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

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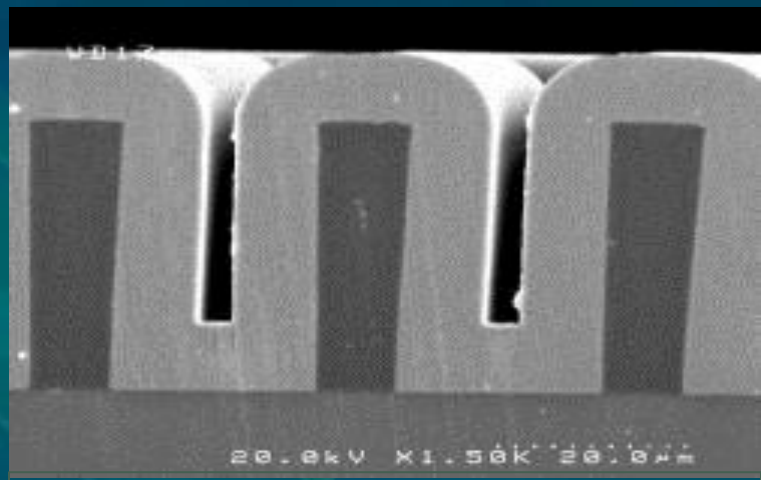
Motivation

- 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

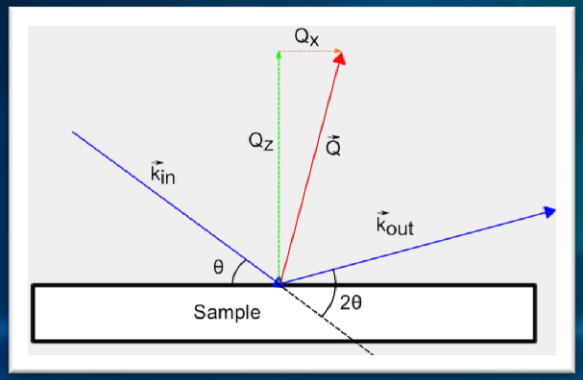
X-Ray Off-specular Scattering

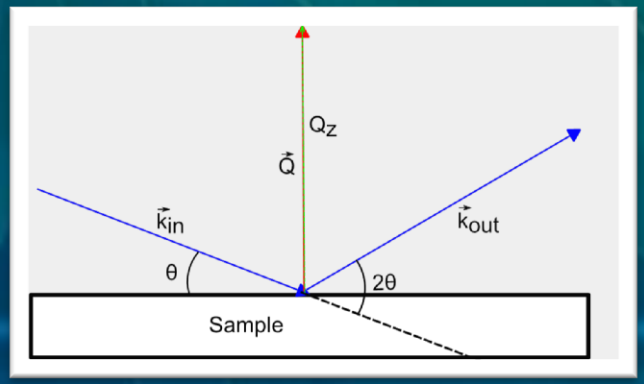
- Rocking Curves
- Vary θ, 2θ constant
- For each θ
  - Measure k_{out} intensity
  - Compute Q_x
- Features on flat sample

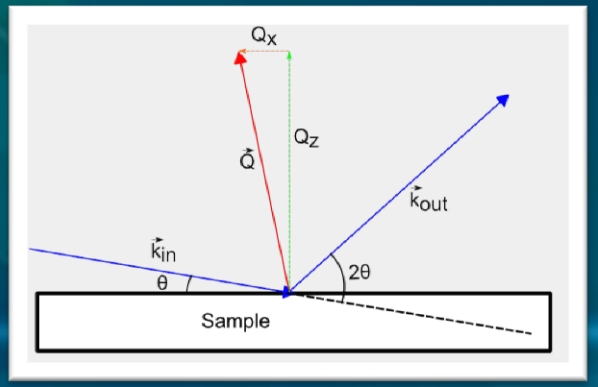
$$\left|\vec{Q}\right| = \frac{4\pi}{\lambda}\sin\left(\frac{2\theta}{2}\right)$$

