

# Reflectometry in BornAgain: overview

Dmitry Yurov

MLZ is a cooperation between:

# Helmholtz equation

- Schrödinger equation:

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

- Electromagnetic wave equation:

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

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



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

- Helmholtz equation:

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



Contains all information about the media

## Fundamental solution for homogeneous media

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

# 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:

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

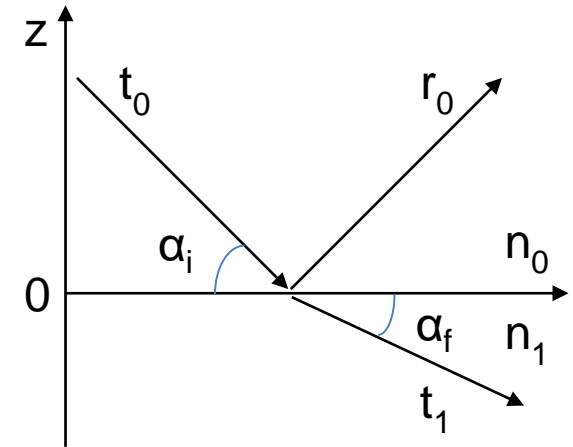
- Boundary conditions:

$$t_0 = 1$$

$$r_1 = 0$$

$$\hat{\xi}(z = 0+) = \hat{\xi}(z = 0-)$$

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



## 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:

$$\xi_{zl}(z) = t_l e^{ik_{zl}(z-p_{l-1})} + r_l e^{-ik_{zl}(z-p_{l-1})}, \quad l = 1, \dots, i$$

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

- Boundary conditions:

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

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

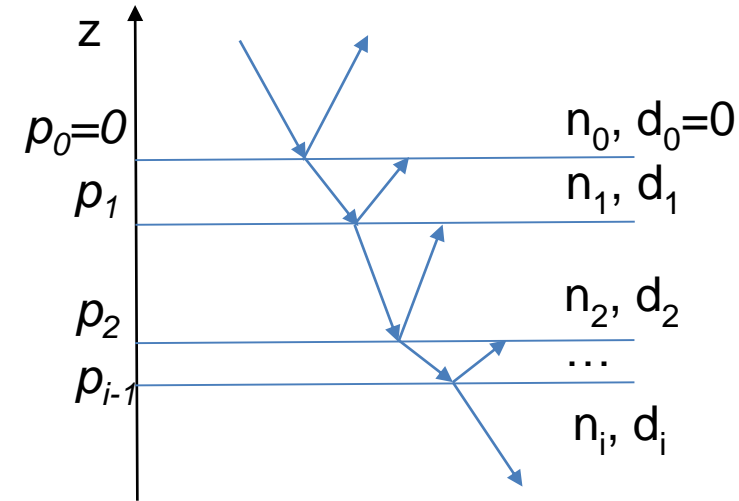
$$\frac{\partial \xi_{zl-1}}{\partial z}(p_l +) = \frac{\partial \xi_{zl}}{\partial z}(p_l -)$$

- Backward matrix relation:

