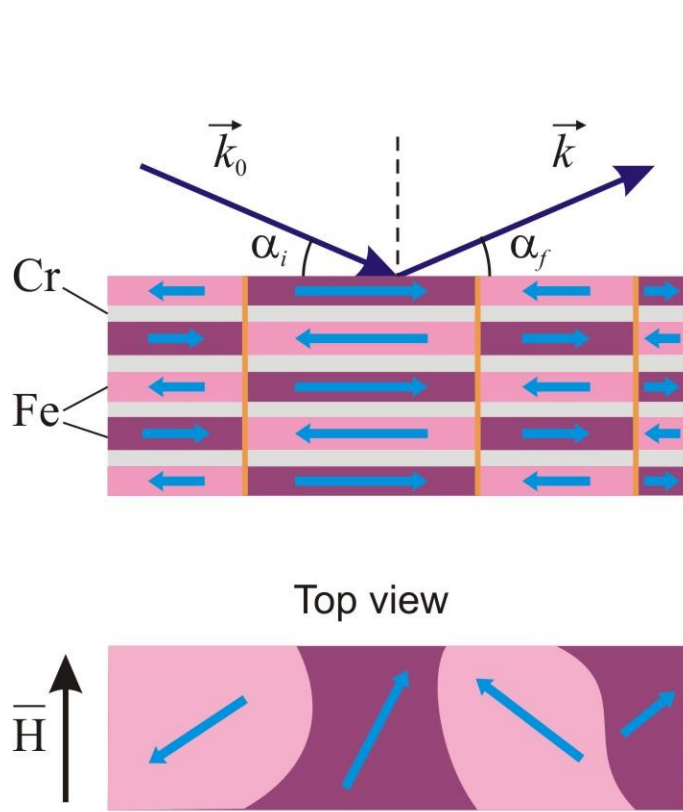
non-spin-flip reflectivities give  $\overline{M}_{\parallel}(Q)$



spin-flip reflectivities give  $\overline{M}_{\perp}^2(Q)$



# Magnetic multilayers

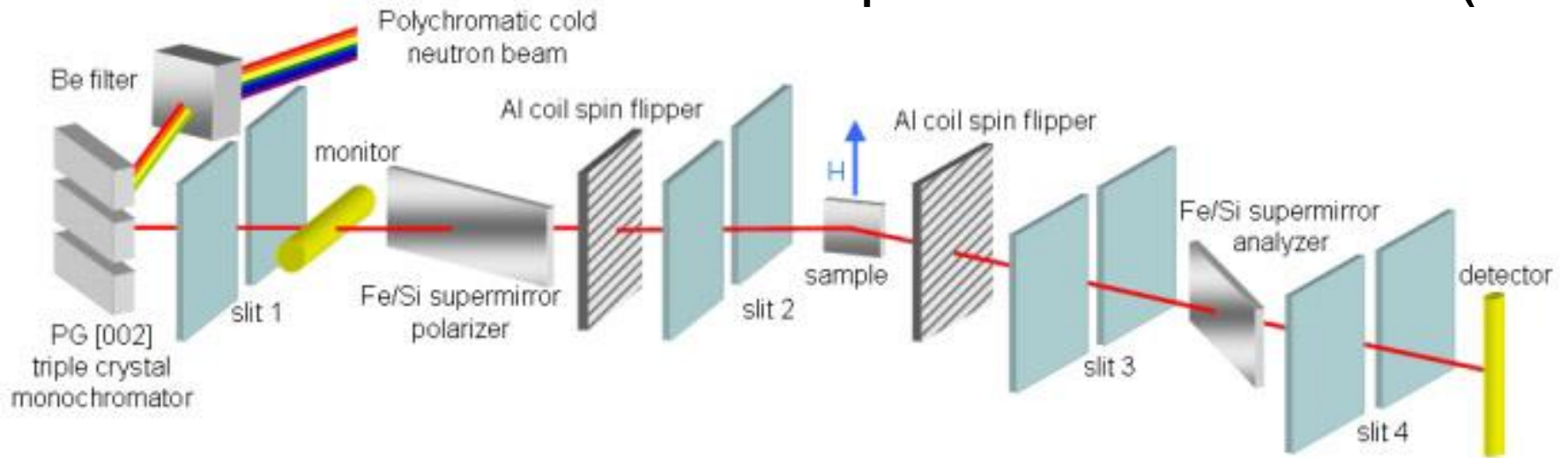


V. Lauter-Pasyuk, J. Phys. IV France 1 (2007)

**Software:** FitSuite L. Deák et al, PRB 76 224420 (2007 )

# Neutron reflectometer

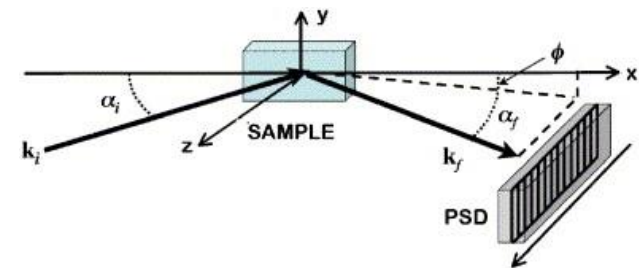
## PBR polarized beam reflectometer (NIST)



### Main units

- **Polarizer** (spin polarization of neutron beam)
- **Spin-flippers** (change of beam polarization at given polarization after polarizer or sample)
- **Analyzer** (analysis of polarization after sample)
- **Detector** (detection of scattered and transmitted beams)

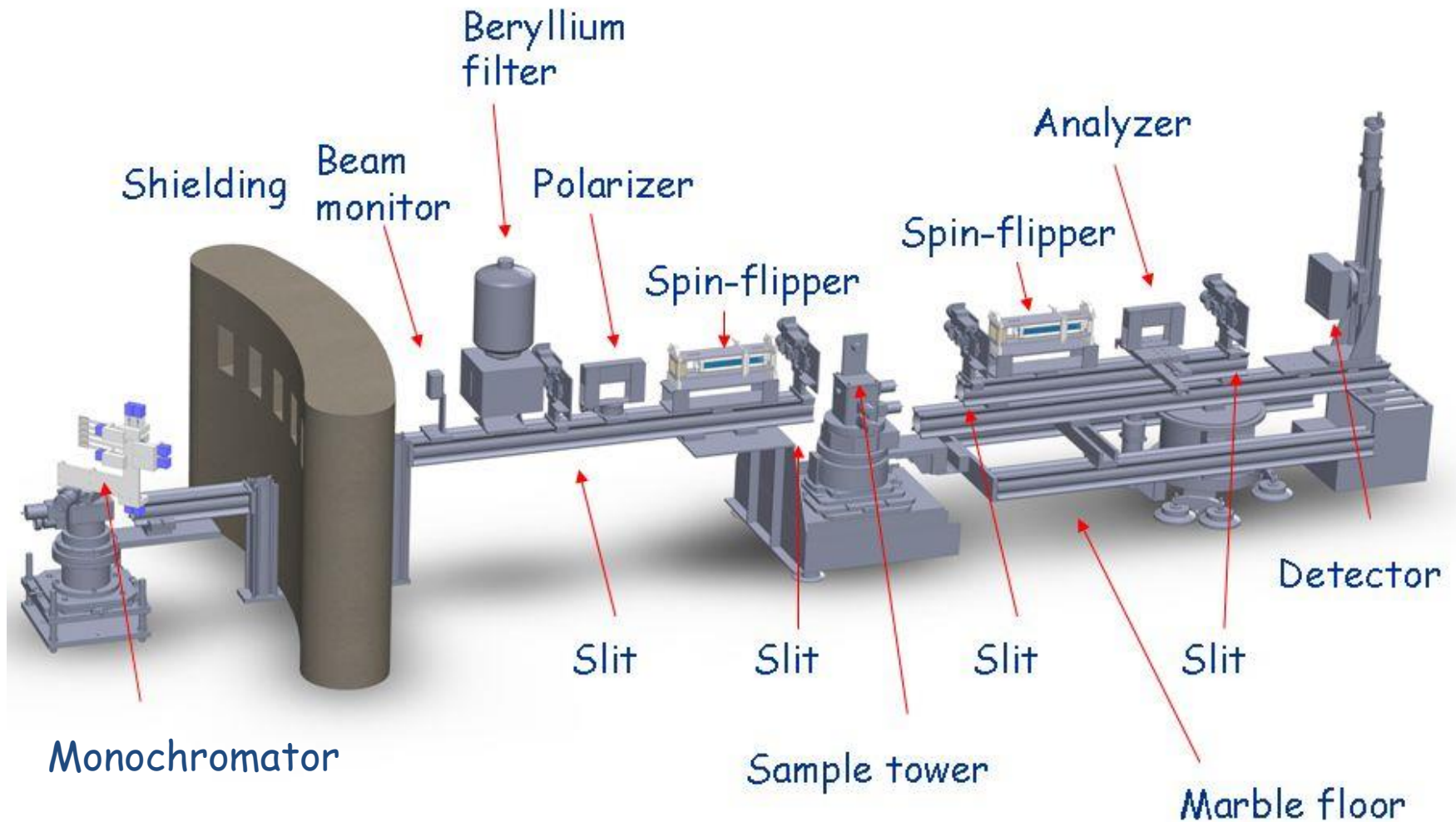
### Vertical sample geometry





# Neutron reflectometer

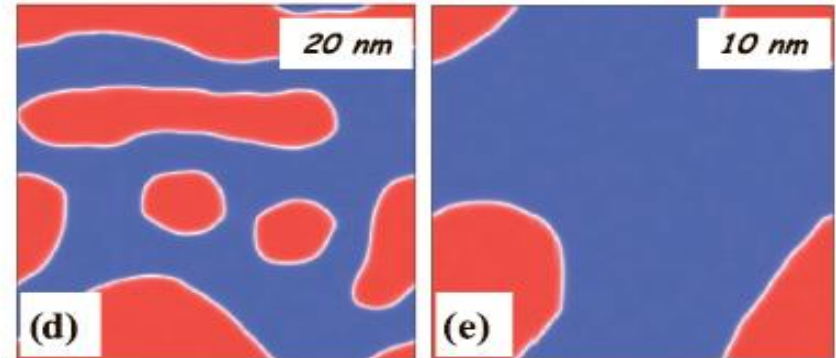
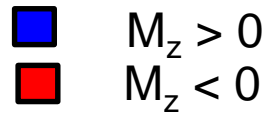
## GINA reflectometer (BNC, Budapest)



# Domain structure in thin films with perpendicular anisotropy

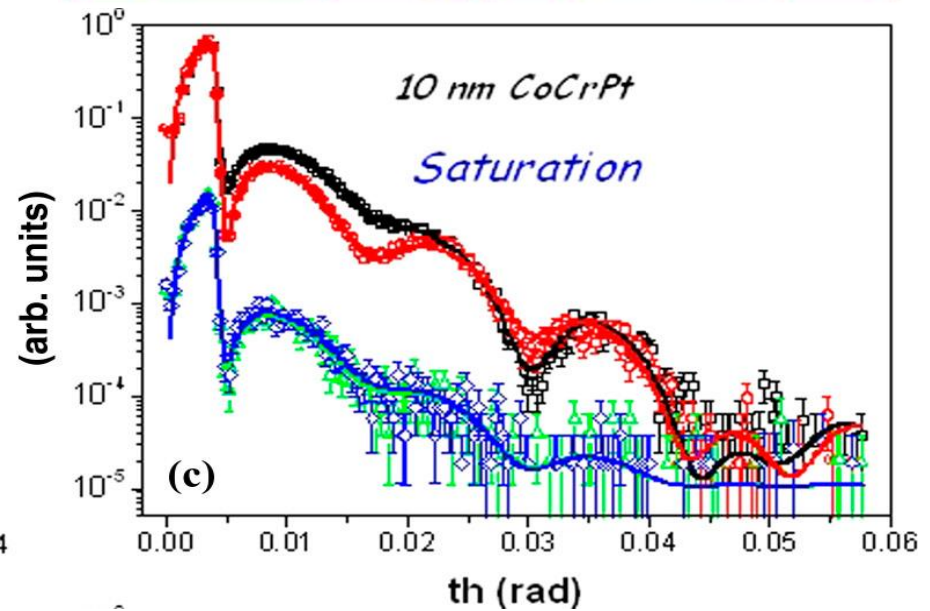
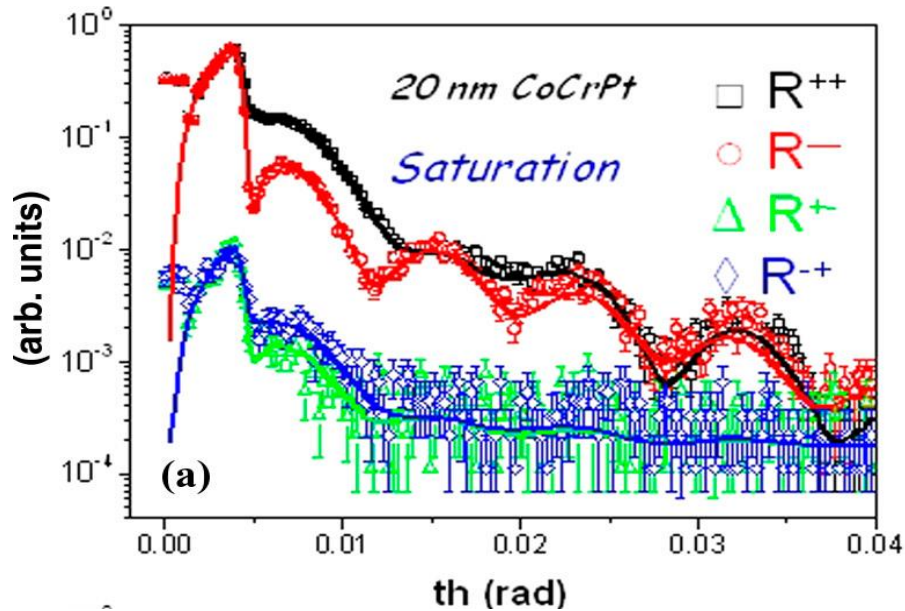
CoCrPt films

Micromagnetic simulations



SuperADAM, ILL

NR



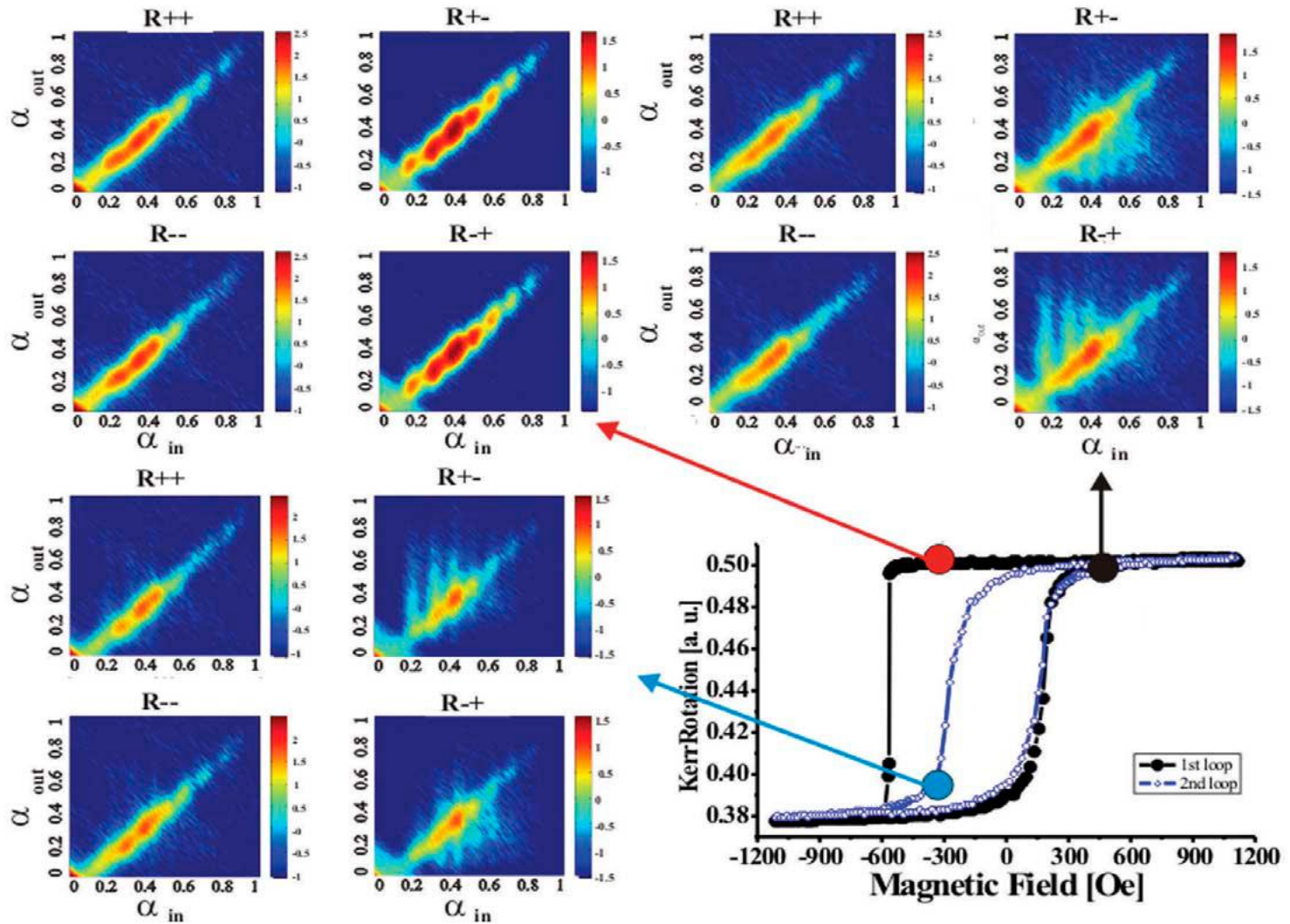
D. Navas, PRB **90**, 054425 (2014)



# Magnetic bilayer with exchange bias

CoO [2 nm] / Co [20 nm]

HZB



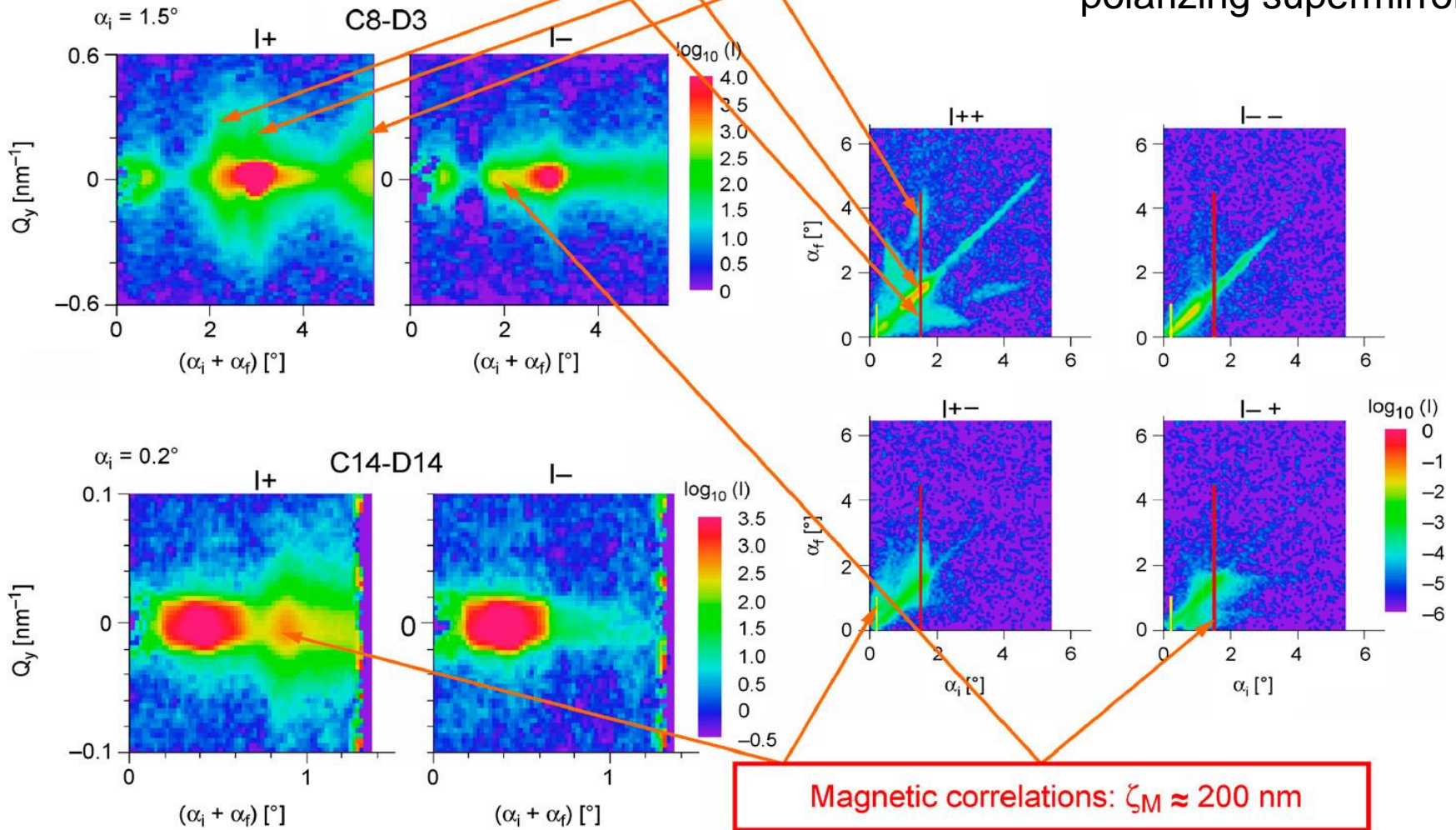
H. Zabel, Materials Today 9 (2006)

# GISANS. Polarized neutrons

KWS-2, FRJ-2

Roughness:  $\zeta_R \approx 15$  nm

FeCoV/TiN<sub>x</sub>  
polarizing supermirror



## Summary to

### 'Reflectometry of non-polarized and polarized neutrons from solid interfaces'

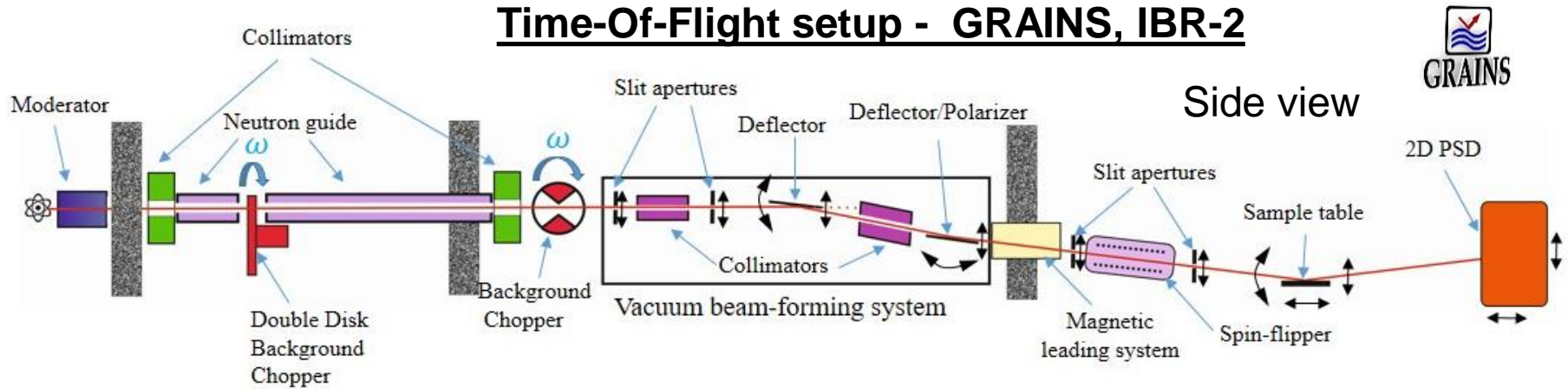
- ***Three neutron reflectometry modes are efficient in the characterization of the multilayered interface structures at interfaces. In addition to the structure, modulation along the depth profile, the characteristic of the distributions in in-plane and out-of-plane correlations are well determined using specific features in off-specular scattering and GISANS patterns.***
- ***Polarized neutron reflectometry is very efficient in the study of magnetic layered interface structures. The characteristics of the magnetic scattering length density distribution at interfaces are related to the magnetization distribution. Thus, the method represents a spatial magnetometry.***

- Principles of Neutron Reflectometry
- Reflectometry of Non-Polarized and Polarized Neutrons from Solid Interfaces
- Neutron Reflectometry from Interfaces with Liquids**
- Experimental Aspects of Neutron Reflectometry



# Horizontal reflectometers

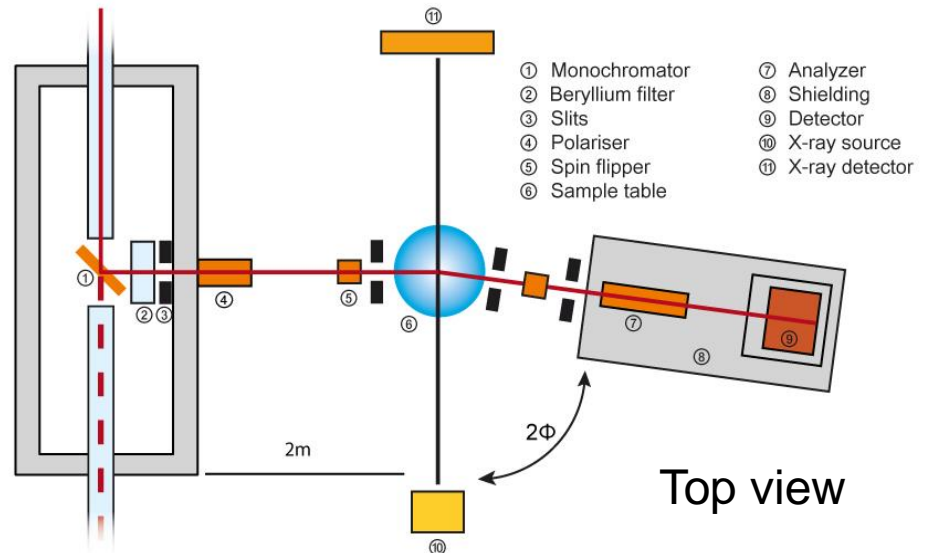
## Time-Of-Flight setup - GRAINS, IBR-2



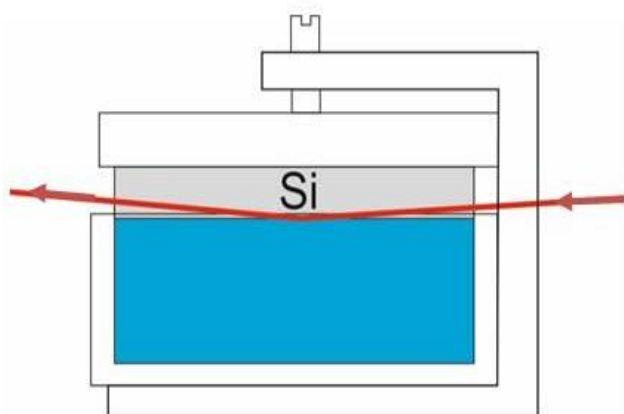
## Steady-State setup - N-REX, MLZ

Horizontal sample plane → studies of interfaces with liquids:

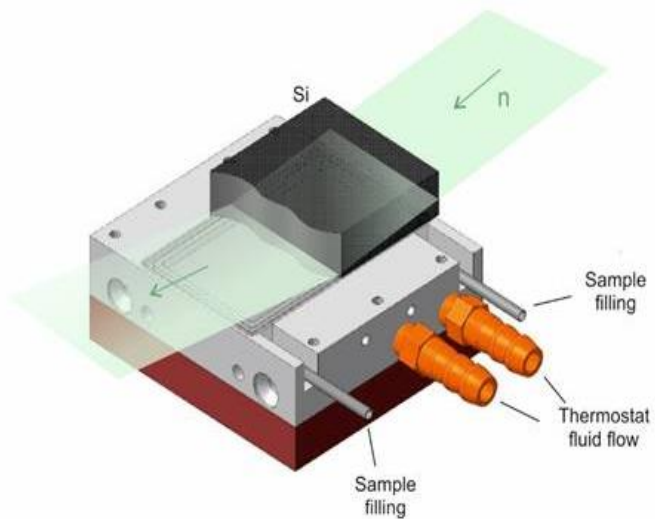
- Solid – Liquid;
- Air – Liquid;
- Liquid – Liquid



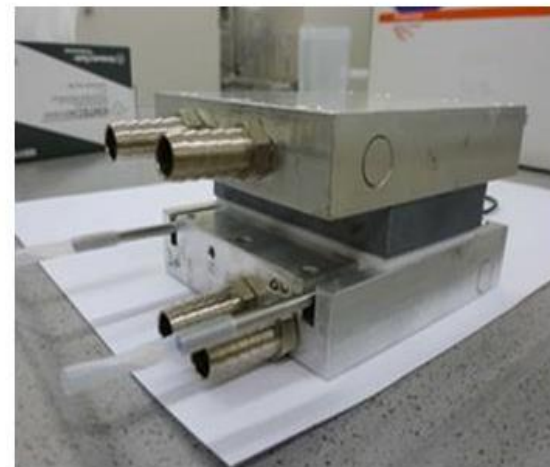
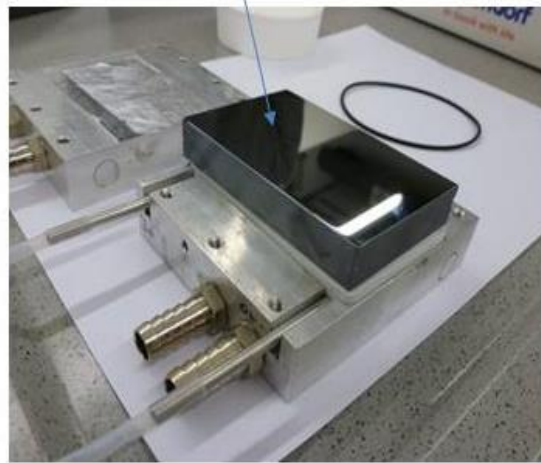
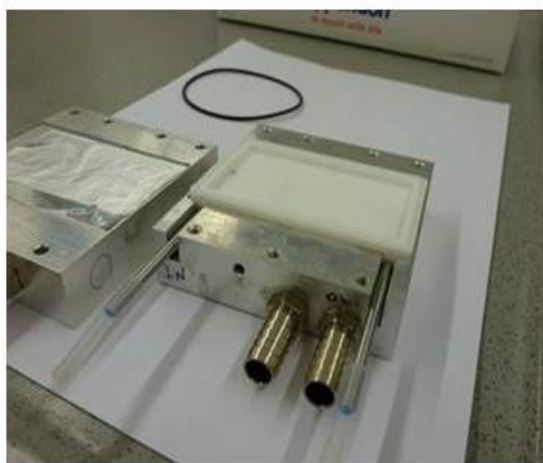
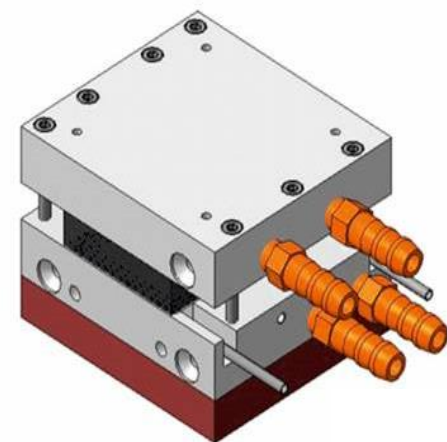
# NR from Solid-Liquid interfaces



**Sample volume  
5-10 ml**

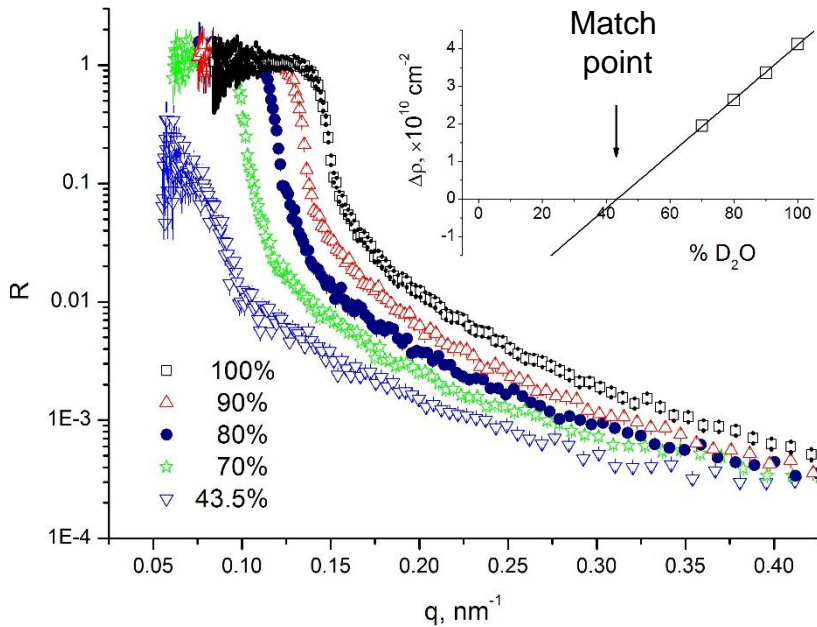


**Si crystal block  
(5 × 7.5 × 1.5 cm<sup>3</sup>)**

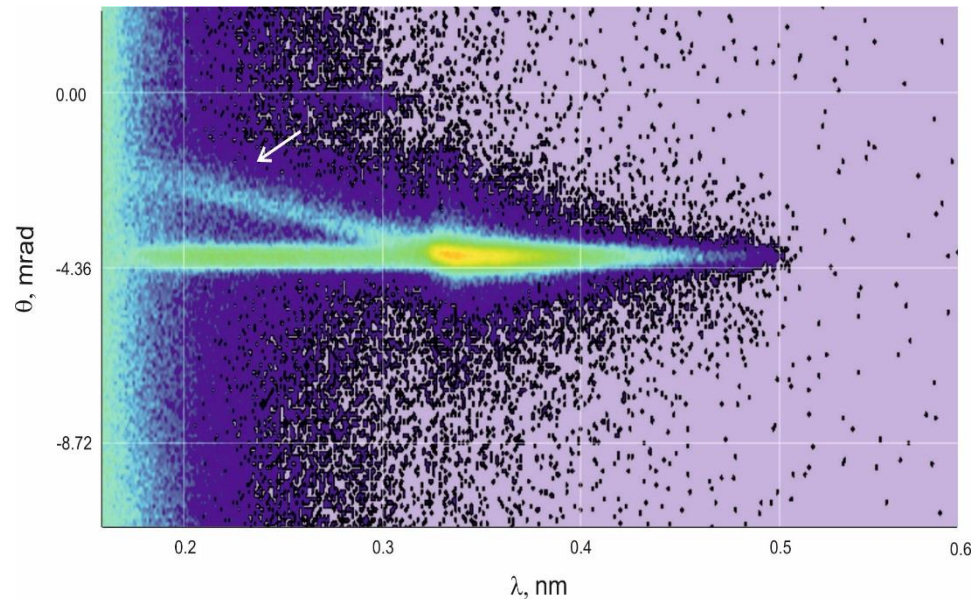


# Simplest interface: Silicon - Water

Specular reflectivity: contrast variation



Diffuse scattering:  
long-period non-homogeneities of substrate



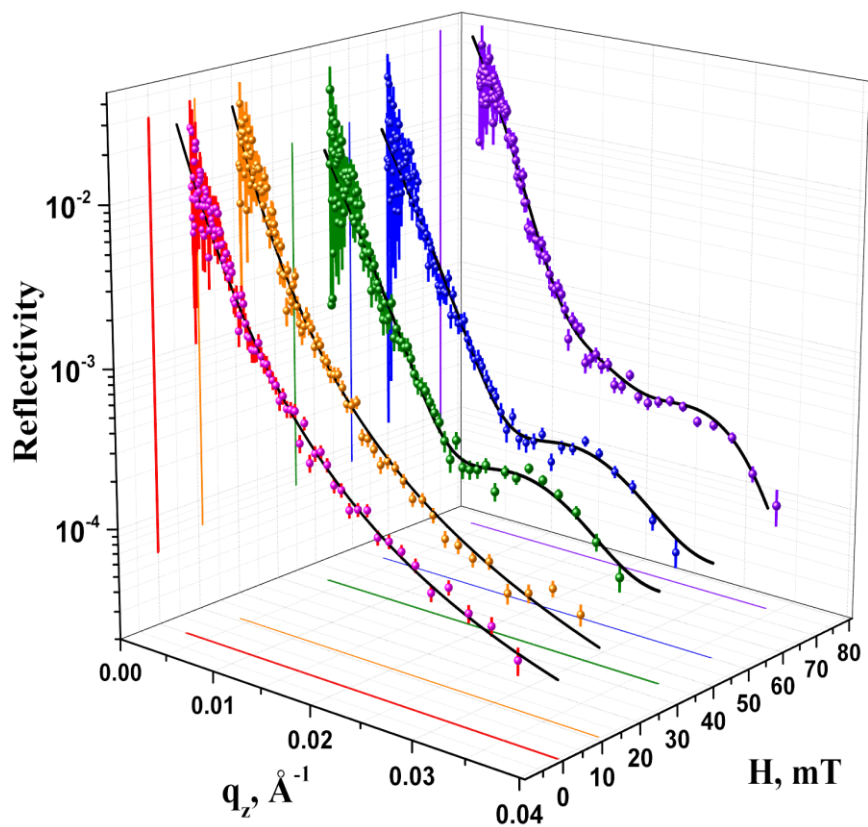
TOF mode (GRAINS, Dubna)

M.V. Avdeev, V.I. Bodnarchuk, V.I. Petrenko, I.V. Gapon, O.V. Tomchuk, A.V. Nagornyi, V.A. Ulyanov, L.A. Bulavin, V.L. Aksenov, Crystallography Reports 62 (6) (2017) 1002–1008

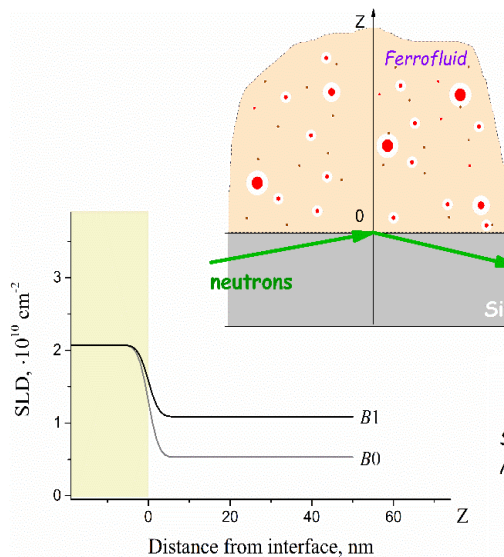


# Interface Assembling of Magnetic Nanoparticle from Ferrofluids Induced by Non-Homogeneous Magnetic Field

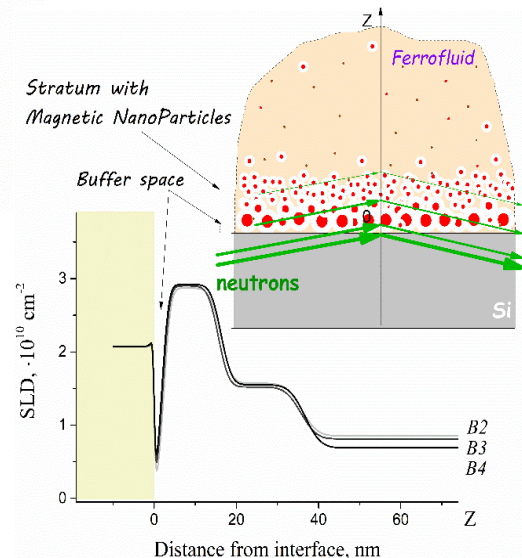
Nanomagnetite ( $\varnothing$  2-200 nm) in transformer oil,  $\varphi_m \sim 6\%$



GRAINS, IBR-2, Dubna



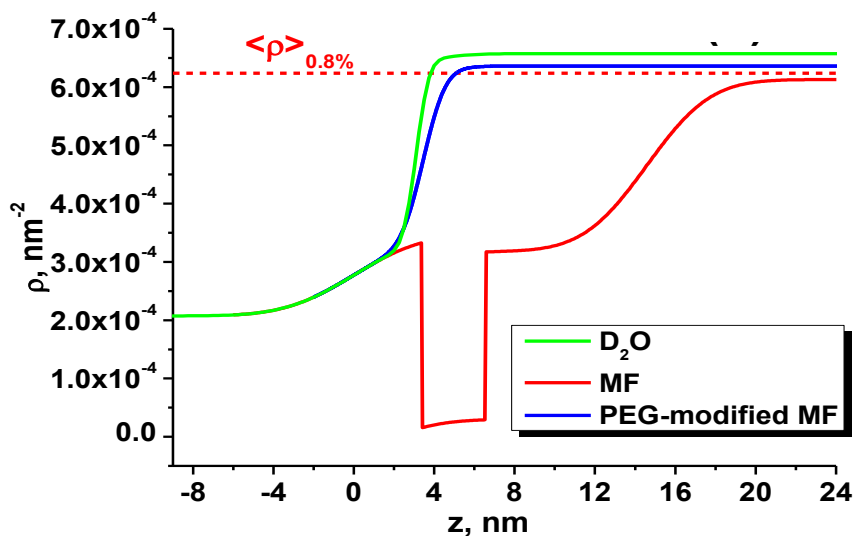
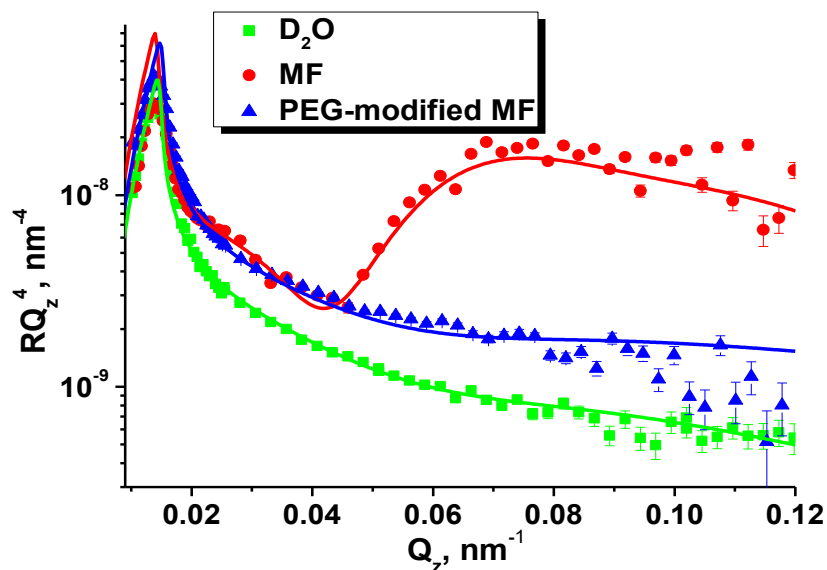
zero and weak magnetic fields



higher magnetic flux density (35-75 mT)

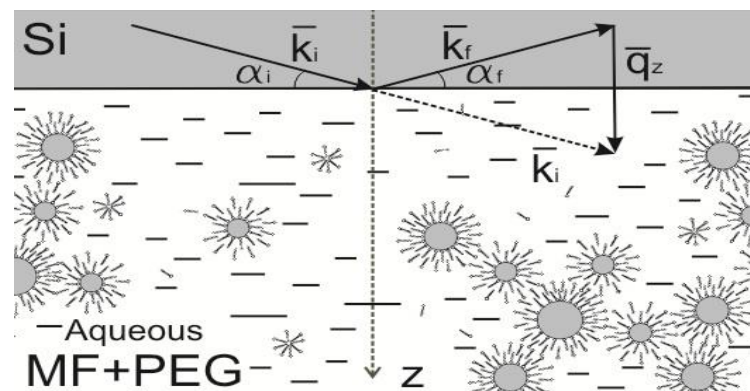
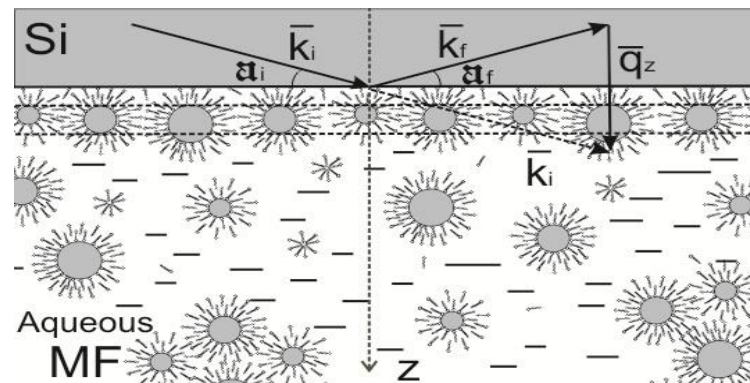


# Adsorption of nanoparticles from aqueous magnetic fluids on silicon substrate



NREX+, FRM-II, Munich

Effect of polymer (PEG) modification



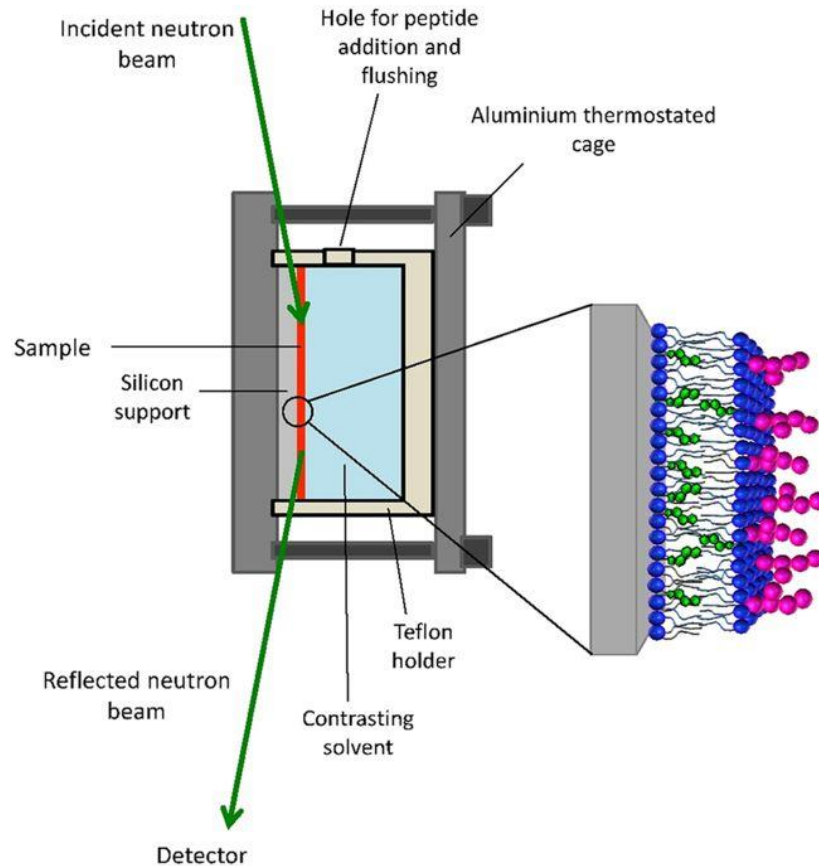
PEG – poly(ethylene glycol)

M.V. Avdeev, V.I. Petrenko, I.V. Gapon, L.A. Bulavin, A.A. Vorobiev, O. Soltwedel, M. Balasoiiu, L. Vekas, V. Zavisova, P. Kopcansky, *Appl. Surf. Sci.* 352 (2015) 49

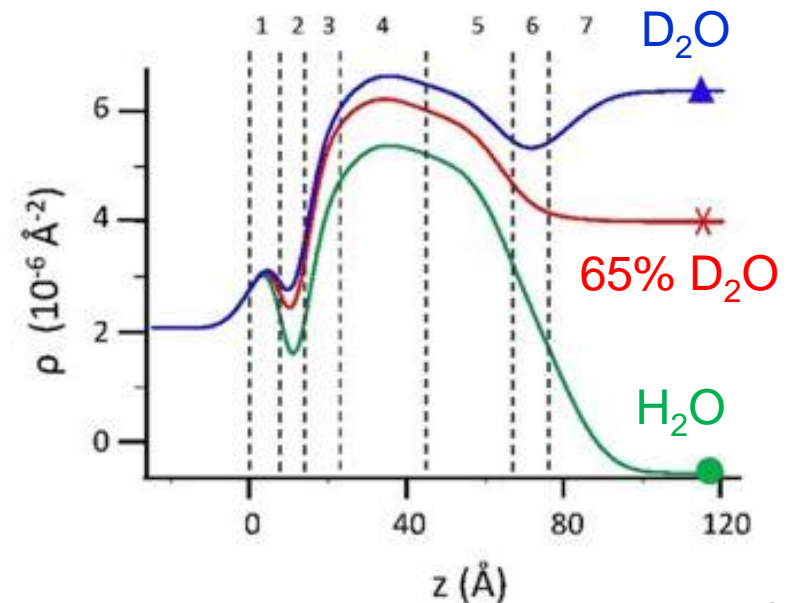
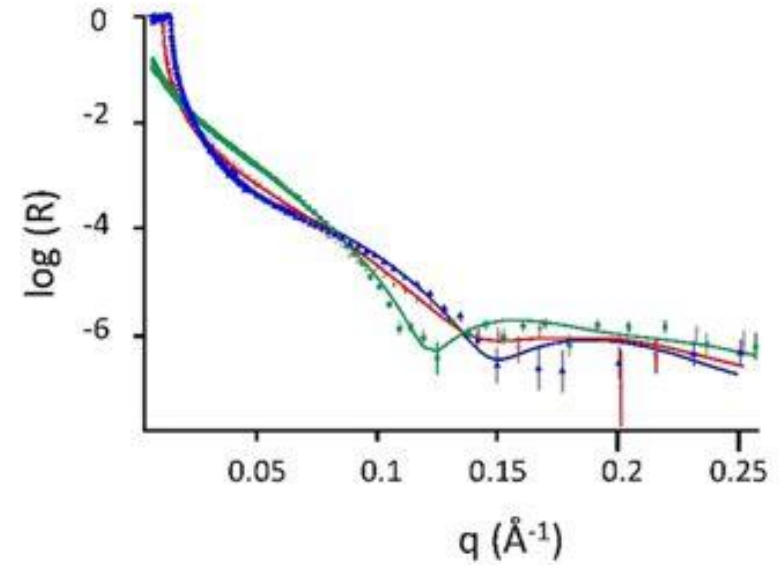
M.Kubovcikova, I.V.Gapon, V.Zavisova, M.Koneracka, V.I.Petrenko, O.Soltwedel, L.Almasy, M.V. Avdeev, P.Kopcansky, *J. Magn. Magn. Mater.* 427 (2017) 67

# Amyloid $\beta$ Peptides in interaction with raft-mime model membranes

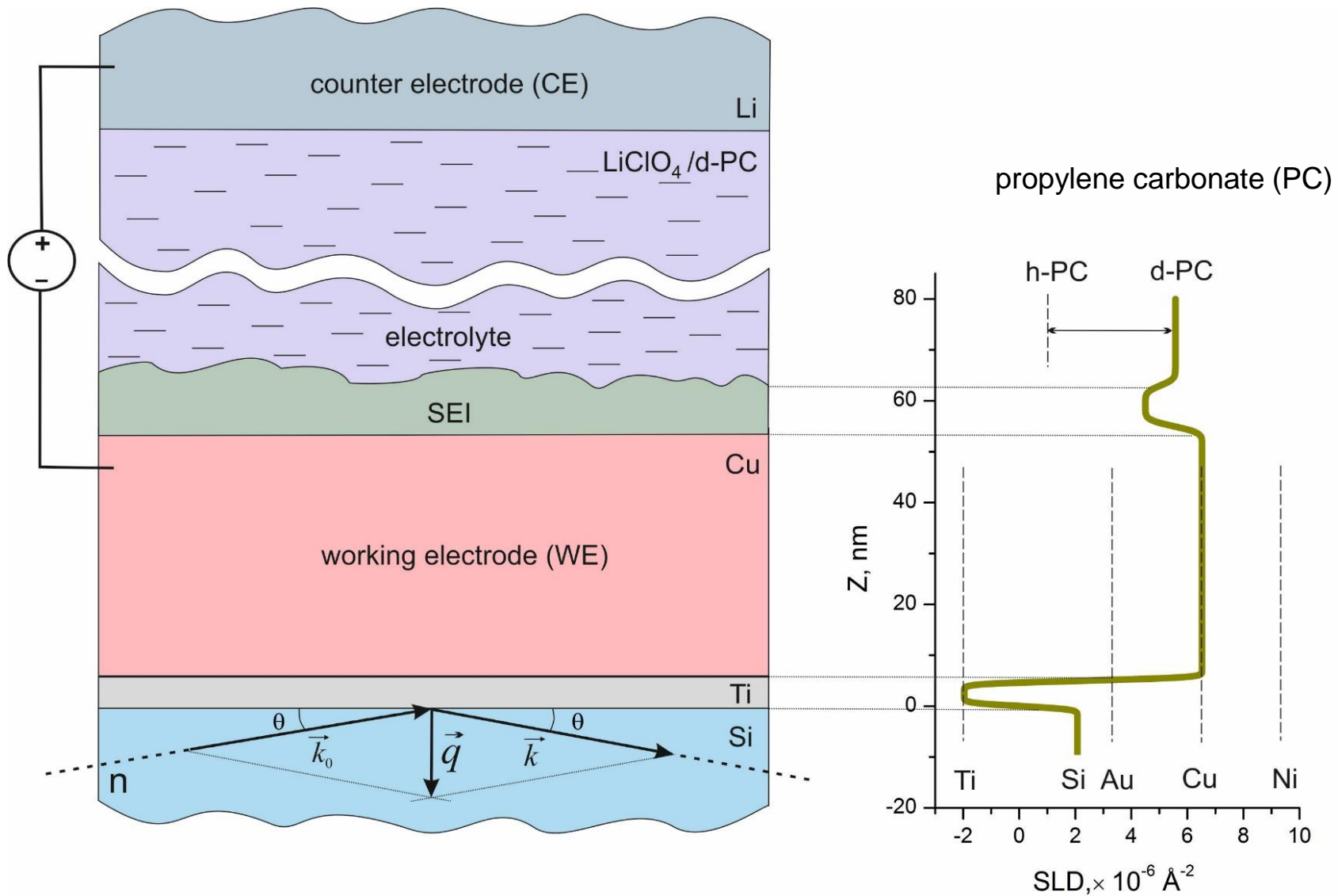
## Vertical geometry



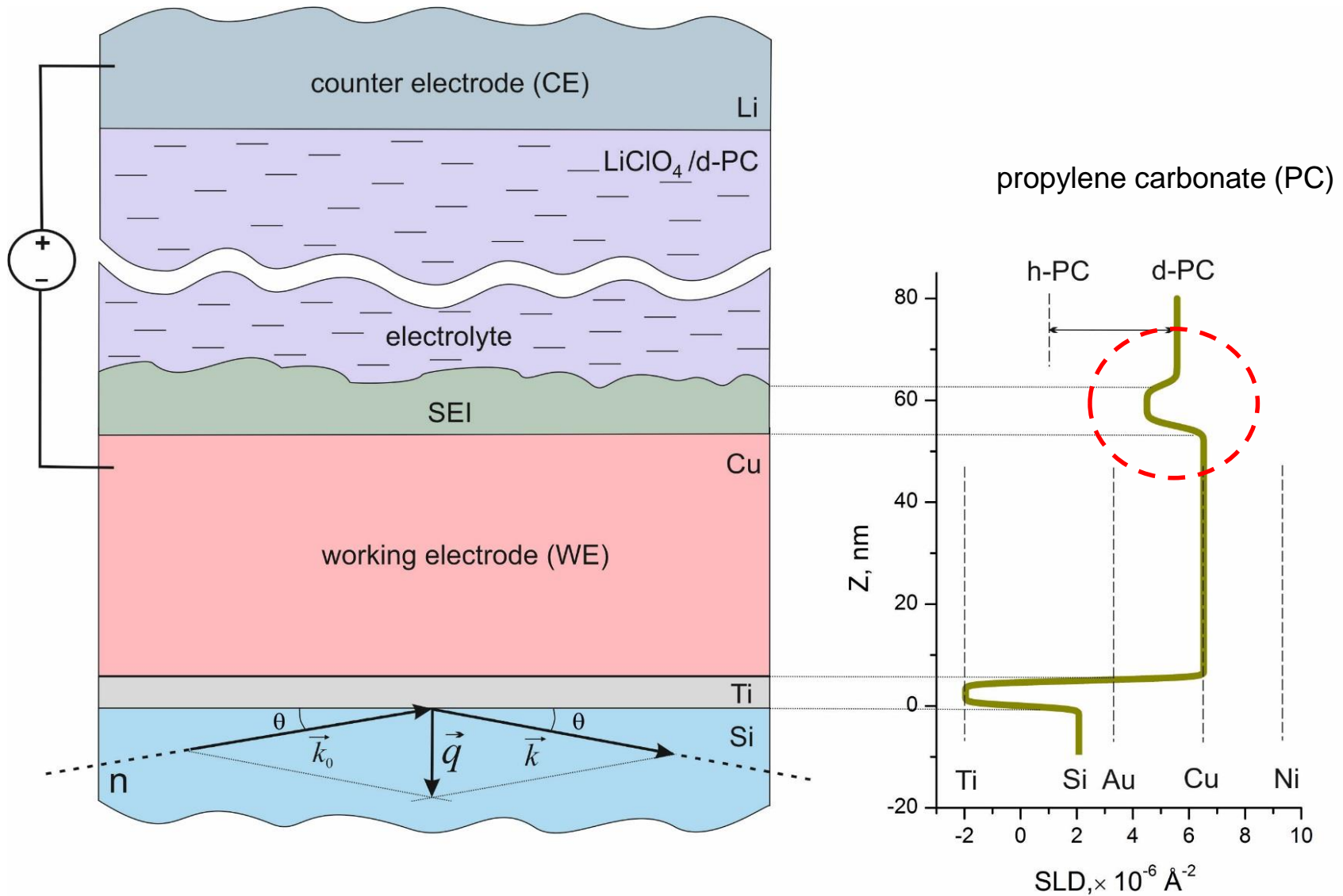
D17, ILL, Grenoble



# Study of Electrolyte-Electrode Interfaces by NR

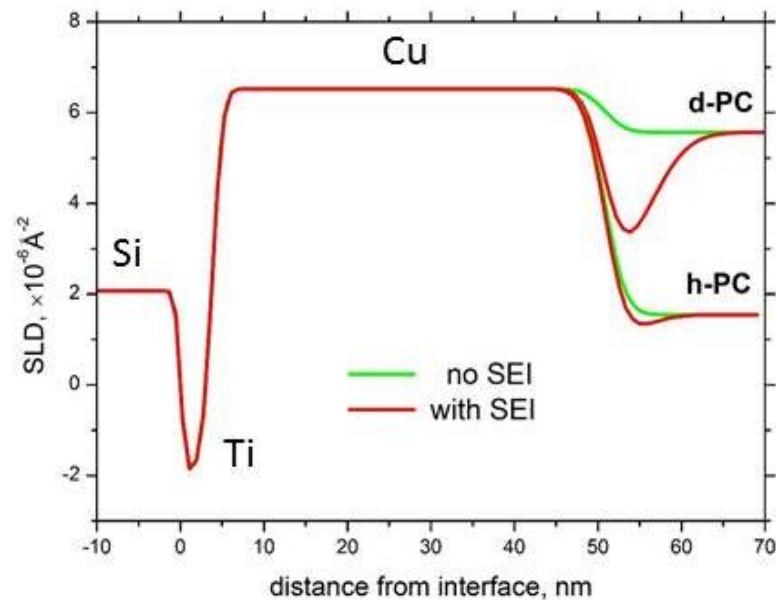
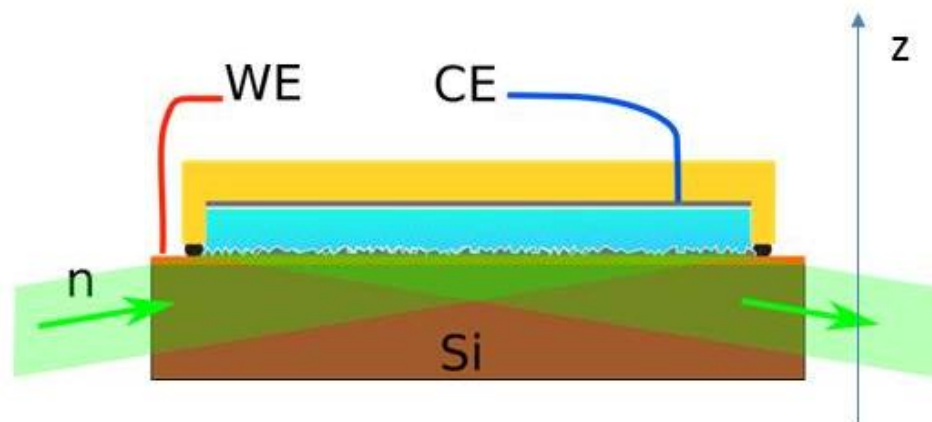
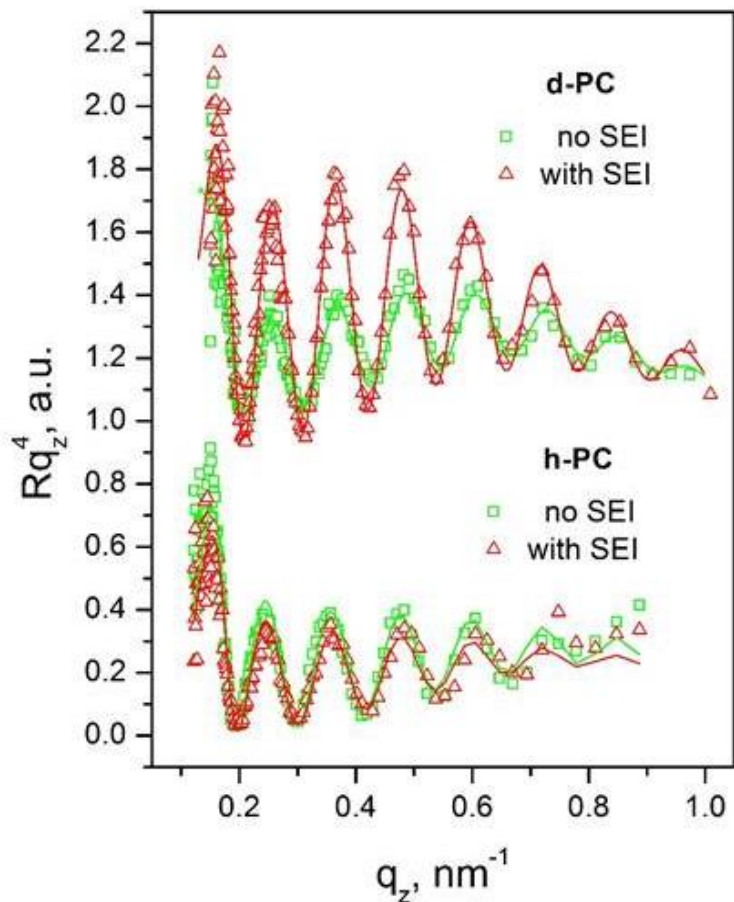


# Study of Electrolyte-Electrode Interfaces by NR



# Study of Electrolyte-Electrode Interfaces by NR

Formation of Solid Electrolyte Interphase (SEI) on plane metal anodes

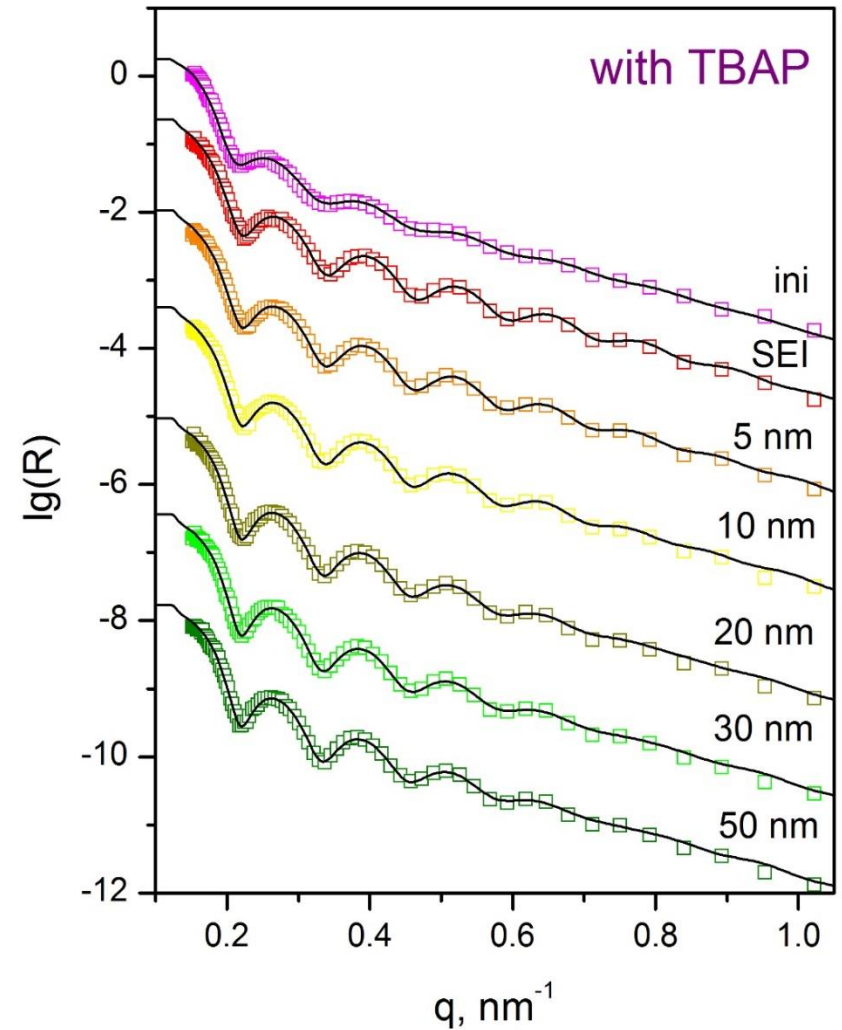
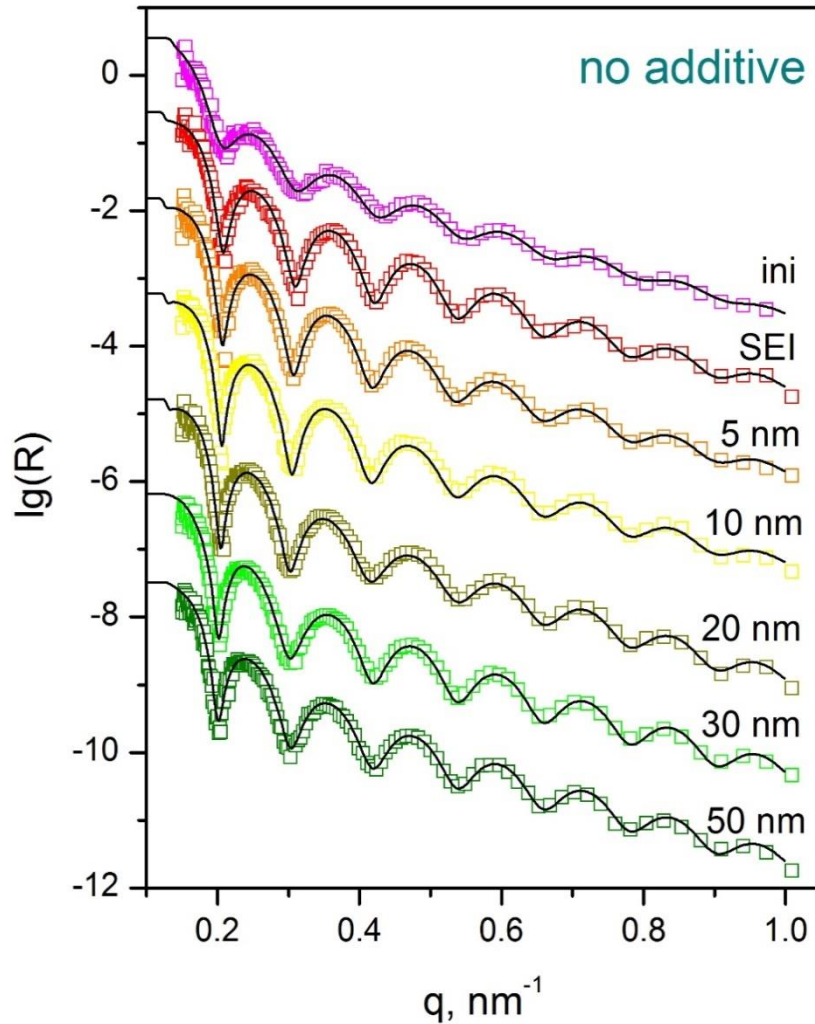


GRAINS TOF Reflectometer, IBR-2, Dubna



# Effect of TBAP: neutron reflectometry

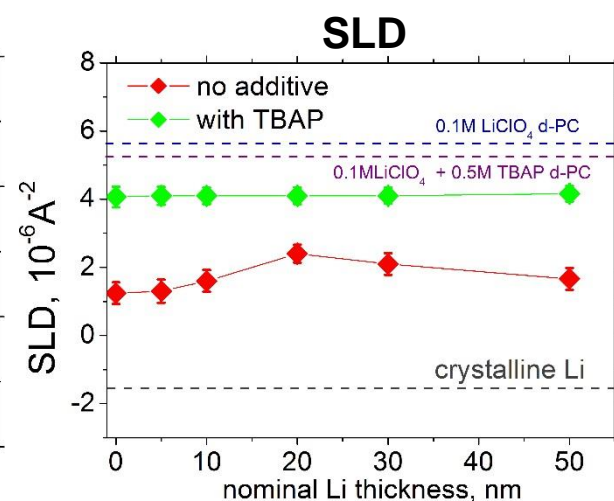
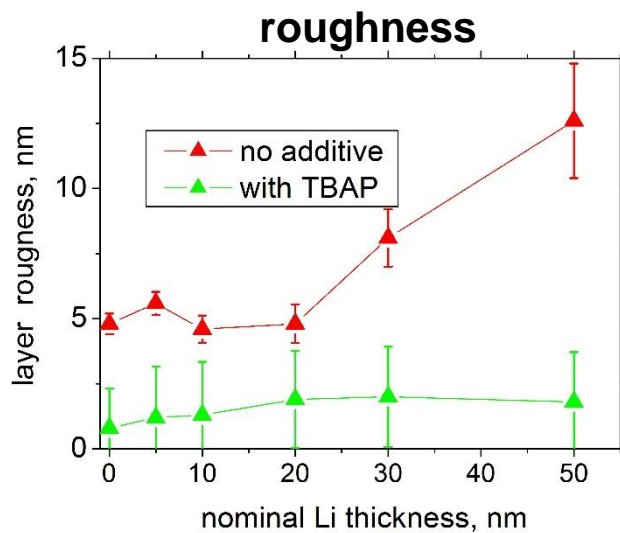
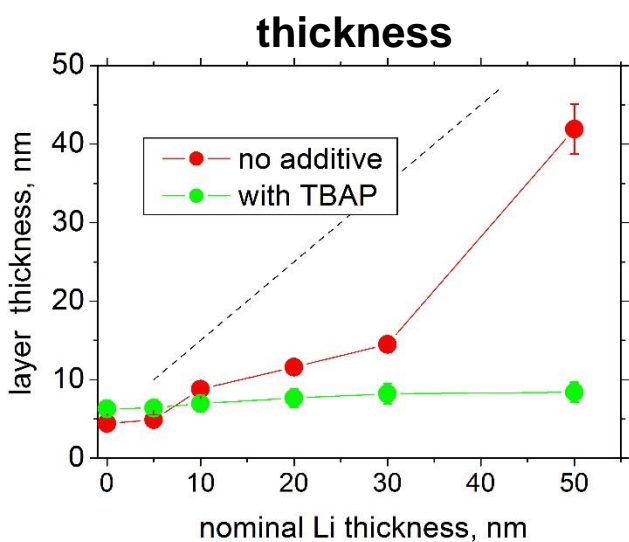
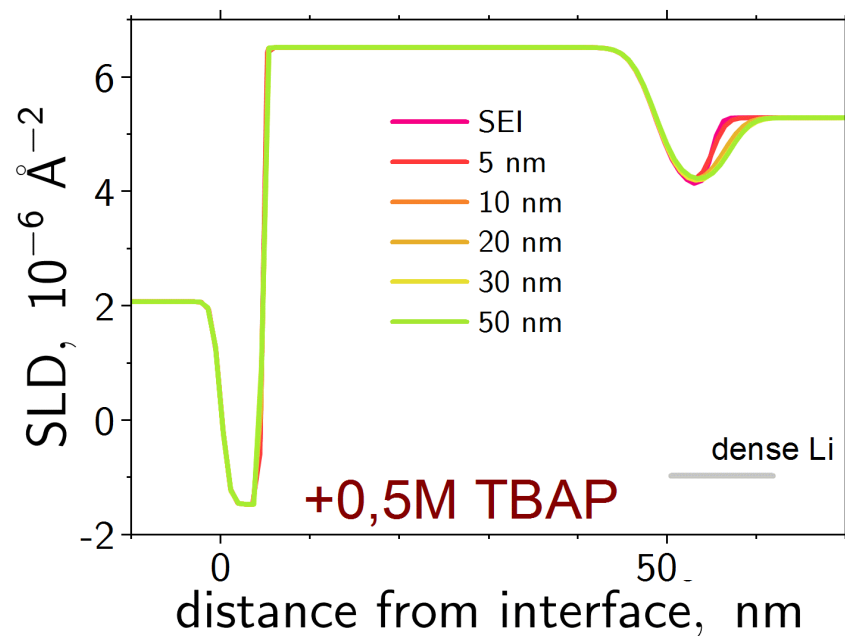
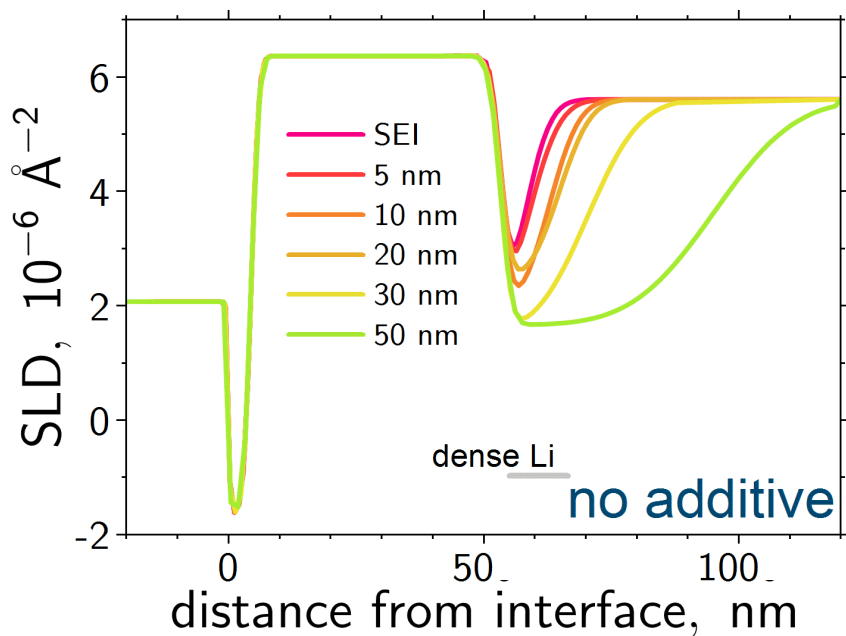
tetra-n-butylammonium perchlorate (TBAP)



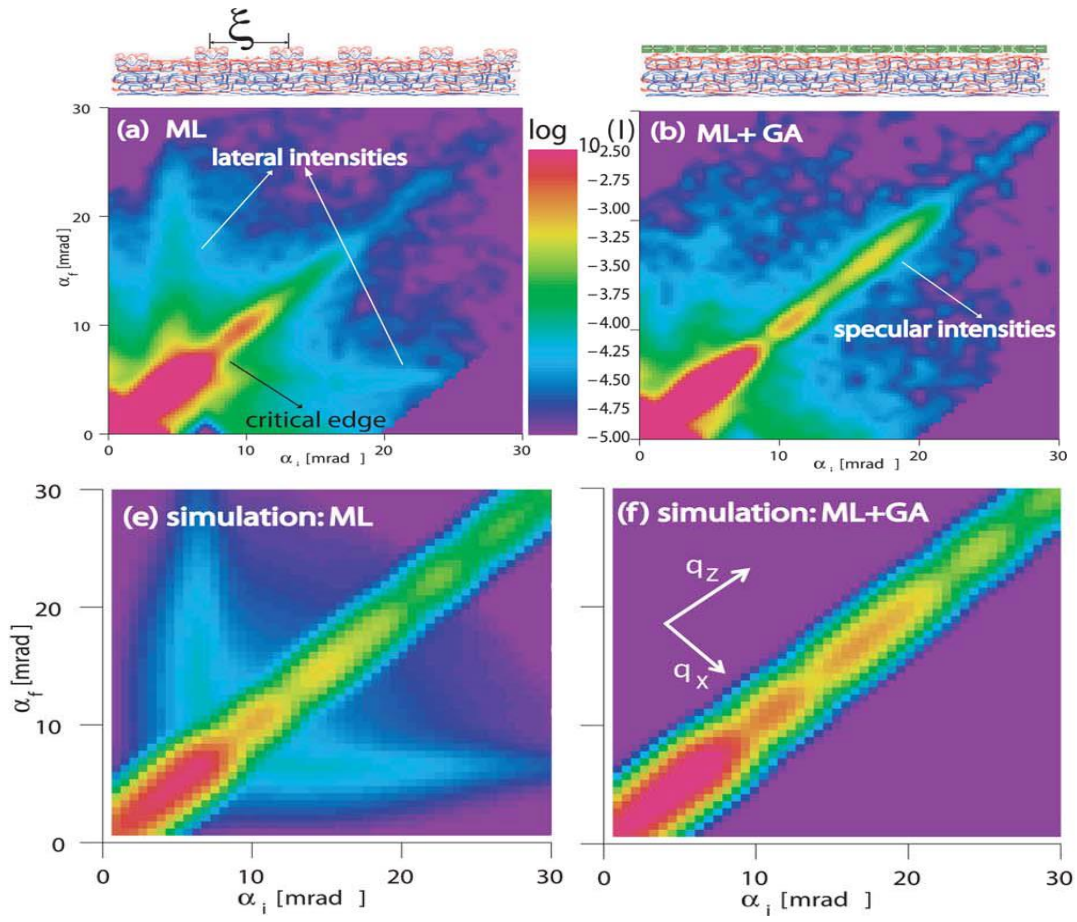
M.V.Avdeev, Rulev A.A., Bodnarchuk V.I., et al. Appl. Surf. Sci, 424 (2017) 378

