Modeling off-specular x-ray scattering from patterned thin films using the Born Approximation.

ANDRÉ GUZMÁN
BRIAN MARANVILLE
PAUL KIENZLE

POOLESVILLE HIGH SCHOOL
NIST CENTER FOR NEUTRON RESEARCH
NIST CENTER FOR NEUTRON RESEARCH
Motivation

• Off-specular scattering with neutrons
• Developing technique at NCNR
• Born Approximation to model other data
  • SANS, Triple Axis
• Testing Born Approximation for use with off-specular
Patterned Permalloy Gratings

- Permalloy is magnetically soft
- Nickel has high neutron SLD
- Patterned on silicon substrate

Permalloy diffraction grating
X-Ray Off-specular Scattering

- Rocking Curves
- Vary $\theta$, $2\theta$ constant
- For each $\theta$
  - Measure $k_{\text{out}}$ intensity
  - Compute $Q_x$
- Features on flat sample

\[
|\vec{Q}| = \frac{4\pi}{\lambda} \sin\left(\frac{2\theta}{2}\right)
\]

\[
Q_{x} = Q \sin(\theta_{\text{tilt}})
\]

\[
Q_{z} = Q \cos(\theta_{\text{tilt}})
\]
Specular Measurements

- Taken before Rocking Curves
- Low Q, Mid Q, High Q
- Peak $\theta$s used for Rocking Curves
- $2\theta > 2$ data too noisy
Mesh Scans

- Rocking curves
- Did not use specular peaks
- Incremented $2\theta$
- Vbscript data collection
Born Approximation Fourier Transforms

- Approximates x-ray scattering
- Assumes weak scattering
- Fourier transform of structure
- Measuring in waves
- Real space to reciprocal Q-space

\[ F(v) = \int_{-\infty}^{+\infty} f(t)e^{-i\nu t} dt \]

\[ x(t) \rightarrow x^{-1}(\nu) \]

\[ FT(q_x) = \int_0^{S_x} \rho e^{-iq_xx} dx \]

\[ x(\text{Å}) \rightarrow q_x (\text{Å}^{-1}) \]
Preliminary Data Analysis

- Property of Fourier Transform
- Equation must hold true
- Detect false peaks

\[
\frac{2\pi}{q_x \text{ peak spacing}} = D_x \text{ Realspace Å}
\]
Square Model

- Uses Born Approximation
- Equation is Fourier Transform of structure
- Parameters in equation correspond to material structure

\[ FT(q_x) = \frac{1}{2D_x n_{max}} \sum_{n=-n_{max}}^{n_{max}} \left( e^{-\frac{(nD_x)^2}{2\sigma^2}} \right) \left( e^{-iq_x nD_x} \right) \left( \frac{i\rho}{q_x} \right) \left( e^{-iq_x S_x} - 1 \right) \]
Trapezoidal Model

- Also uses Born Approximation
- Slightly more complicated
- Structure not perfect square

\[
\begin{align*}
\left( \frac{-nD_x}{2\sigma^2} e^{-iq_x nD_x} \right) & \frac{l_{1z}}{l_{1x}} \left[ e^{-iq_x l_{1x}} \left( 1 + iq_x (l_{1x} + nD_x) \right) \frac{q_x^2}{q_x^2} - 1 + iq_x nD_x \right] \\
+ \frac{i\rho}{q_x} & \left[ e^{-iq_x (S_x - l_{2x})} - e^{-iq_x l_{1x}} \right] \\
+ \frac{l_{2z}}{l_{2x}} & \left[ e^{-iq_x S_x (1 + iq_x (S_x + nD_x))} - e^{-iq_x (S_x - l_{2x})} (1 + iq_x (S_x - l_{2x} + nD_x)) \right]
\end{align*}
\]
BUMPS Data Analysis

- Bayesian Uncertainty Modeling for Parametric Systems
- General purpose fitting program
- Varies parameters
- Finds best fit for data
Model Comparison

- Used part of lowq data
- Both stop matching at end
- Trapezoid fits more closely
- Neither works in left half
Structure and Form Factor

- Form factor is constant over summation
- Form factor more dynamic
- Structure factor determines peak location
- Form factor determines shape

\[
\sum_{n=-n_{\text{max}}}^{n_{\text{max}}} \left[ \frac{(nD_x)^2}{2\sigma^2} \left( e^{-iq_xnD_x} \right) \left( \frac{i\rho}{q_x} \right) \left( e^{-iq_xS_x} - 1 \right) \right]
\]
Conclusions and Future Work

- Trapezoidal model works slightly better
- Born Approximation works lowq and midq right side
- Further refine data model
- Test on more complicated sample
- Test on real samples
Acknowledgements

• Advisor:
  • Brian Maranville

• BUMPS and C Programming Support:
  • Paul Kienzle

• NCNR SHIP Coordinators
  • Yamali Hernandez
  • Julie Borchers

• NCNR SHIP Sponsor
  • Center for High Resolution Neutron Scattering
Questions?