$$Q_x = Q\sin(\theta_{tilt})$$

$$Q_z = Q\cos(\theta_{tilt})$$

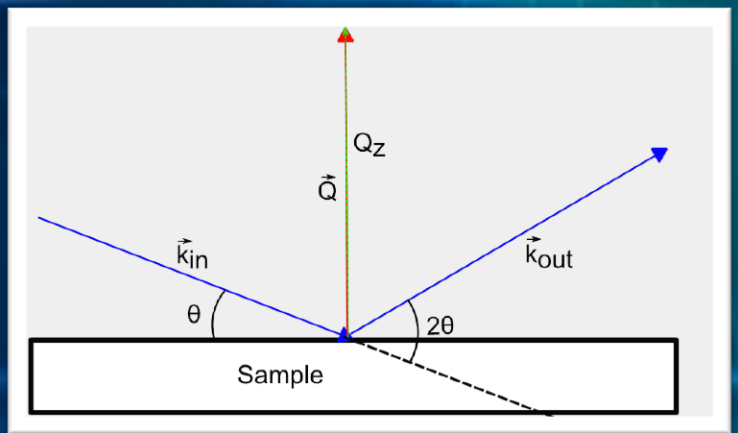


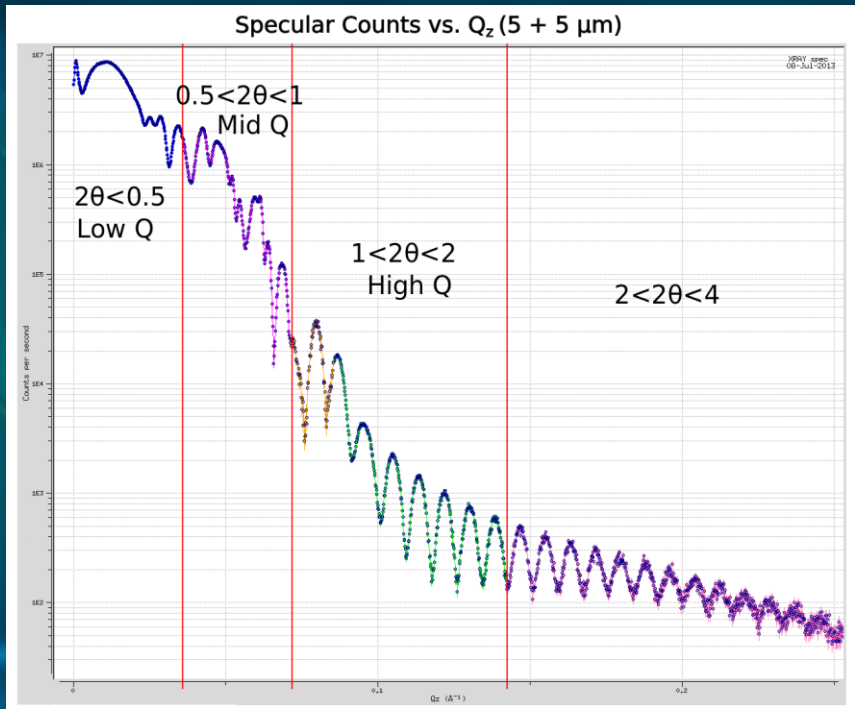




Specular Measurements

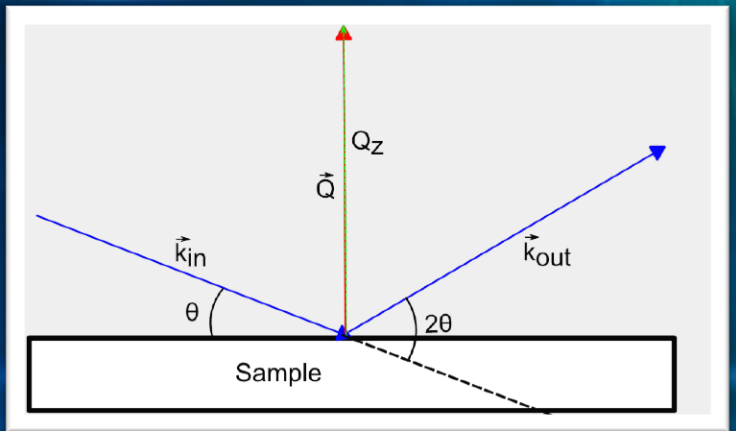
- Taken before Rocking Curves
- Low Q, Mid Q, High Q
- Peak θs used for Rocking Curves
- 2θ > 2 data too noisy

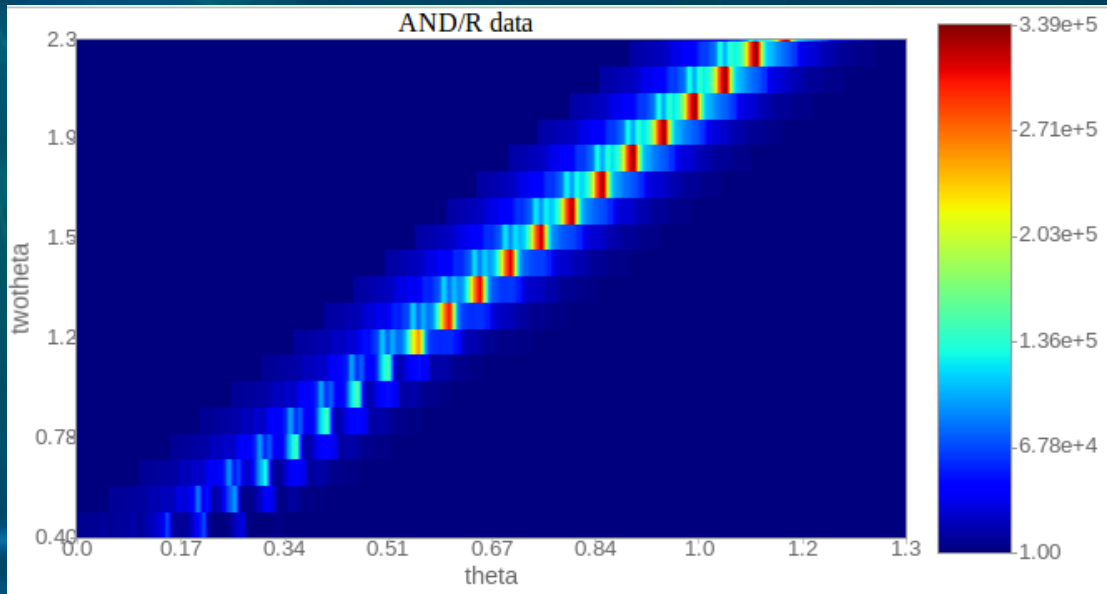




Mesh Scans

- Rocking curves
- Did not use specular peaks
- Incremented 2θ
- Vbscript data collection





Born Approximation Fourier Transforms

$$F(\nu) = \int_{}^{+\infty} f(t) e^{-i\nu t} \mathrm{d}t$$

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

$$FT(q_x) = \int_{0}^{S_x} \rho e^{-iq_x x} \mathrm{d}x$$

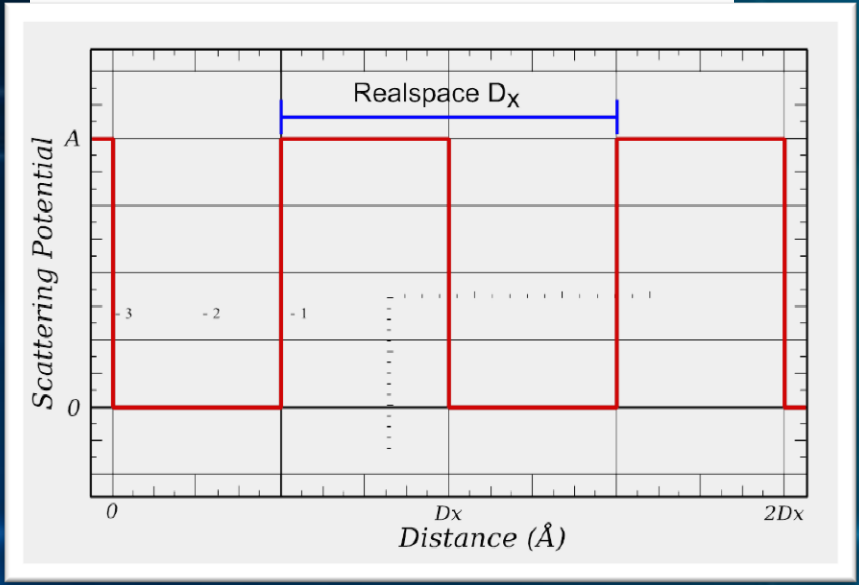
$$x(\text{Å}) \rightarrow q_x(\text{Å}^{-1})$$

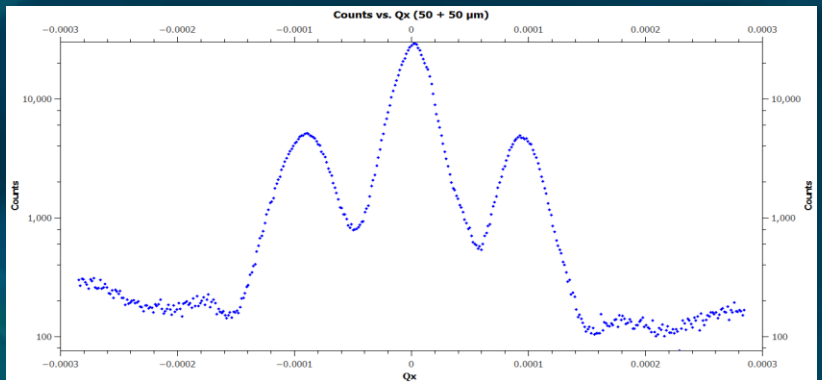
- Approximates x-ray scattering
- Assumes weak scattering
- Fourier transform of structure
- Measuring in waves
- Real space to reciprocal Q-space

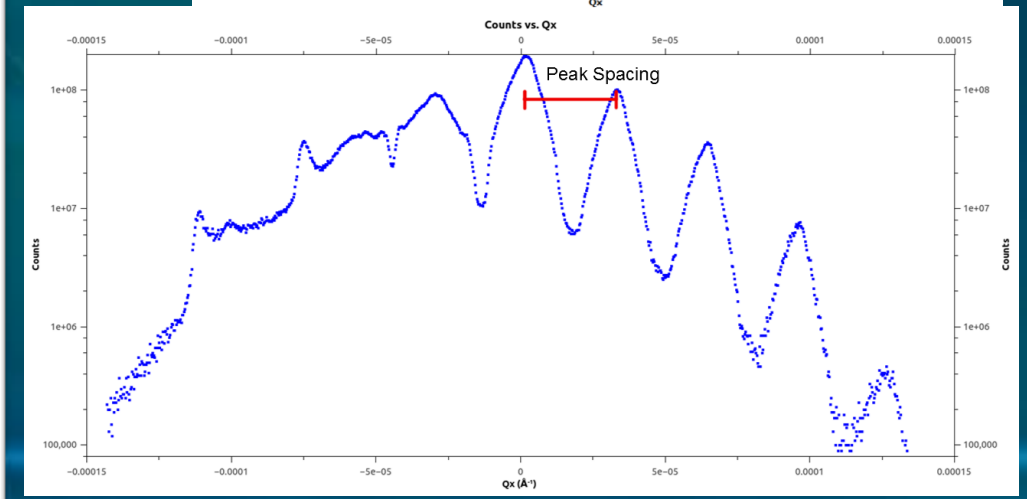
Preliminary Data Analysis

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

$$\frac{2\pi}{q_x \text{ peak spacing}} = D_x \text{ Realspace } \mathring{A}$$



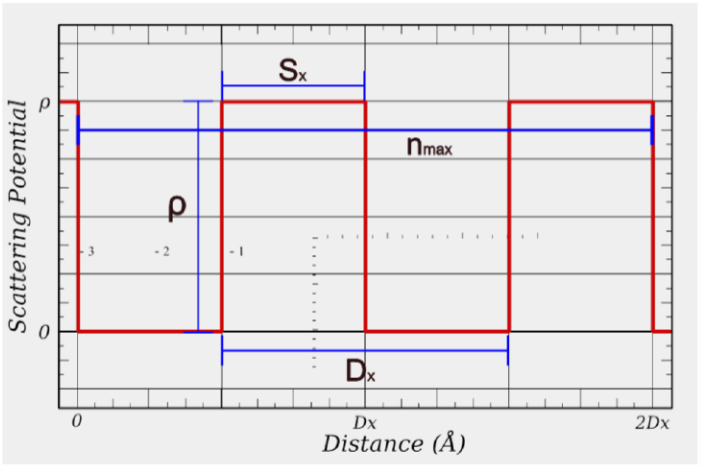


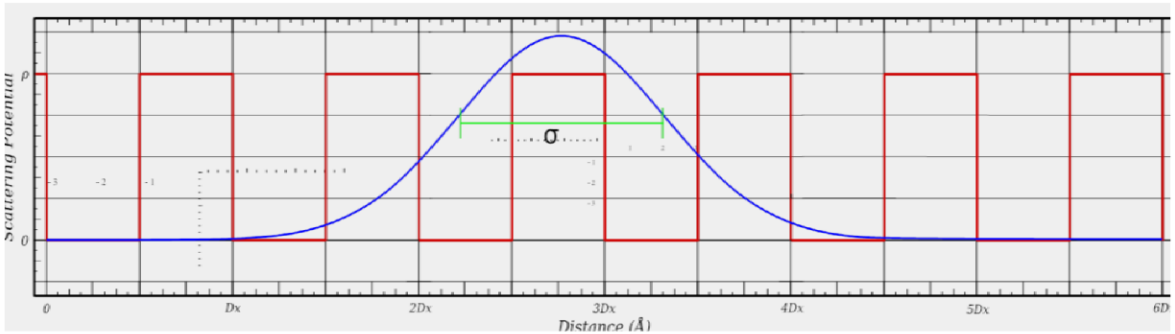


Square Model

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

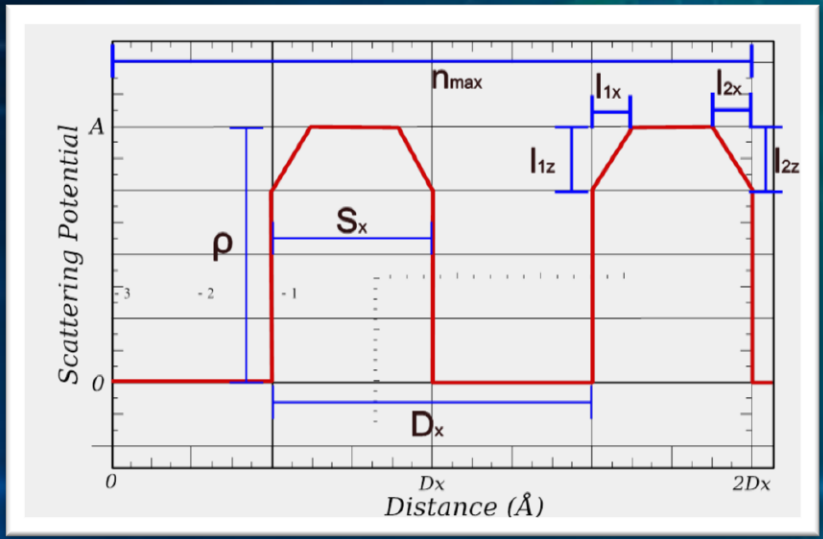
$$FT(q_x) = \frac{1}{2D_x n_{max}} \sum_{n=-n_{max}}^{n_{max}} \left[\left(e^{\frac{-(nD_x)^2}{2\sigma^2}} \right) \left(e^{-iq_x nD_x} \right) \left(\frac{i\rho}{q_x} \right) \left(e^{-iq_x S_x} - 1 \right) \right]$$





Trapezoidal Model

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



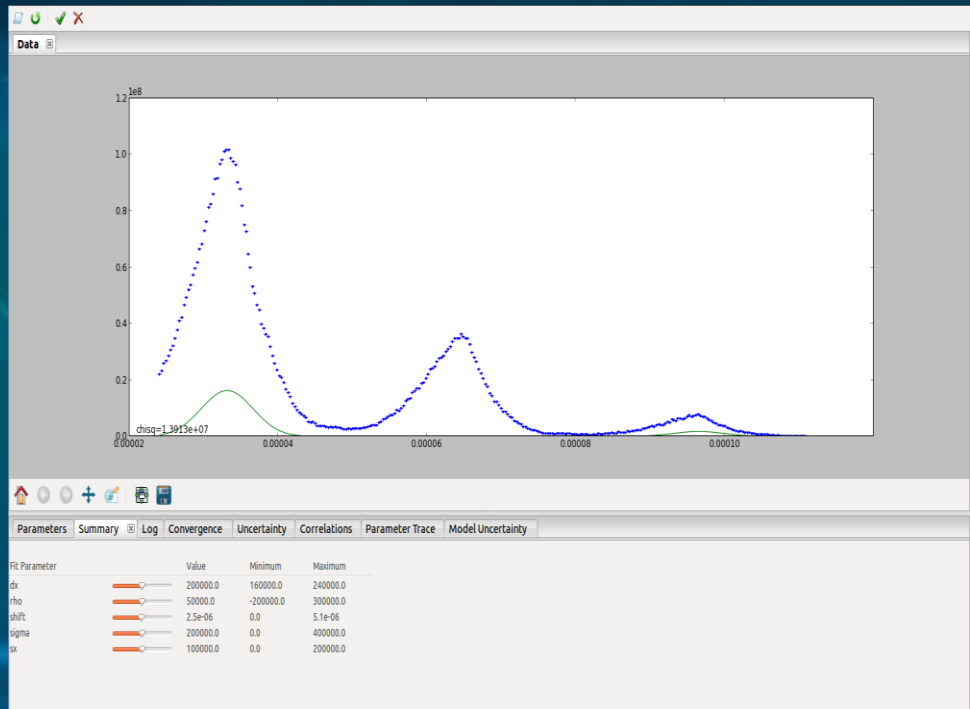
$$\left(e^{\frac{-nD_x}{2\sigma^2}}e^{-iq_x nD_x}\right)\frac{l_{1z}}{l_{1x}}\left[\frac{e^{-iq_x l_{1x}}(1+iq_x(l_{1x}+nD_x))}{q_x^2}-\frac{1+iq_x nD_x}{q_x^2}\right]$$

$$+\frac{i\rho}{q_x}\left[e^{-iq_x(S_x-l_{2x})}-e^{-iq_x l_{1x}}\right]$$

$$+\frac{l_{2z}}{l_{2x}}\left[\frac{e^{-iq_x S_x}(1+iq_x(S_x+nD_x))}{q_x^2}-\frac{e^{-iq_x(S_x-l_{2x})}(1+iq_x(S_x-l_{2x}+nD_x))}{q_x^2}\right]$$

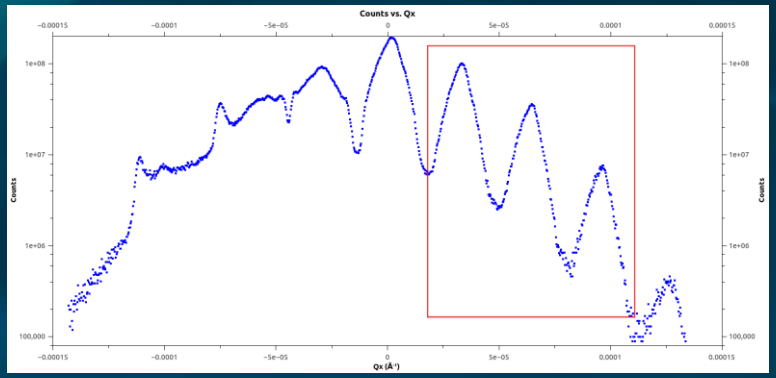
BUMPS Data Analysis

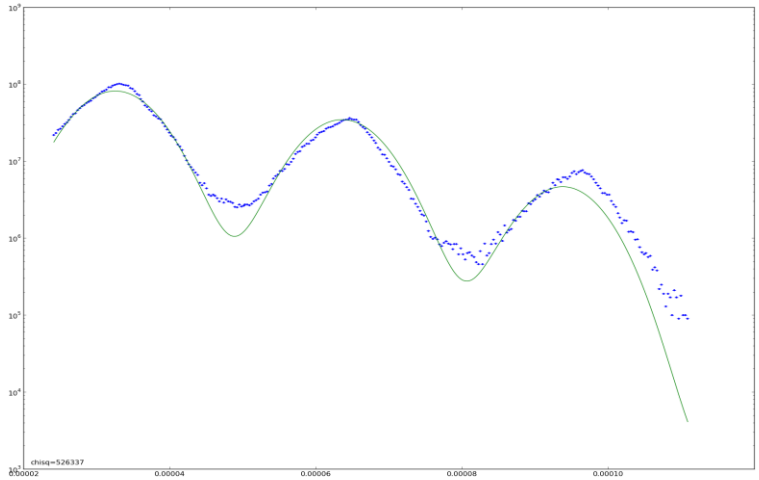
- Bayesian Uncertainty Modeling for Parametric Systems
- General purpose fitting program
- Varies parameters
- Finds best fit for data

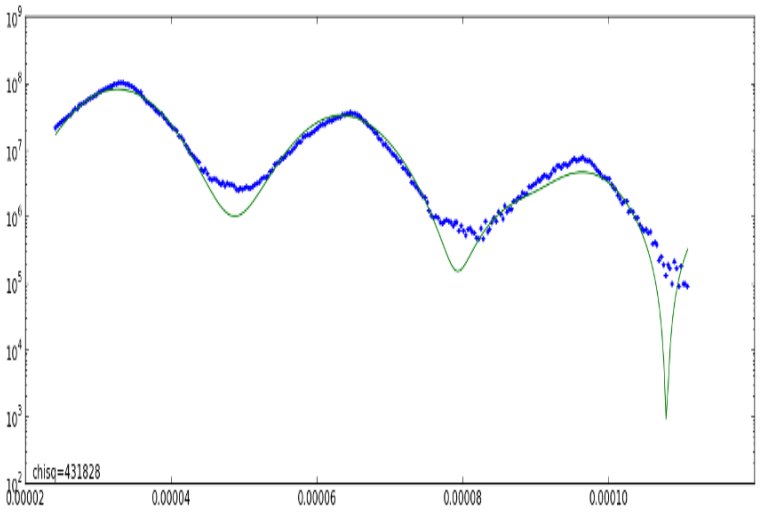


Model Comparison

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





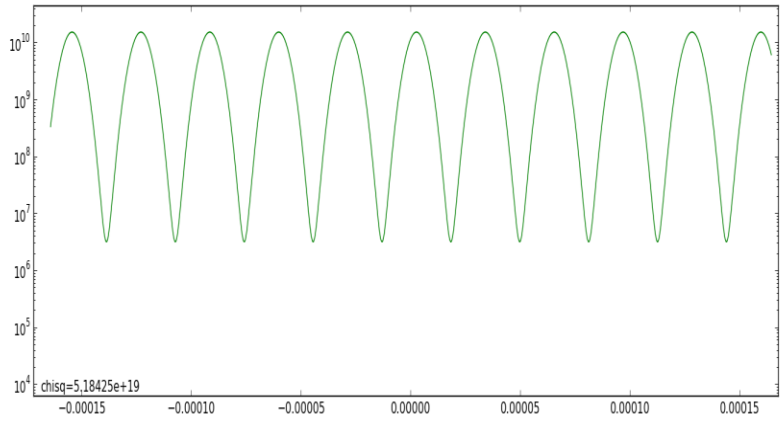


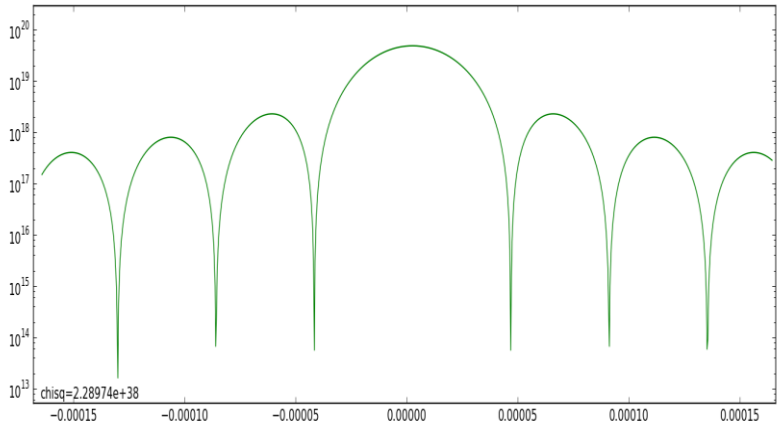
Structure and Form Factor

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

Structure Factor Form Factor

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





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

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Questions?