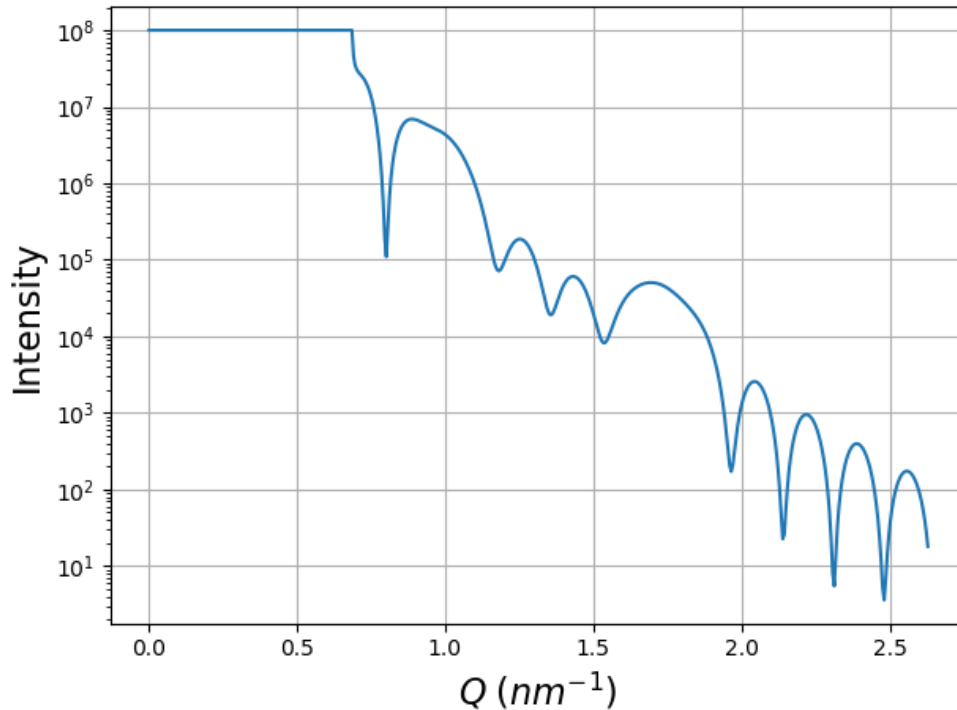
$$\begin{pmatrix} t_{l-1} \\ r_{l-1} \end{pmatrix} = \underbrace{\begin{pmatrix} \exp(-ik_{zl-1}d_{l-1}) & 0 \\ 0 & \exp(ik_{zl-1}d_{l-1}) \end{pmatrix}}_{\text{Phase shift}} \underbrace{\frac{1}{2k_{zl-1}} \begin{pmatrix} k_{zl-1} + k_{zl} & k_{zl-1} - k_{zl} \\ k_{zl-1} - k_{zl} & k_{zl-1} + k_{zl}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

Phase shift

"Sewing" amplitudes together

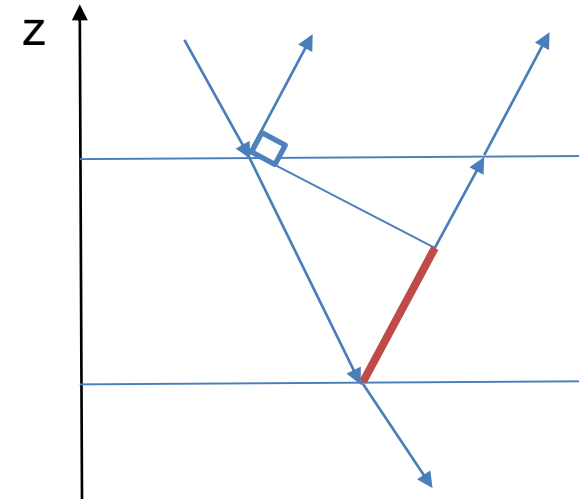


# Typical reflectometry image



Scattering wave vector:

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



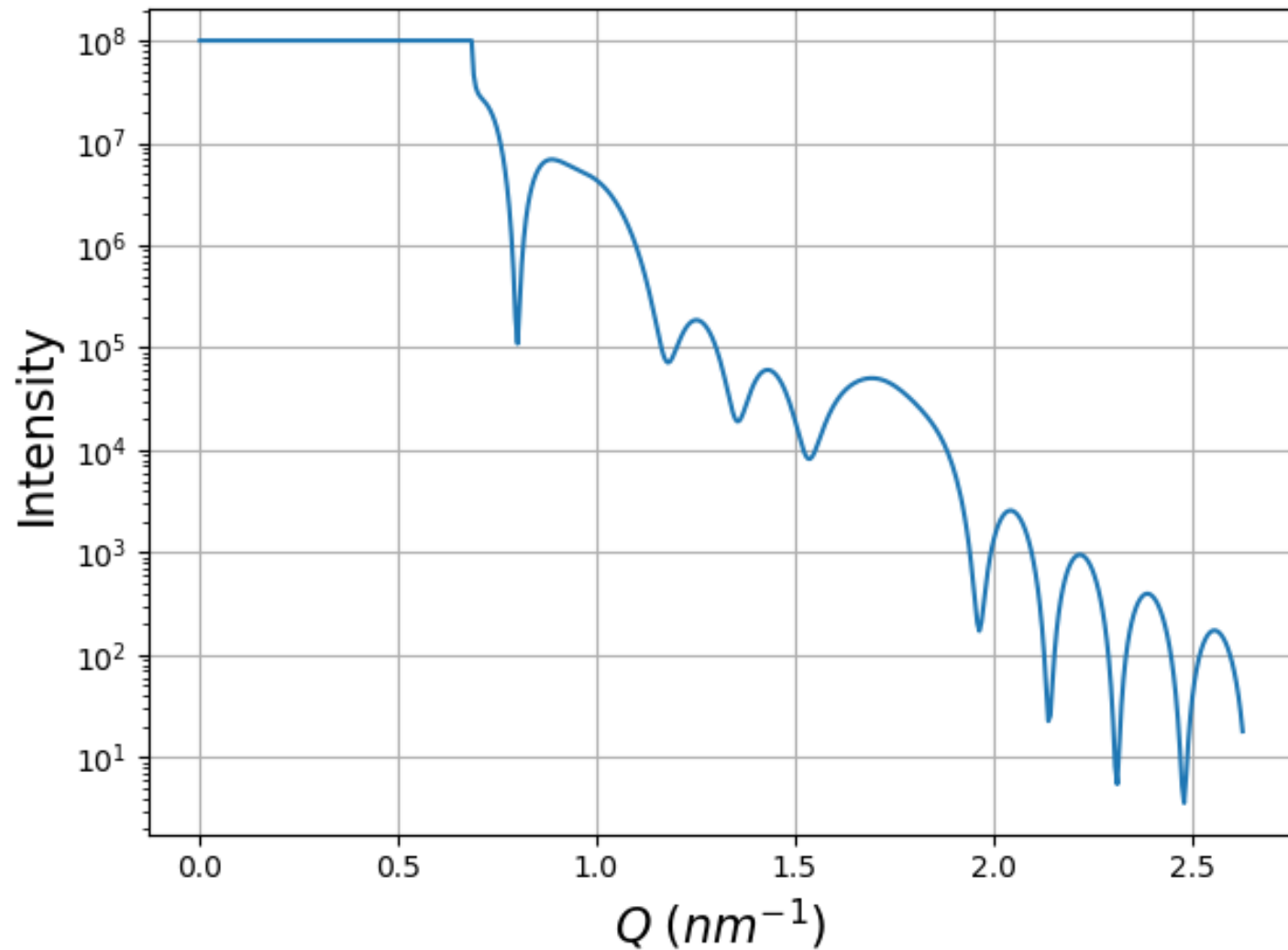
Interference maximum:

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

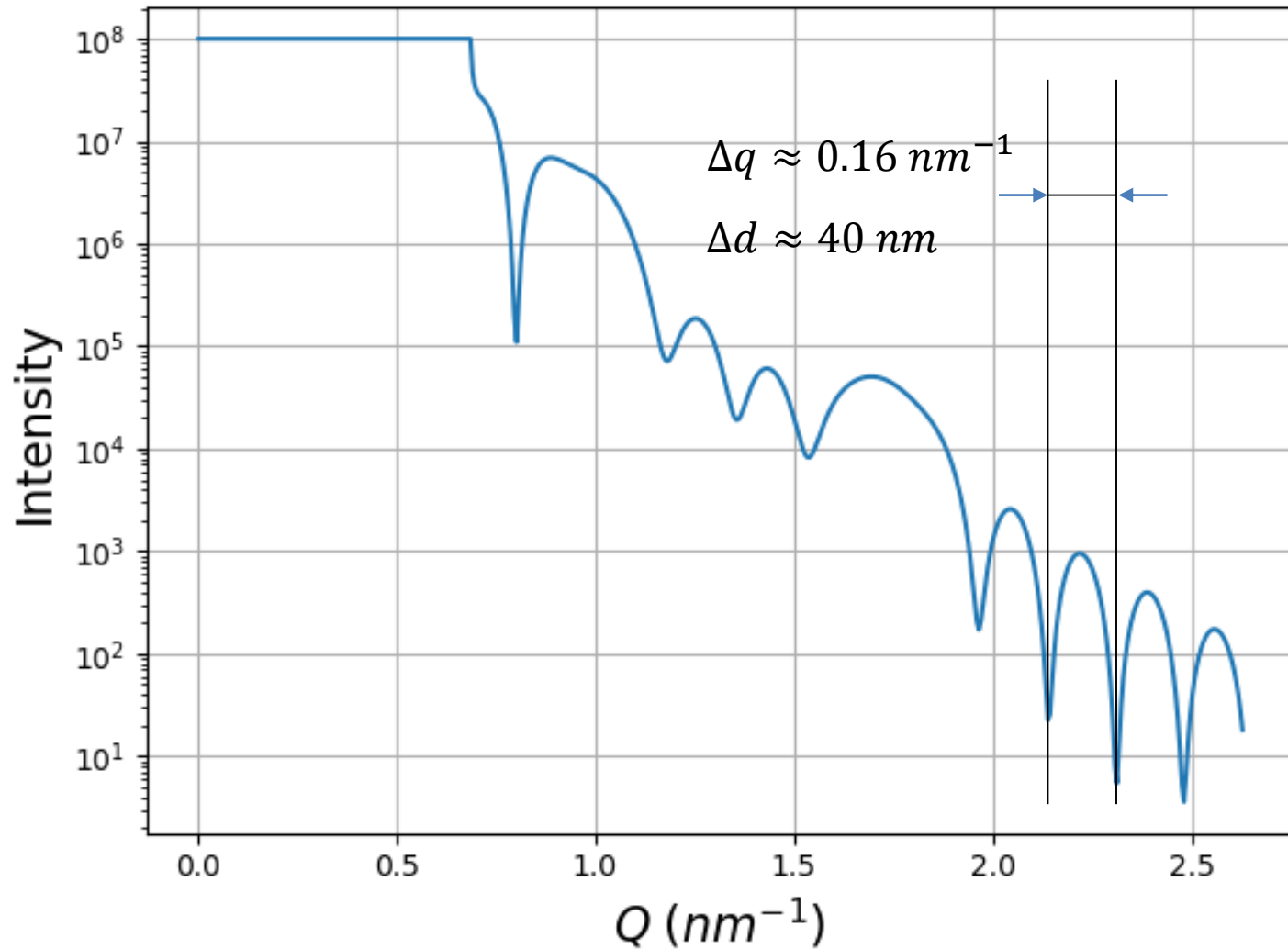
Peak width:

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

# Task: sample thickness from reflectometry image

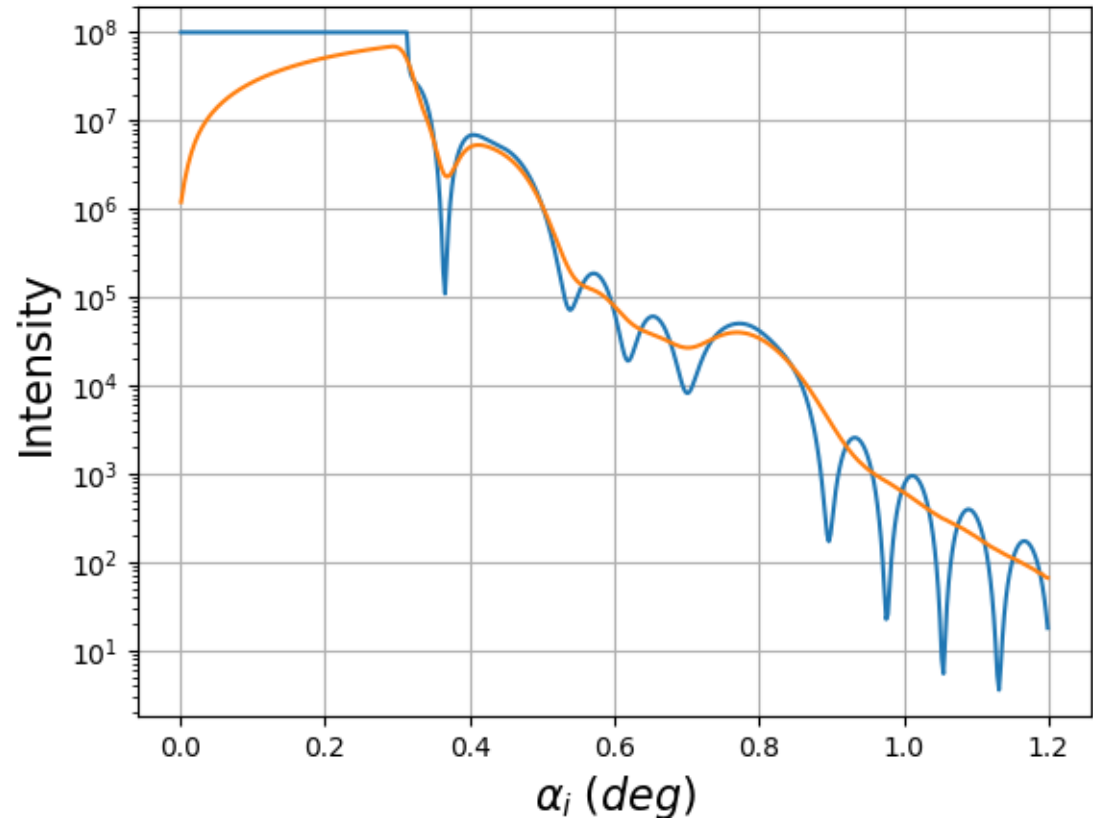


# Task: sample thickness from reflectometry image



# Beam effects: overview

- Footprint correction
- Beam divergence
- Background noise





# Beam effects: footprint correction

- Depends on beam-to-sample width ratio

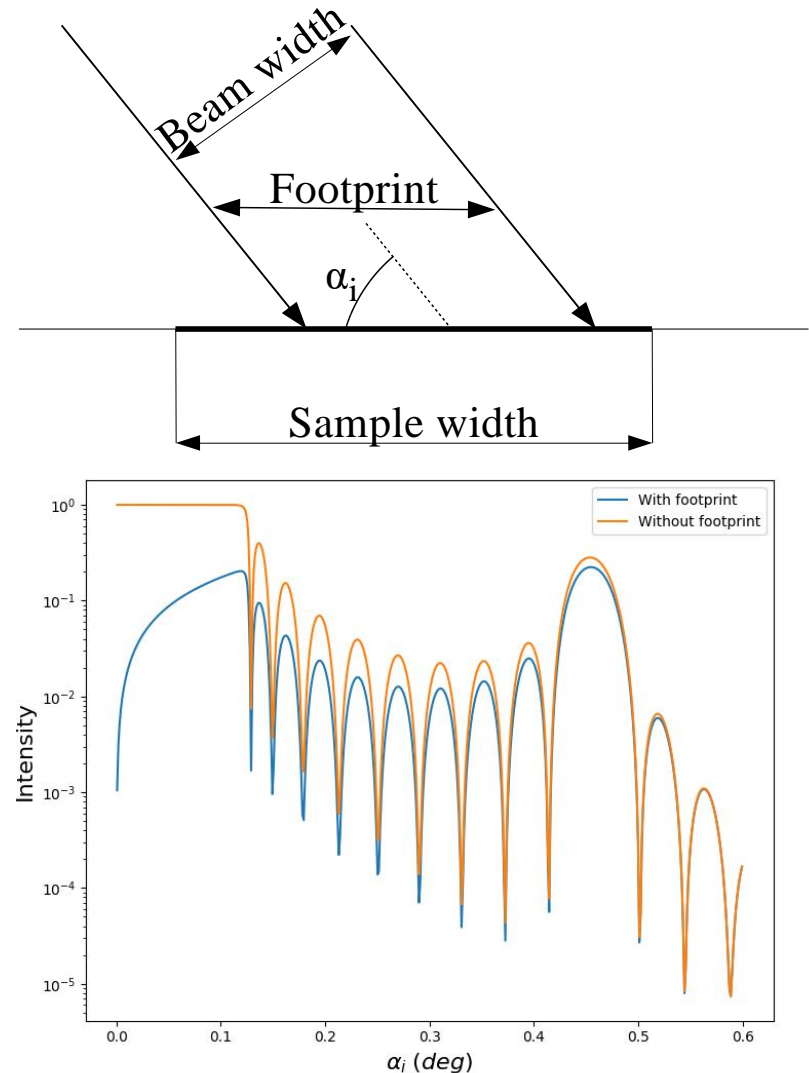
$$Z = \frac{w_{beam}}{w_{sample}}$$

- 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  $q$ :