M.V. Avdeev, A.A. Rulev, E.E. Ushakova, et al., Appl. Surf. Sci. 486 (2019) 287

# Effect of TBAP: neutron reflectometry



# Off-specular mode. Solid-liquid interfaces



Smoothing of polyelectrolyte multilayers with molecular additive (glutamic acid)

Adsorption of polyelectrolytes on Si from  $D_2O$  sample ML:

$PEI/((PSS/PAH)_2/(dPSS/PAH))$

sample ML + GA:

$PEI/((PSS/PAH)_2/(dPSS/PAH/GA))_3$

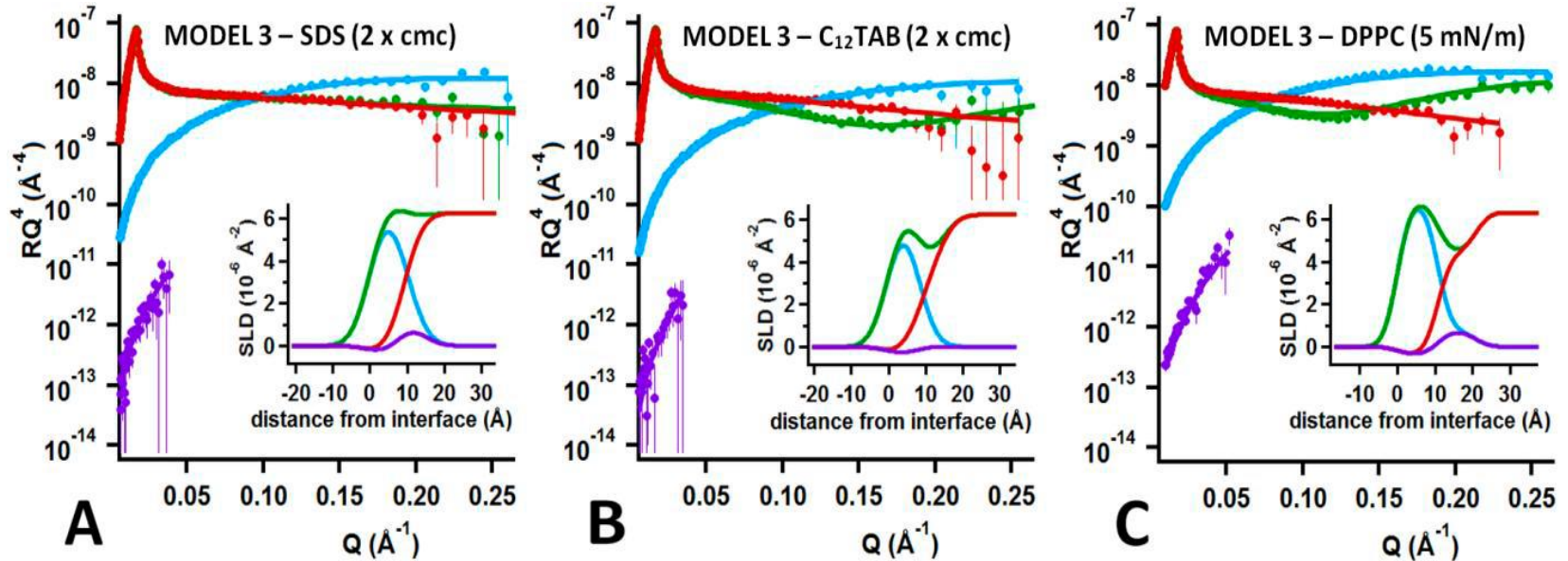
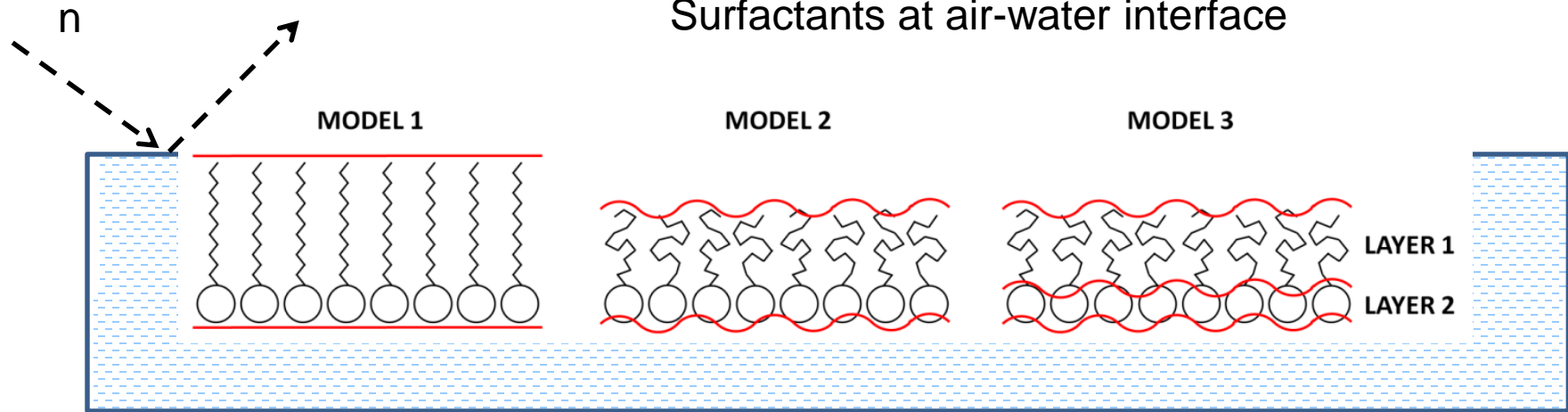
TREFF, MLZ

N. Paul, A. Paul, S. Mattauch, et al., Soft Matter 9 (2013) 10117



# Neutron reflectometry from free surfaces

## Surfactants at air-water interface



FIGARO, ILL

R.A. Campbell, et al., J. Coll. Interface Sci. 531 (2018) 98-108.

## Summary to 'Reflectometry from Interfaces with Liquids'

- ***Neutron reflectometry experiments for interfaces with liquids require special cells and sample environment. The active development of such kind of experiments for soft matter research is due to high penetrating power of neutrons and possibilities for enhancing reflectivity by varying the contrast (using deuteration).***
- ***The behavior of colloidal liquid solutions at interfaces with solids is an important area of research with the practical impact.***
- ***Off specular scattering is sensitive to fine structural effects in liquid-solid interfaces with colloidal solutions.***
- ***Study of structural organization of free surfaces of air-liquid interfaces is of current interest.***

- Principles of Neutron Reflectometry
- Reflectometry of Non-Polarized and Polarized Neutrons from Solid Interfaces
- Neutron Reflectometry from Interfaces with Liquids
- Experimental Aspects of Neutron Reflectometry**

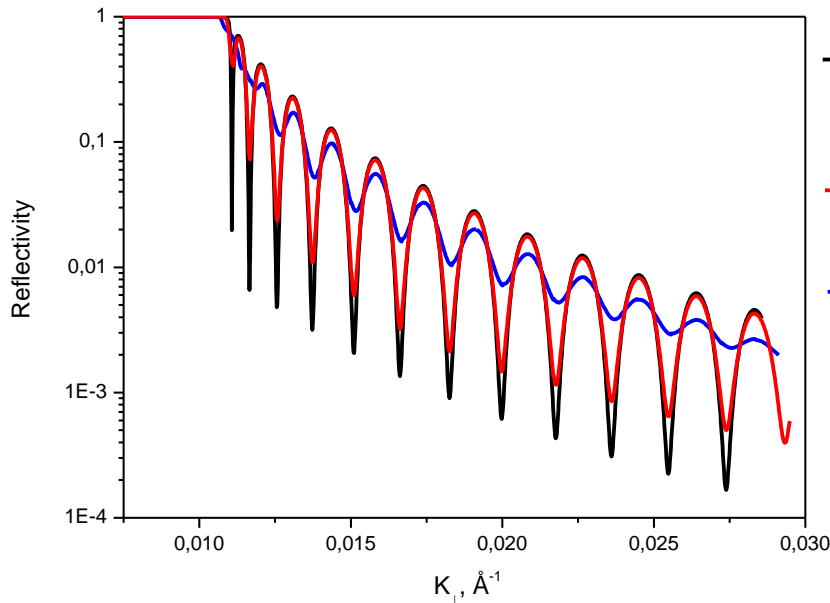
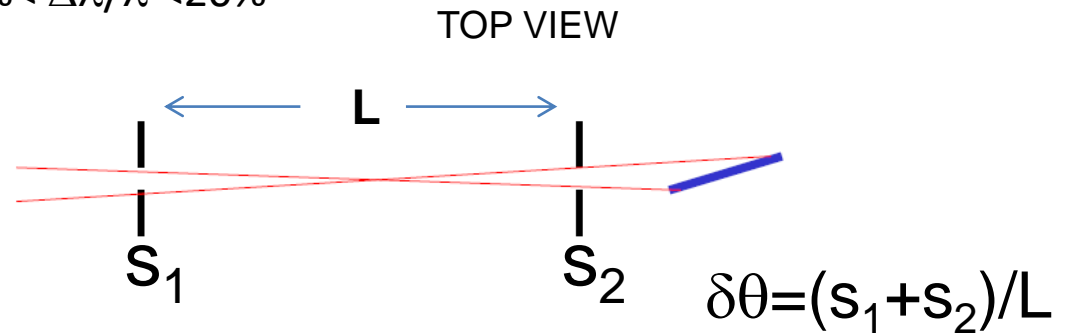
# Resolution function: vertical sample geometry

## Wavelength resolution:

- Graphite monochromator  $\Delta\lambda/\lambda \sim 1\%$
- Multilayered monochromator  $5\% < \Delta\lambda/\lambda < 20\%$
- TOF-mode  $1\% < \Delta\lambda/\lambda < 20\%$

## Angular resolution:

- Determined by aperture sizes



—  $\Delta\theta/\theta = 0$

—  $\Delta\theta/\theta = 1\%$

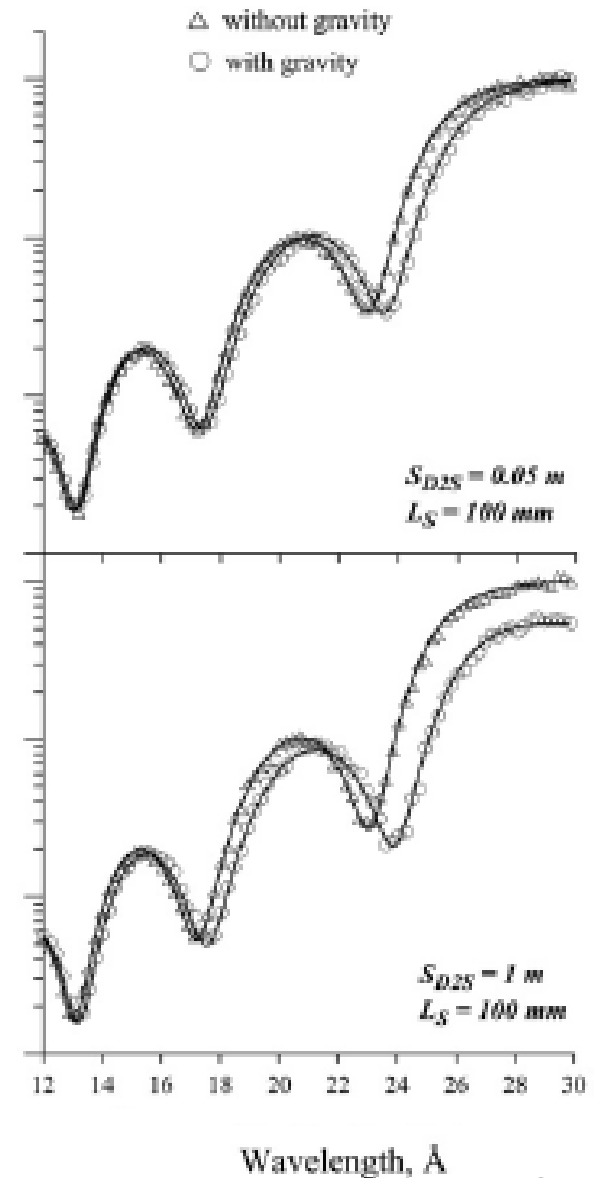
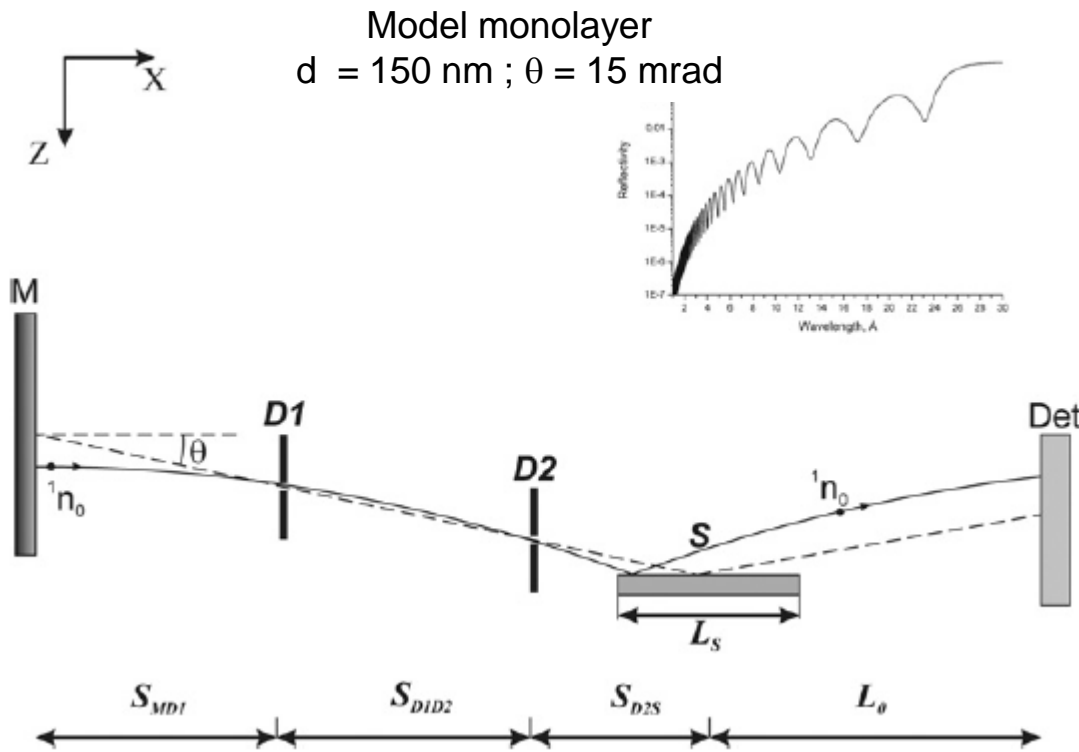
—  $\Delta\theta/\theta = 3\%$

For analytical representation see

**W.G.Bouwman, J.S.Pedersen,  
*J. Appl. Cryst.* 29 (1996) 152-158**

# Resolution function: horizontal sample geometry

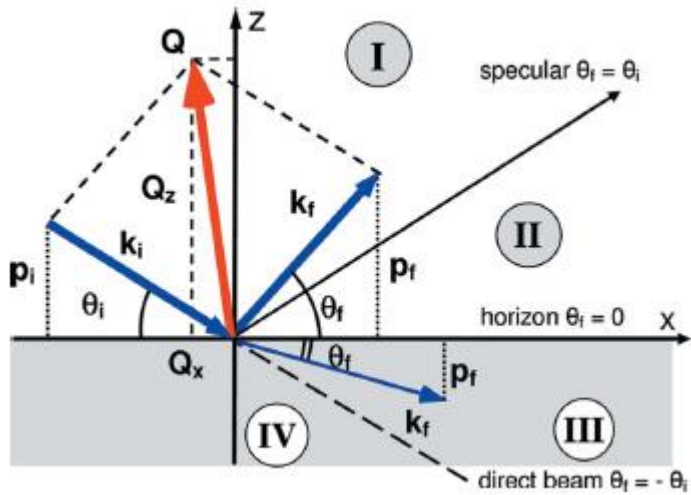
Additional gravity effect is important for  $\lambda > 1 \text{ nm}$



For analytical representation see

I. Bodnarchuk, et al.,  
 Nucl. Instr. Methods A 631 (2011) 121–124

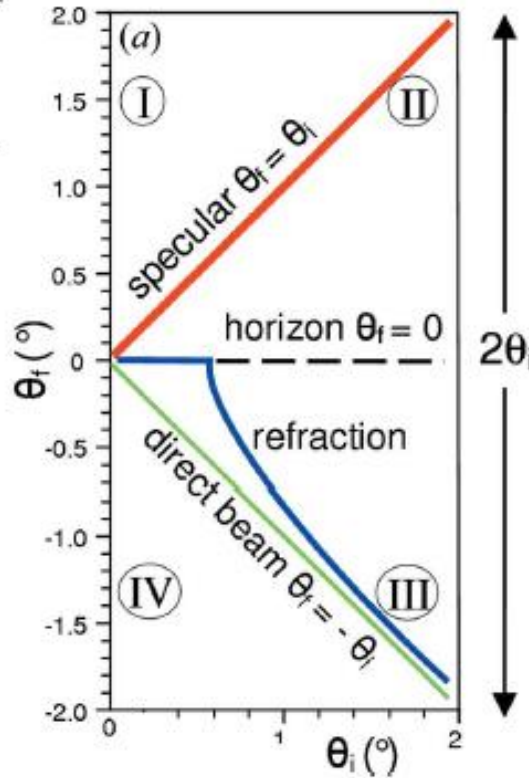
# Representation of NR data: specular scattering



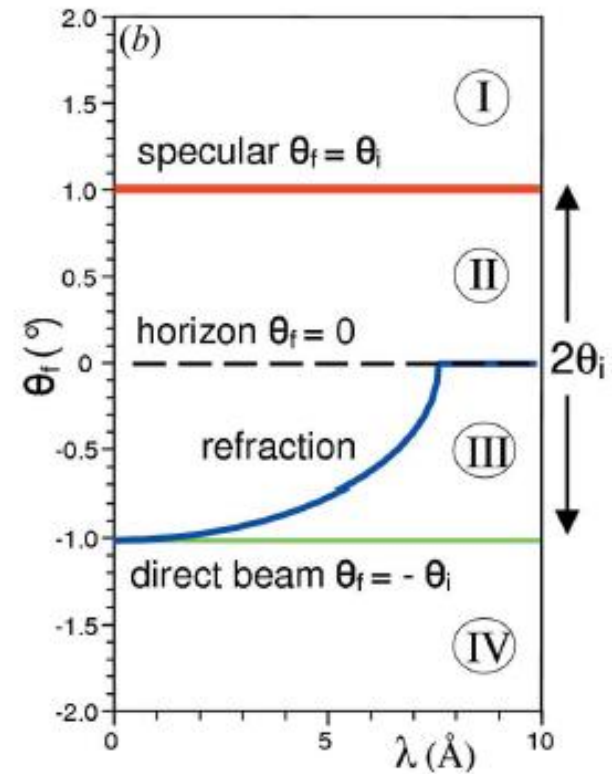
$$Q_x = (\pi/\lambda)(\theta_i + \theta_f)(\theta_i - \theta_f)$$

$$Q_z = (2\pi/\lambda)(\theta_i + \theta_f).$$

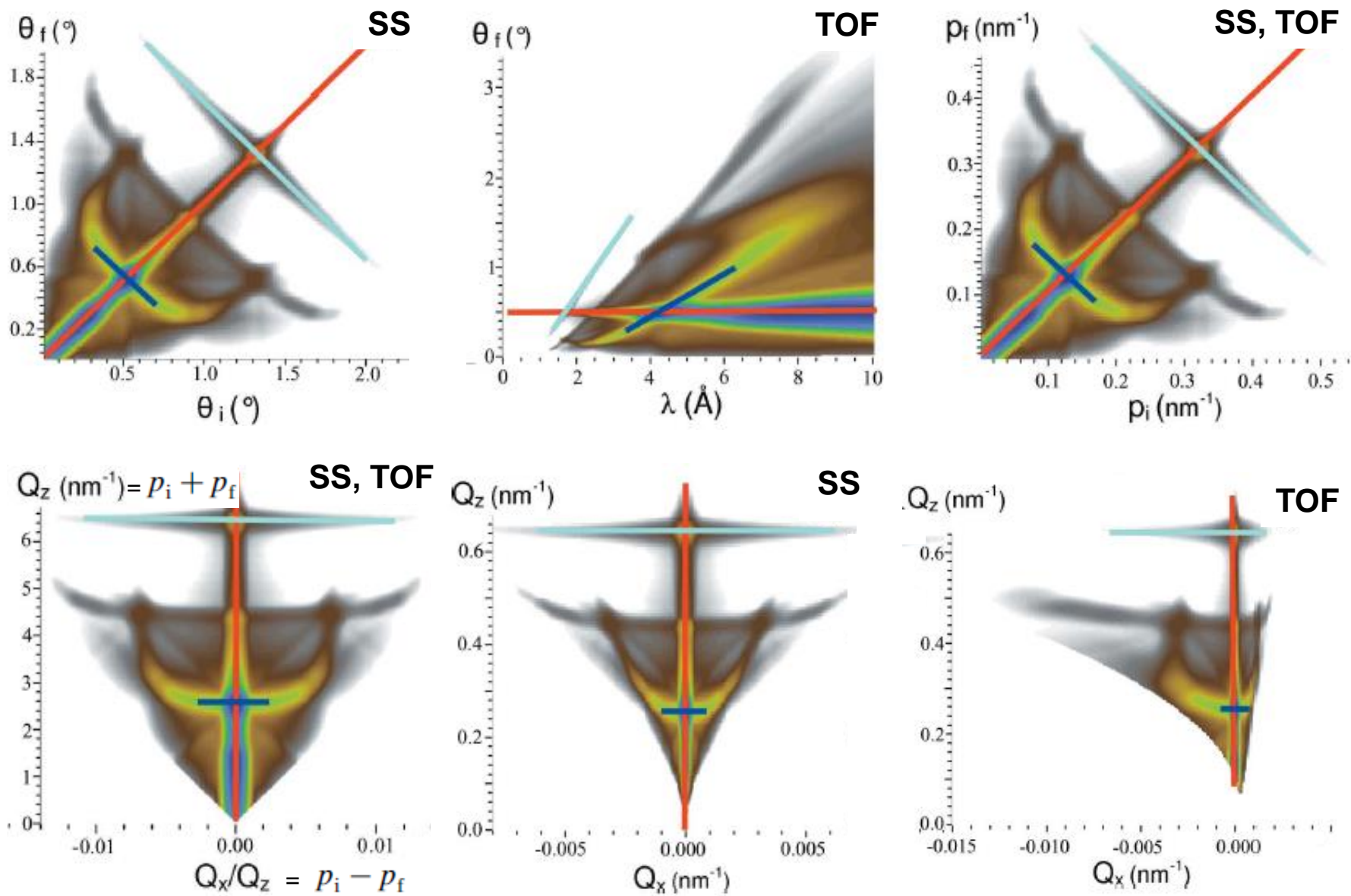
Steady state mode



TOF mode



# Representation of NR data: diffuse scattering

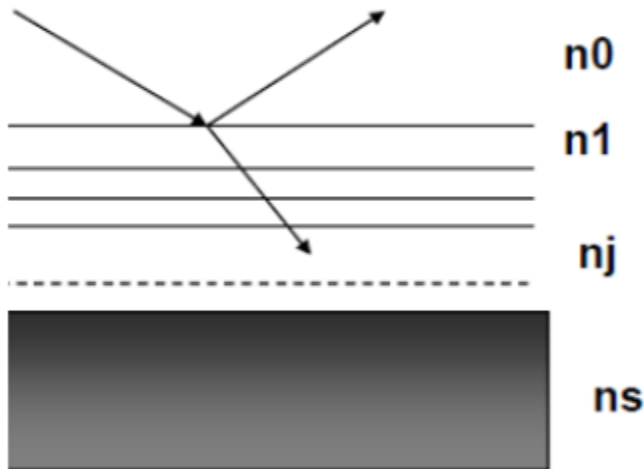


For details see F.Ott, S.Kozhevnikov J. Appl. Cryst. 44 (2011) 359–369



# Analysis of NR data: matrix formalism for specular reflectivity

for multilayers



*(Born & Wolf, 'Principles in Optics', 6th Ed, Pergammon, Oxford, 1980)*

For  $j$ -th layer

$$M_j = \begin{bmatrix} \cos \beta_j & -(i/p_j) \sin \beta_j \\ -ip_j \sin \beta_j & \cos \beta_j \end{bmatrix}$$

$$p_j = n_j \sin \theta_j \quad \beta_j = (2\pi/\lambda) n_j d_j \sin \theta_j$$



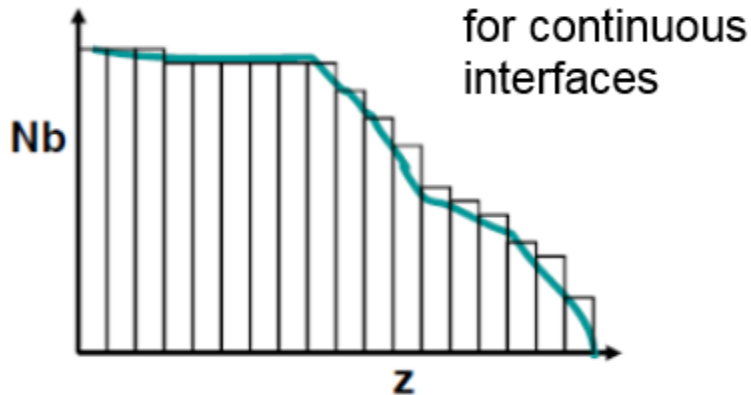
Total reflectivity matrix

$$M = [M_1][M_2] \dots [M_n]$$



**Reflectivity**

$$R^2 = \left| \frac{(M_{11} + M_{12} p_s) p_0 - (M_{21} + M_{22}) p_s}{(M_{11} + M_{12} p_s) p_0 + (M_{21} + M_{22}) p_s} \right|^2$$



Parrat formalism

**Software: Parrat32, Motofit / IGOR PRO, EFFI, SansView, MAUD ...**



## Summary to 'Experimental Aspects of Neutron Reflectometry'

- ***Resolution function of neutron reflectometer contains wavelength and angular components which in optimum should be close. For reflectometers with horizontal sample plane gravitational effect for long-wave neutrons should be taken into account;***
- ***Off-specular scattering patterns can be represented in different systems of coordinates depending on the mode of experiment and specific scattering features;***
- ***Matrix formalism is one of the mostly used approaches for calculating specular reflectivity and fitting it to experimental curves.***