Reflectometry in BornAgain: overview

Dmitry Yurov

Helmholtz equation

- Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\Delta + U\right]\psi = i\hbar\frac{\partial\psi}{\partial t}$$

- Electromagnetic wave equation:

$$\Delta\vec{E} = \frac{\epsilon\mu}{c^2}\frac{\partial^2\vec{E}}{\partial t^2}$$

$$\frac{\partial U}{\partial t}, \frac{\partial\epsilon}{\partial t}, \frac{\partial\mu}{\partial t} = 0$$

$$\left(\vec{E}, \psi\right) = \hat{\xi}(\vec{r}) \cdot T(t)$$

- Helmholtz equation:

$$[\Delta + k_0^2 n^2]\hat{\xi} = 0$$

Contains all information about the media

Fundamental solution for homogeneous media

$$\hat{\xi} = \hat{A}exp\left(i\vec{k}\cdot\vec{r}\right), \left|\vec{k}\right|^2 = k_0^2 n^2$$

Plane wave in semi-infinite media

- Helmholtz equation:

$$[\Delta + k^2]\hat{\xi} = 0$$

- Doing separation of variables once again:

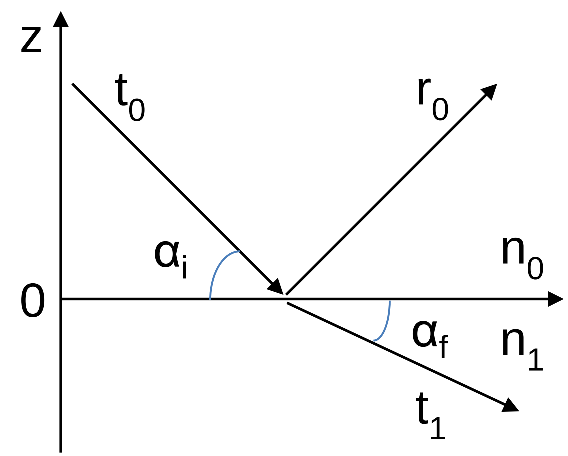
$$\hat{\xi}(\vec{r}) = \hat{A}e^{i(k_x \cdot x + k_y \cdot y)}\xi_z(z)$$
$$\frac{d^2\xi_z}{dz^2} + k_z^2(z)\xi_z = 0$$

- Generic solution:

$$\xi_{zl}(z) = t_l e^{ik_{zl}z} + r_l e^{-ik_{zl}z}$$

- Boundary conditions:

$$t_0 = 1$$
$$r_1 = 0$$
$$\hat{\xi}(z = 0+) = \hat{\xi}(z = 0-)$$
$$\frac{\partial\hat{\xi}}{\partial z}(z = 0+) = \frac{\partial\hat{\xi}}{\partial z}(z = 0-)$$



Important implications

Fresnel's formulas: $R = |r_0|^2 = \left|\frac{k_{z0}-k_{z1}}{k_{z0}+k_{z1}}\right|^2$, $T = |t_1|^2 = \left|\frac{2k_{z0}}{k_{z0}+k_{z1}}\right|^2$

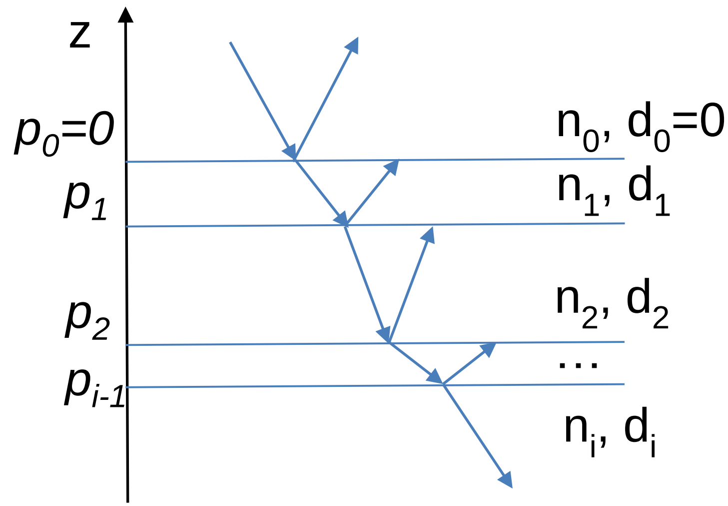
Snell's law: $\frac{\cos\alpha_i}{\cos\alpha_f} = \frac{n_1}{n_0}$, $\cos\alpha_{i,c} = \frac{n_1}{n_0}$

Matrix formalism for multi-layer systems

- Generic solution for z-component:

$$\xi_{zl}(z) = t_l e^{ik_{zl}(z-\mathrm{p}_{l-1})} + r_l e^{-ik_{zl}(z-\mathrm{p}_{l-1})}, \qquad l = 1, \dots, i$$

$$\xi_{z0}(z) = t_0 e^{ik_{z0}z} + r_0 e^{-ik_{z0}z}$$



- Boundary conditions:

$$t_0 = 1, \qquad r_i = 0$$

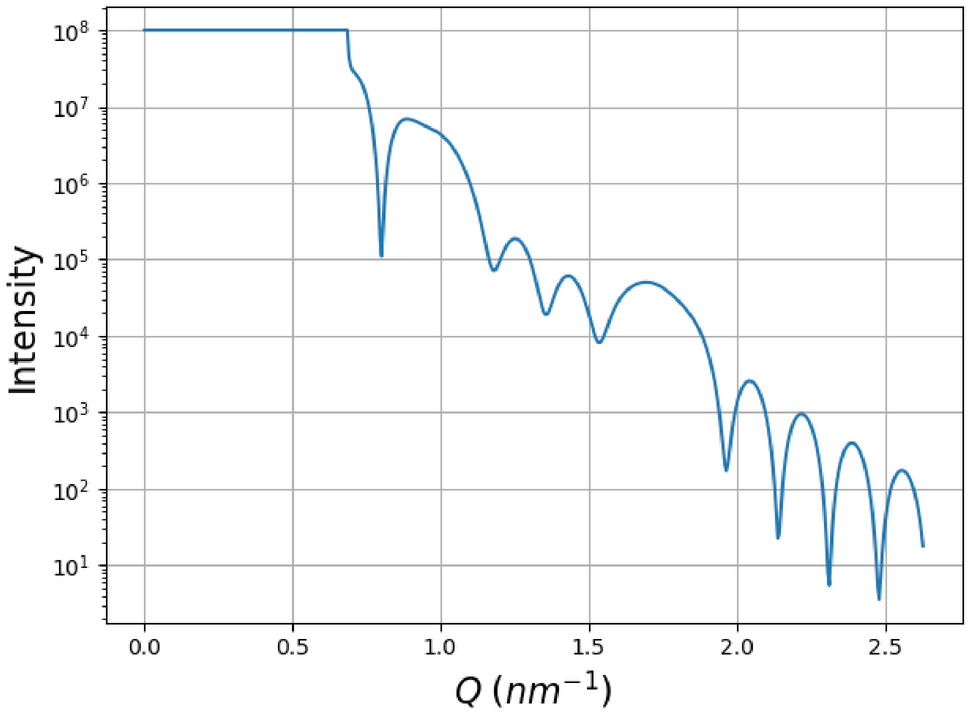
$$\xi_{zl-1}(p_l +) = \xi_{zl}(p_l -)$$

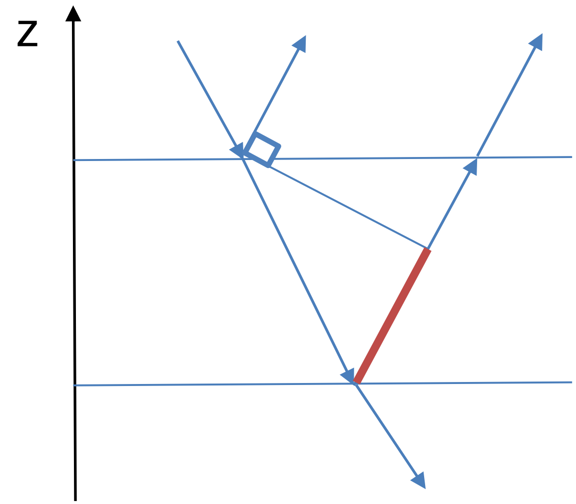
$$\frac{\partial \xi_{zl-1}}{\partial z}(p_l +) = \frac{\partial \xi_{zl}}{\partial z}(p_l -)$$

- Backward matrix relation:

$$\begin{pmatrix} t_{l-1} \\ r_{l-1} \end{pmatrix} = \underbrace{\begin{pmatrix} \exp(-ik_{zl-1}d_{l-1}) & 0 \\ 0 & \exp(ik_{zl-1}d_{l-1}) \end{pmatrix}}_{\text{Phase shift}} \underbrace{\frac{1}{2k_{zl-1}} \begin{pmatrix} k_{zl-1} + k_{zl} & k_{zl-1} - k_{zl} \\ k_{zl-1} - k_{zl} & k_{zl-1} + k_{zl} \end{pmatrix}}_{\text{“Sewing“ amplitudes together}} \begin{pmatrix} t_l \\ r_l \end{pmatrix}$$

Typical reflectometry image





Interference maximum:

$$\Delta\varphi = 2d\sin\alpha_i = \lambda$$

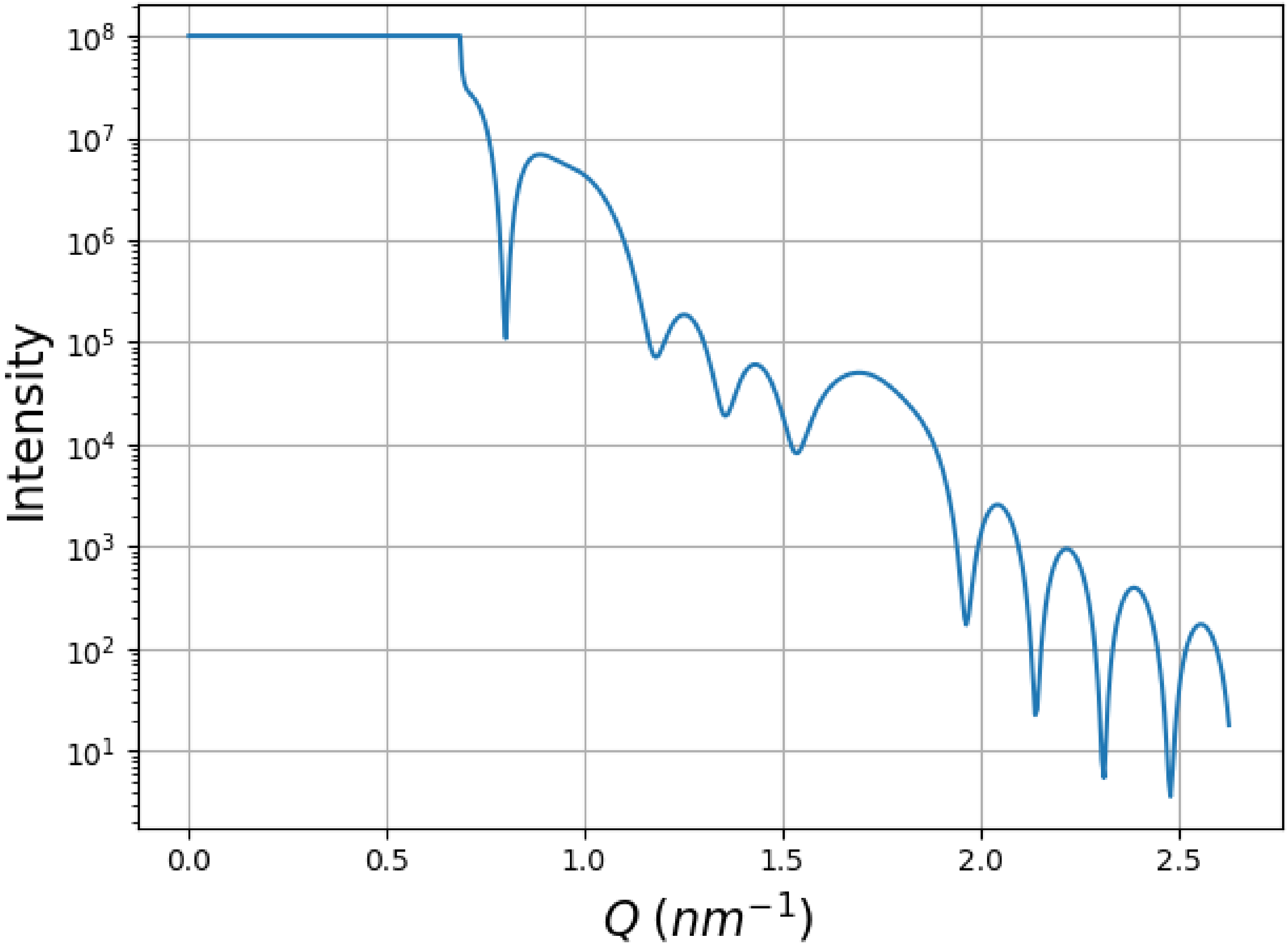
Scattering wave vector:

$$Q = 2k_{z0} = \frac{4\pi}{\lambda}\sin\alpha_i$$

Peak width:

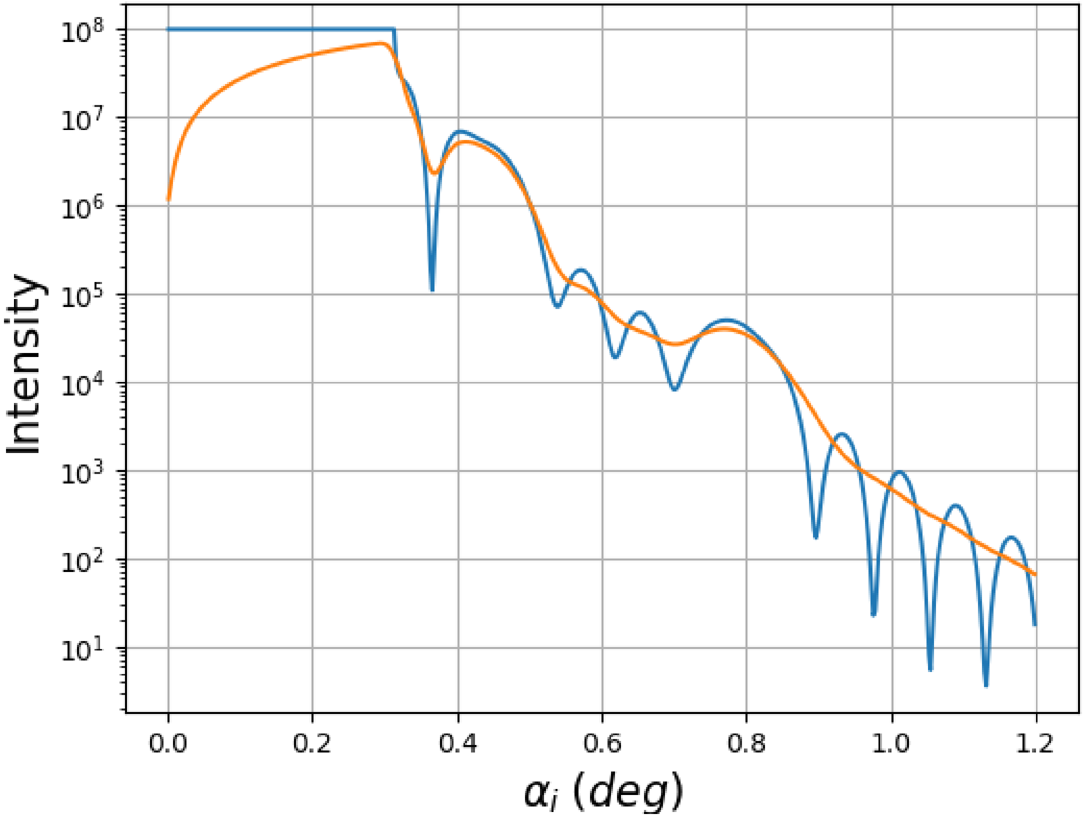
$$\delta Q \approx \frac{2\pi}{d}$$

Task: sample thickness from reflectometry image



Beam effects: overview

- Footprint correction
- Beam divergence
- Background noise



Beam effects: footprint correction

- Depends on beam-to-sample width ratio

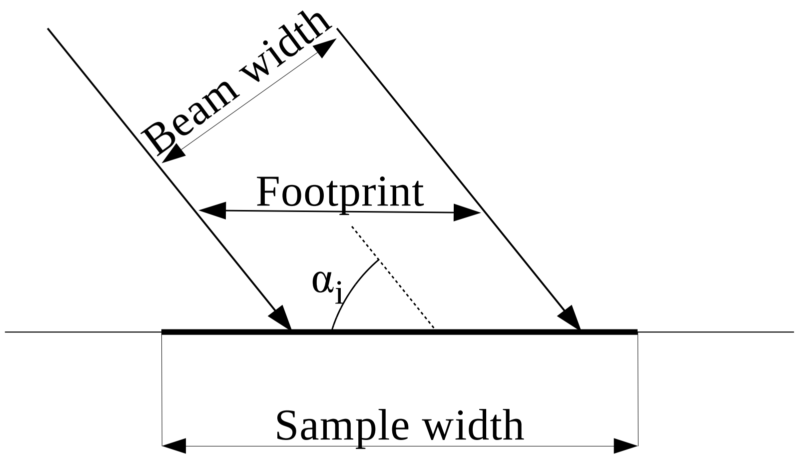
$$Z = \frac{w_{beam}}{w_{sample}}$$

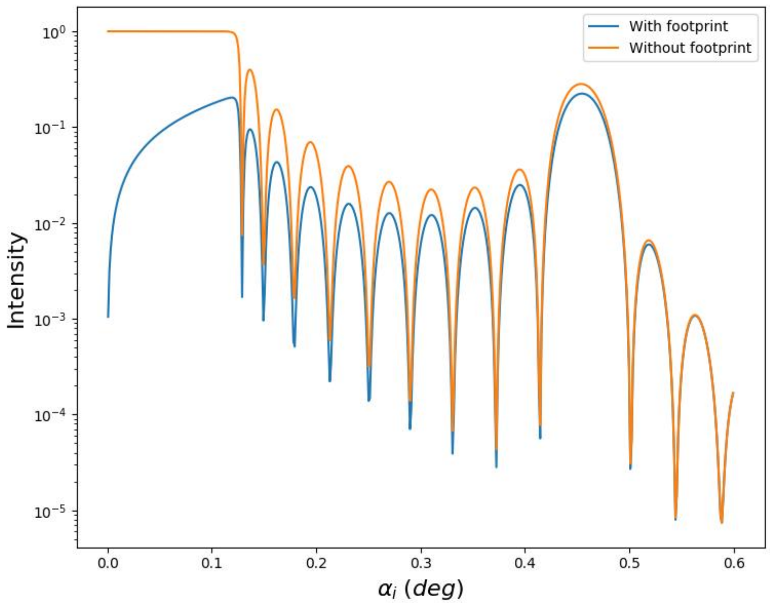
- Gaussian beam

$$F_G(R, \alpha_i) = \operatorname{erf}\left(\frac{\sin \alpha_i}{\sqrt{2}\, Z}\right)$$

- Square beam

$$F_S(R, \alpha_i) = \min\left(\frac{\sin \alpha_i}{Z}, 1\right)$$





Beam effects: divergence

- Total divergence impact on *q*:

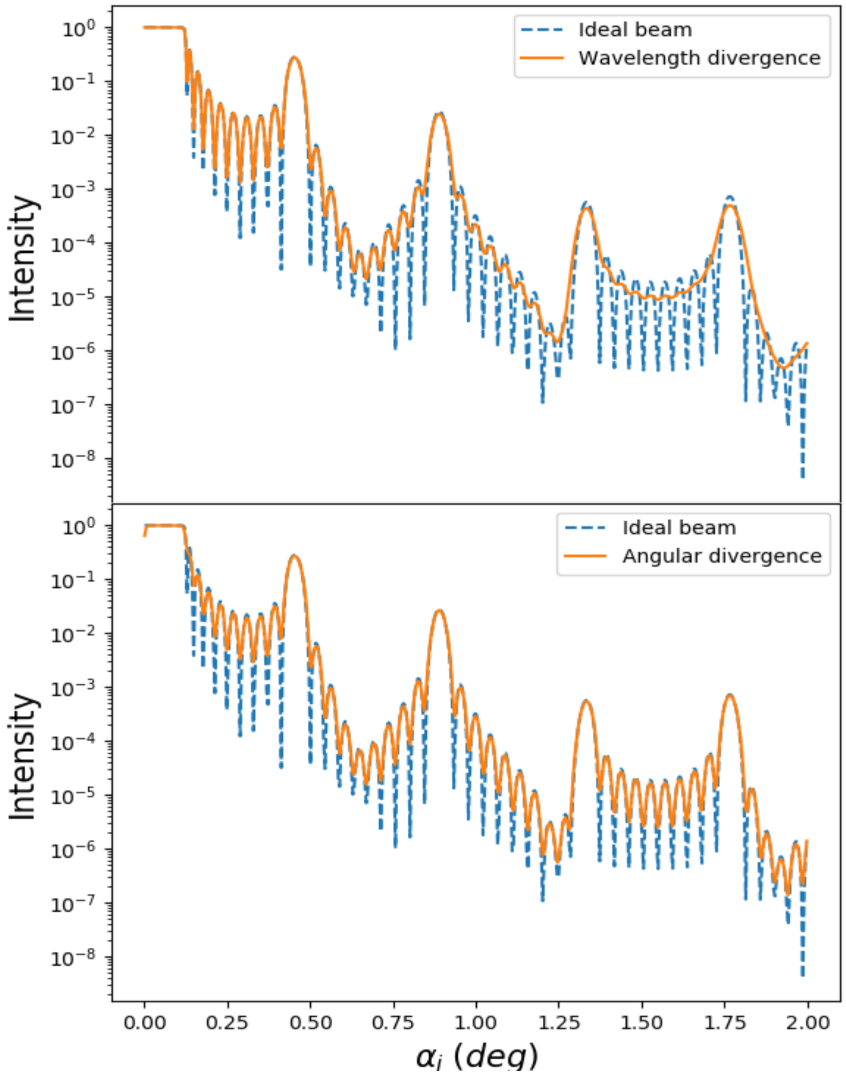
$$\Delta Q = \sqrt{Q^2 \left(\frac{\Delta\lambda}{\lambda}\right)^2 + \left(\frac{4\,\pi}{\lambda}\cos\alpha_i \cdot \Delta\alpha_i\right)^2}$$

- Wavelength divergence at small angles:

$$\Delta Q(\Delta\lambda = 0, \alpha_i \ll 1) \approx \frac{4\,\pi}{\lambda}\Delta\alpha_i$$

- Angular divergence at small angles:

$$\Delta Q(\Delta\alpha_i = 0, \alpha_i \ll 1) \approx \frac{4\,\pi}{\lambda}\alpha_i\frac{\Delta\lambda}{\lambda}$$



Materials: index of refraction vs SLD

Index of refraction

$$n = 1 - \delta + i\beta$$

- Depends on wavelength
- X-ray data at http://henke.lbl.gov/optical_constants/getdb2.html

Scattering length density (SLD)

$$n^2 = 1 - \frac{\lambda^2}{\pi}\rho, \qquad \rho = \rho_r - i\rho_i$$

- Can be interpreted as normalized potential of interaction
- Interaction with neutrons:

$$\sigma_{abs} \propto \lambda \quad \Rightarrow \quad \rho \approx const$$

- Neutron data at https://webapps.frm2.tum.de/intranet/neutroncalc/

Materials: index of refraction vs SLD

`HomogeneousMaterial`

- Based on index of refraction
- Suitable for any probe type
- Provides correct values of refractive index for a monochromatic wave with predefined wavelength
- Main use case: probes with negligible wavelength divergence

`MaterialBySLD`

- Based on SLD
- Provides correct values of refractive index in a range of wavelengths
- Main use case: neutron probes (except for He-3, Cd, Sm, Eu, Gd, Yb, Hg materials)

Reflectometry in BornAgain: tutorials

Dmitry Yurov

GUI: Simulate and fit Ag nano-particles

- Instrument:
  - Direct beam intensity: 10^8
  - Wavelength: 0.1798 nm
  - Angle range: 0 – 3 deg
  - Gaussian angular divergence: σ = 0.01 deg
  - Square footprint: sample width – 10 cm, beam width – 0.1 mm

- Sample:
  - Neutron data at https://webapps.frm2.tum.de/intranet/neutroncalc/

Material	Density, g/cm3	ρ_r, 10^{-6} A^{-2}	ρ_i, 10^{-6} A^{-2}	thickness, nm
Vacuum	-	0	0	Inf
Ag	4			20
SiO_2	2.33			5
Si	2.33			Inf

GUI: Simulate and fit Ag nano-particles

- Fitting parameters
  - Ag density
  - Ag layer thickness
  - SiO_2 density
  - SiO_2 layer thickness

Fit parameter	Start	Min	Max
Ag ρ_r, 10^{-6} A^{-2}	1.322	0.661	2.0
Ag thickness, nm	20	10	30
SiO_2 ρ_r, 10^{-6} A^{-2}	3.681	3.5	4.0
SiO_2 thickness, nm	5	3	8

Thank you for your attention!