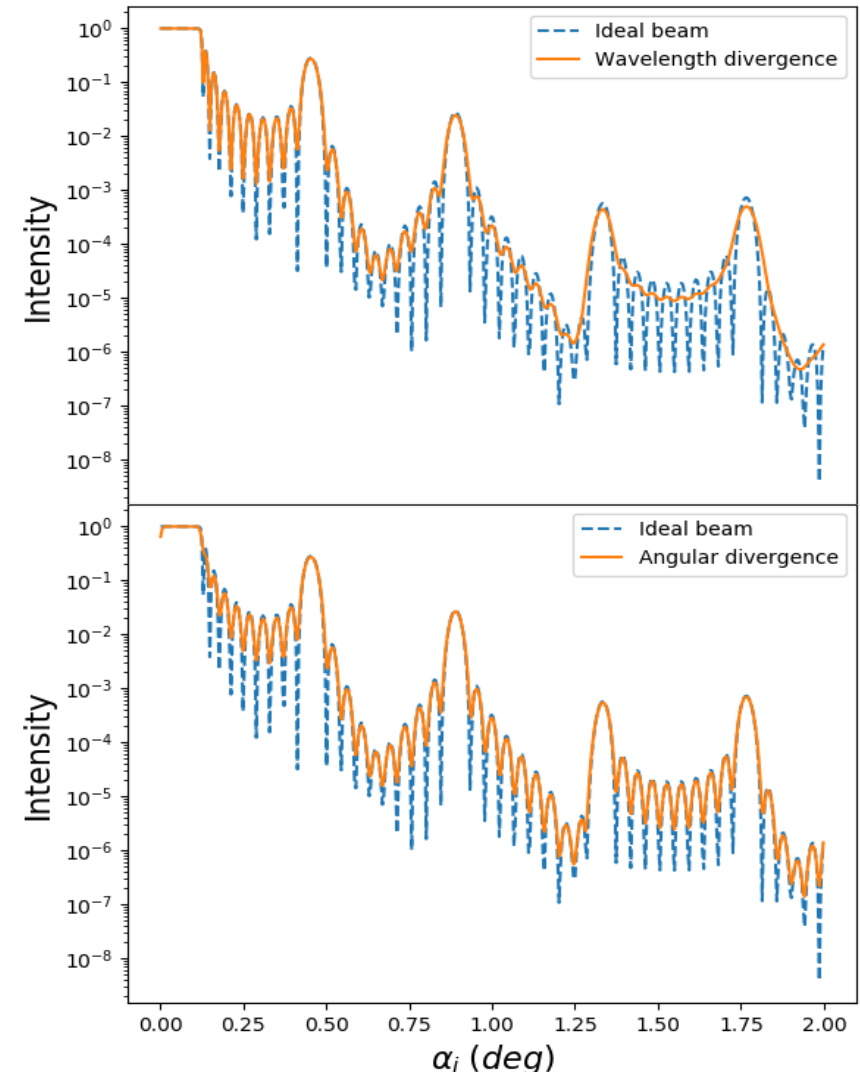
$$\Delta Q = \sqrt{Q^2 \left( \frac{\Delta \lambda}{\lambda} \right)^2 + \left( \frac{4 \pi}{\lambda} \cos \alpha_i \cdot \Delta \alpha_i \right)^2}$$

- 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](http://henke.lbl.gov/optical_constants/getdb2.html)

Scattering length density (SLD)

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

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

$$\left. \begin{array}{l} \sigma_{abs} \gg \sigma_{inc} \\ \sigma_{abs} \propto \lambda \end{array} \right\} \Rightarrow \rho \approx const$$

- 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 and materials with small signal attenuation

# Reflectometry in BornAgain: tutorials

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MLZ is a cooperation between:

# 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:  $\sigma = 0.01$  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	$\rho_r, 10^{-6} \text{ A}^{-2}$	$\rho_i, 10^{-6} \text{ A}^{-2}$	thickness, nm
Vacuum	-	0	0	Inf
Ag	4			20
SiO <sub>2</sub>	2.33			5
Si	2.33			Inf

# 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:  $\sigma = 0.01$  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/cm <sup>3</sup>	$\rho_r$ , $10^{-6}$ A <sup>-2</sup>	$\rho_i$ , $10^{-6}$ A <sup>-2</sup>	thickness, nm
Vacuum	-	0	0	Inf
Ag	4	1.322	0.004	20
SiO <sub>2</sub>	2.33	3.681	0	5
Si	2.33	2.074	0	Inf

# GUI: Simulate and fit Ag nano-particles

- Fitting parameters
  - Ag density
  - Ag layer thickness
  - SiO<sub>2</sub> density
  - SiO<sub>2</sub> layer thickness

Fit parameter	Start	Min	Max
Ag $\rho_r$ , $10^{-6} \text{ A}^{-2}$	1.322	0.661	2.0
Ag thickness, nm	20	10	30
SiO <sub>2</sub> $\rho_r$ , $10^{-6} \text{ A}^{-2}$	3.681	3.5	4.0
SiO <sub>2</sub> thickness, nm	5	3	8



# GUI: Simulate and fit Ag nano-particles

- Fitting parameters
  - Ag density
  - Ag layer thickness
  - SiO<sub>2</sub> density
  - SiO<sub>2</sub> layer thickness

Fit parameter	Target value
Ag $\rho_r$ , $10^{-6} \text{ A}^{-2}$	1.984
Ag thickness, nm	25
SiO <sub>2</sub> $\rho_r$ , $10^{-6} \text{ A}^{-2}$	3.8
SiO <sub>2</sub> thickness, nm	7

# Thank you for your attention!

MLZ is a cooperation between: