Intro to Polarized Neutron Reflectivity

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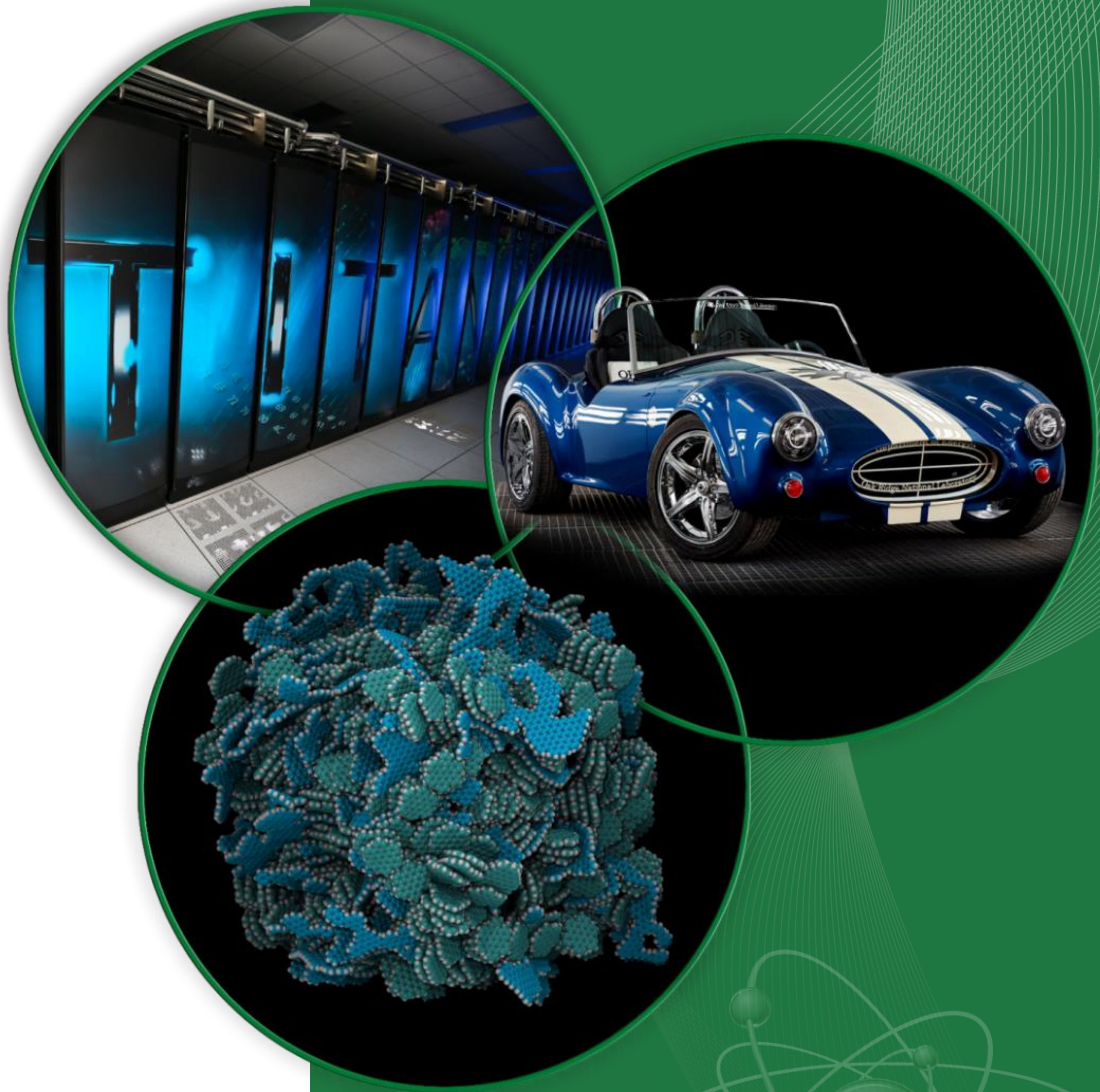
ORNL

BL4A instrument



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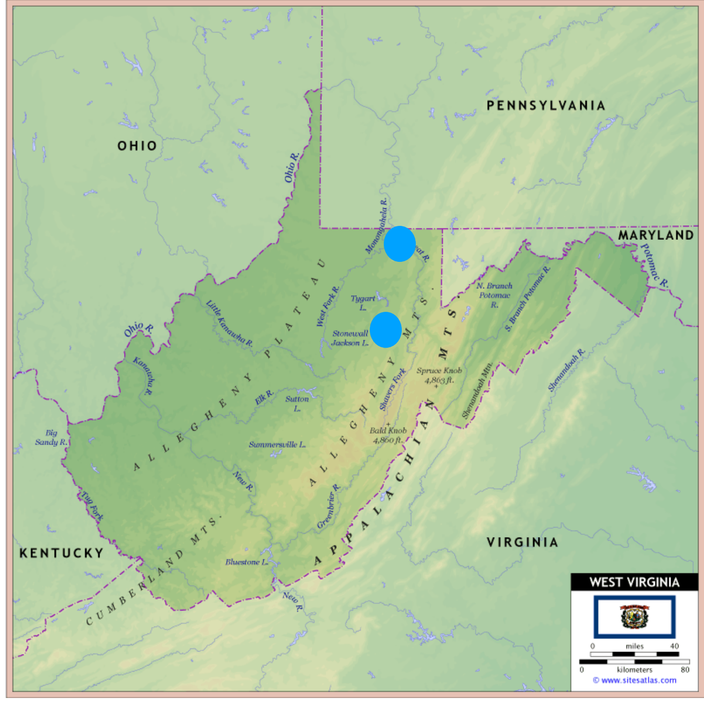
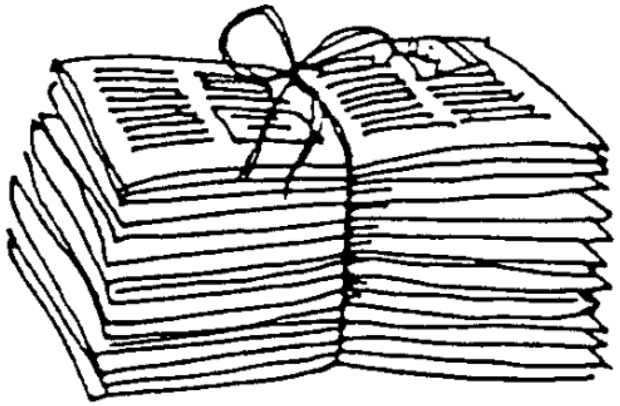
National Laboratory

How did I get here?



- Start: Small Appalachia coal mining town.
- PHD: WVU in Physics (2001)
- DOE Neutron PostDoc stationed at Rutherforc Appleton Lab. Oxfordshire UK
- Transitioned to instrument scientist (2004)
- Moved to ORNL (2015)

Work Flow



Idea / Problem

Experiment and Analysis

Scientific Understanding

Why use neutron reflection?

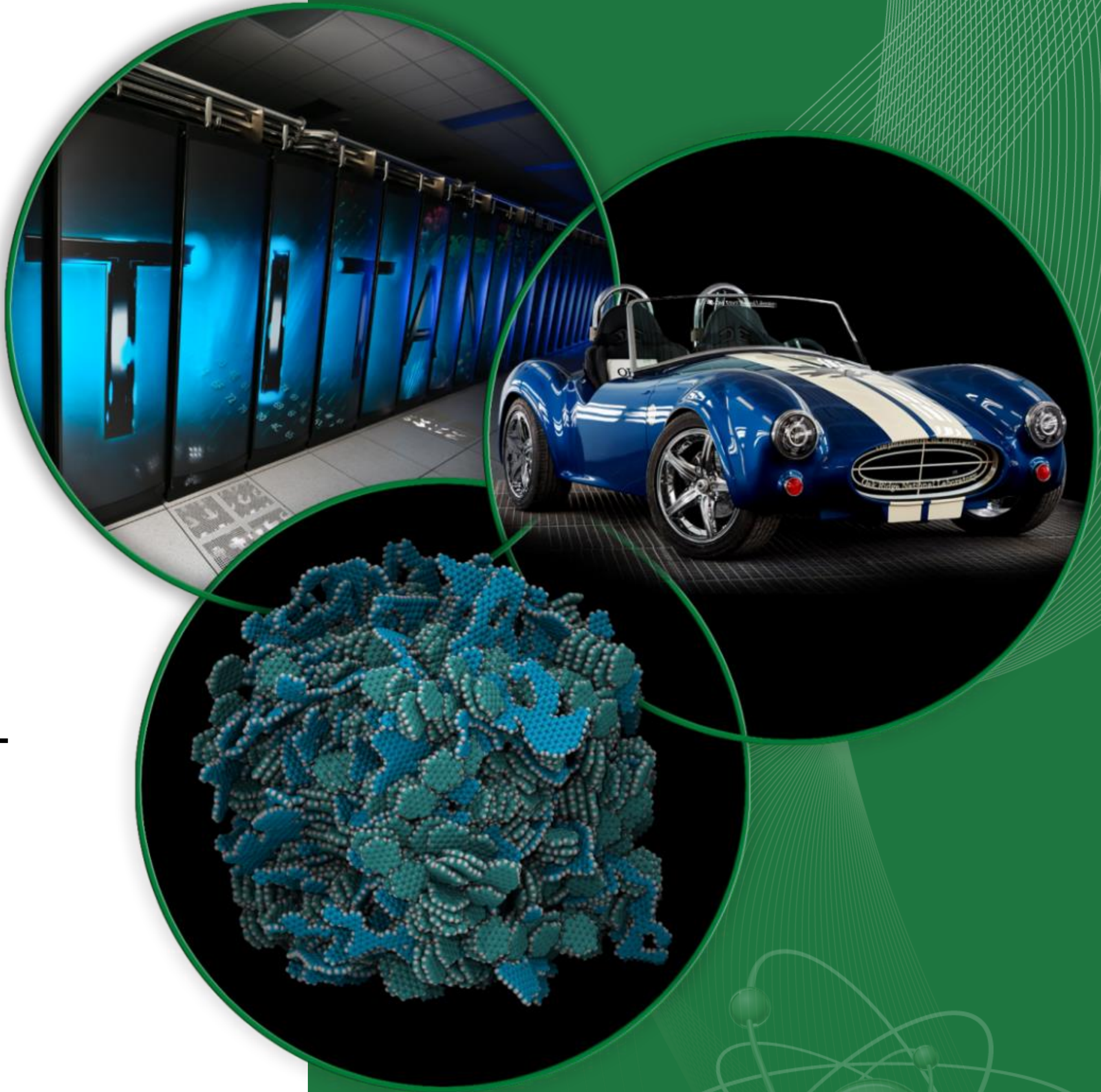
Start with building intuition.

Science examples to motivate.

Math & physics description.

Reading the tea leaves.

Nuts & bolts.



Reflections Come in Many Types

Perfect reflections

Reflections Come in Many Types

Imperfect reflections

Reflections Come in Many Types

Reflections from an imperfect surface with structure

Reflections Come in Many Types

Reflections with some dispersion

Reflections Come in Many Types

Reflections from curved objects

Reflections Come in Many Types

Reflections where below surface features are visible

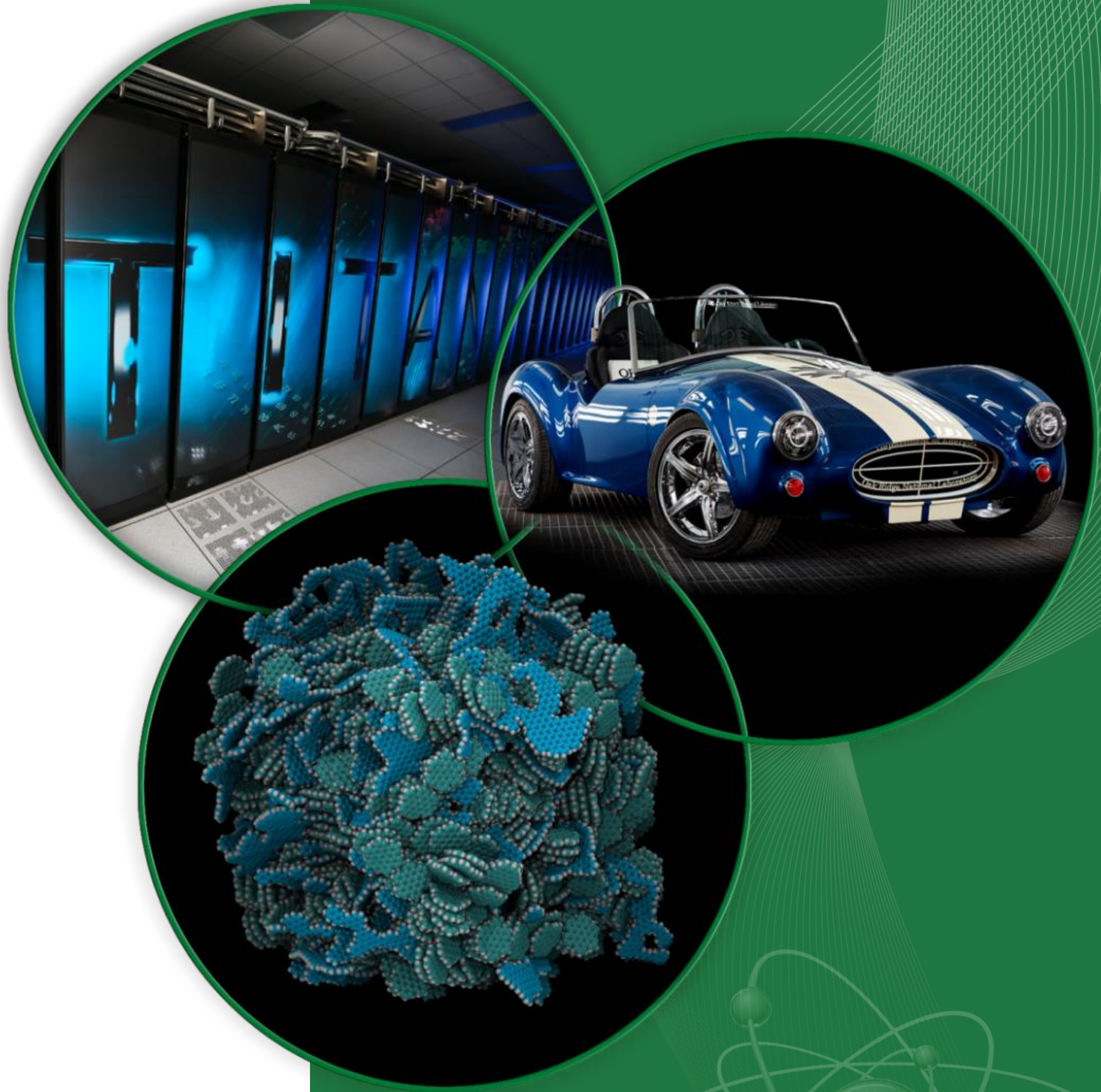
Why use neutron reflection

Spin 1/2

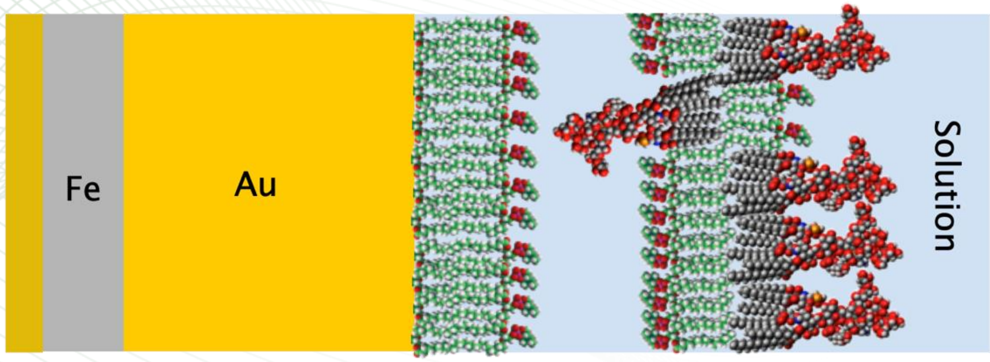
Convenient energies, speeds, wavelength

Great complement to x-ray and other large facility measurements (slow muons)

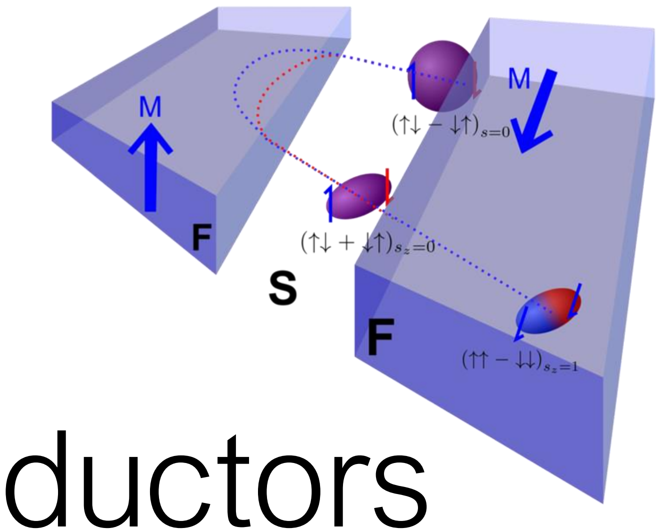
Great complement to lab based imaging & magnetic measurements



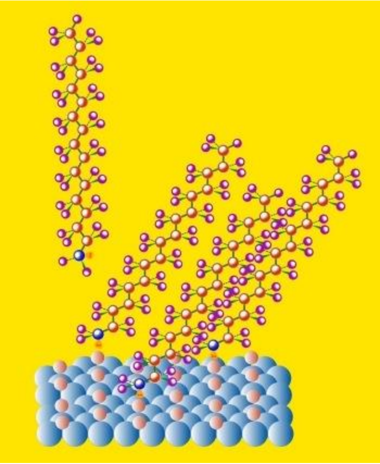
Why use neutron reflection



Biology

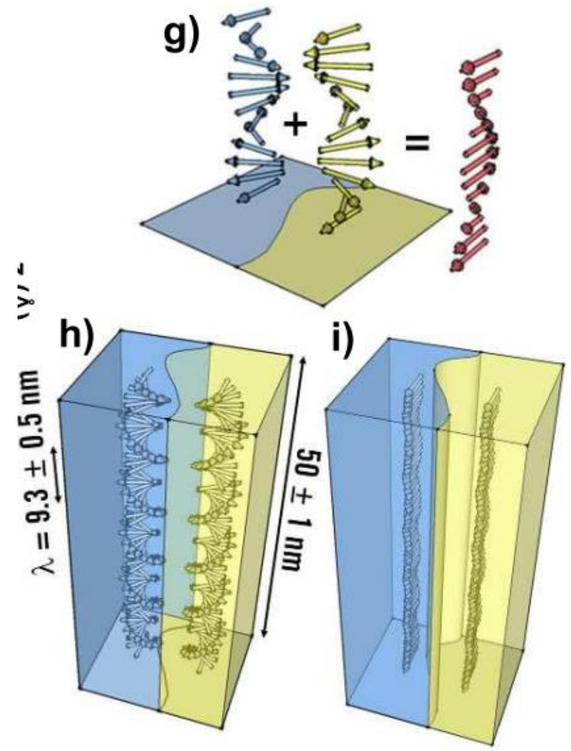


Superconductors



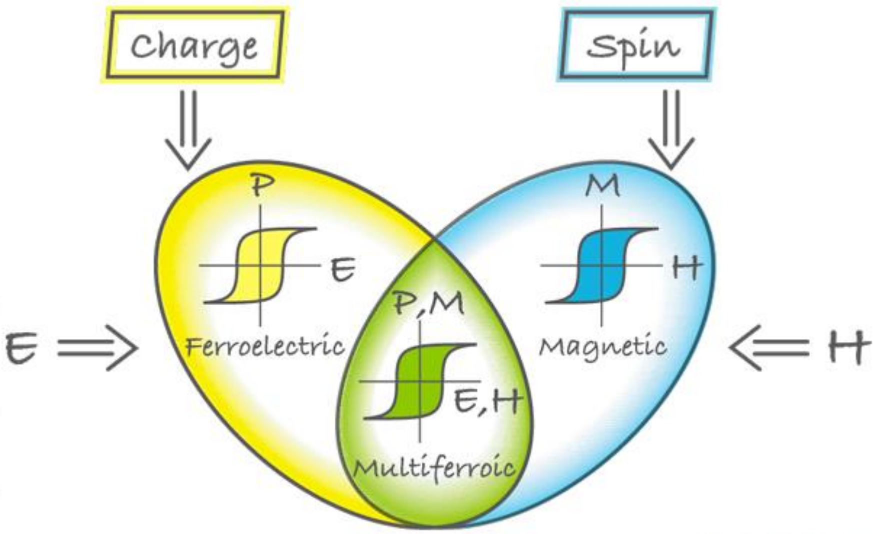
Langmuir 2013, 29, 13735–13742

Soft Matter



Magnetism

Multiferroics

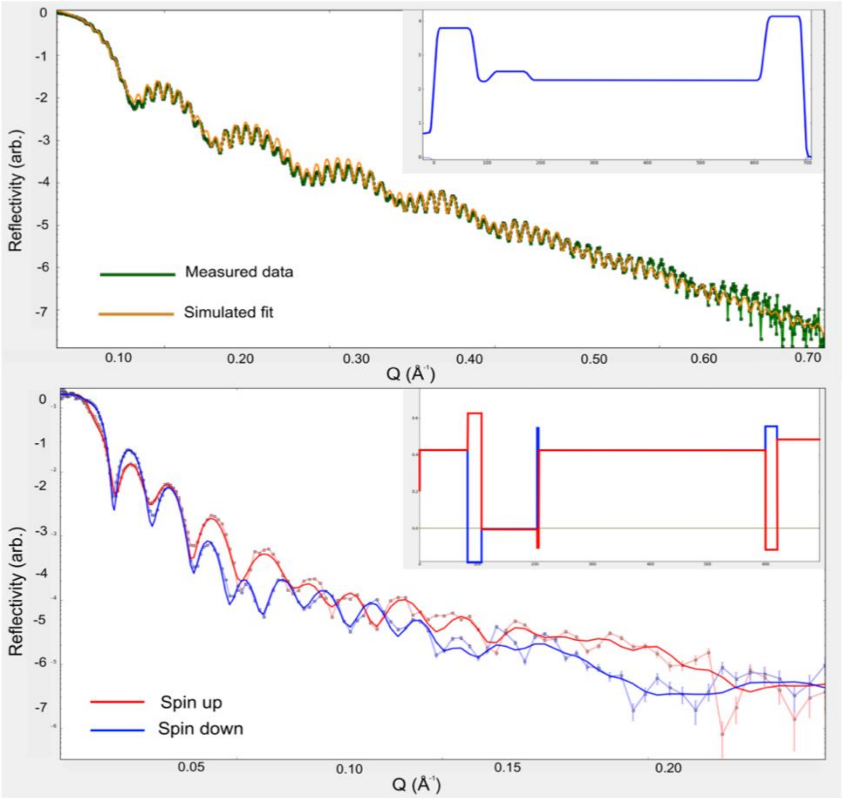


Physics 2, 20 (2009)

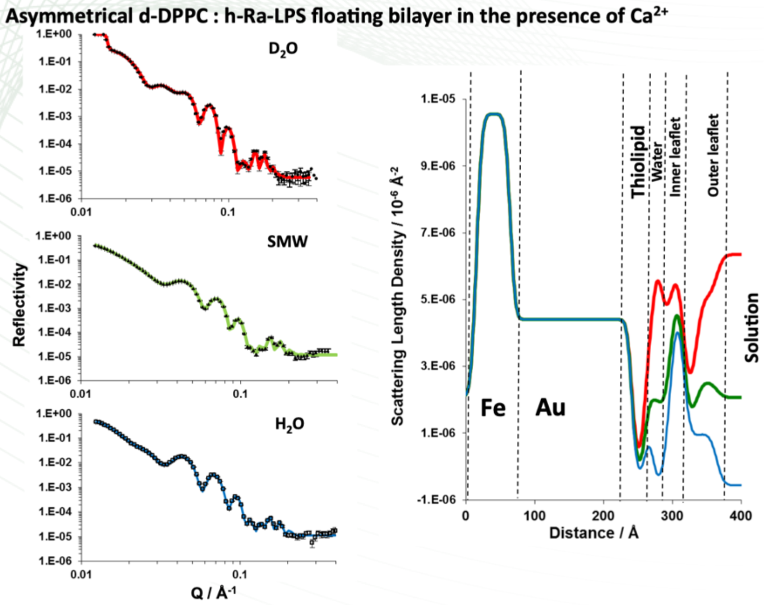
Illustration: Alan Stonebraker

Data Examples

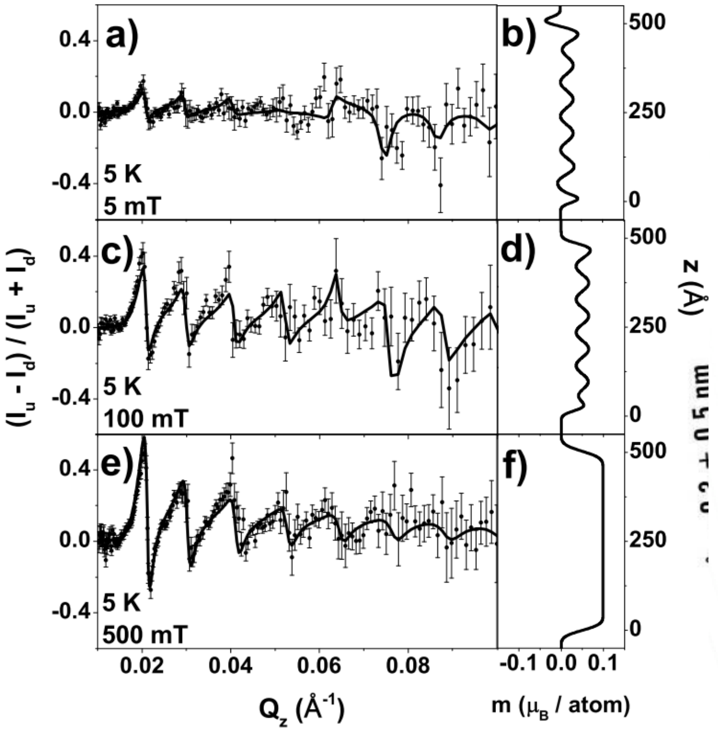
Superconductors



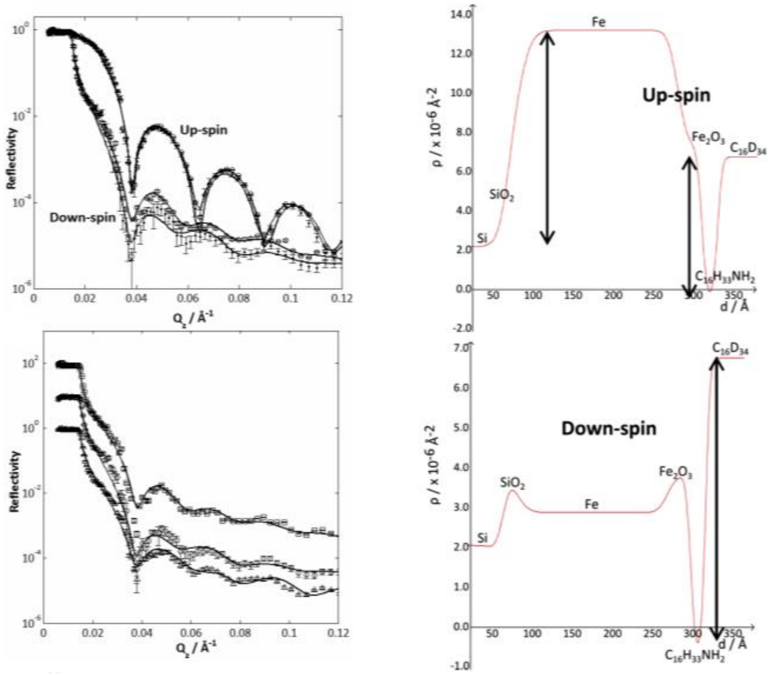
Biology

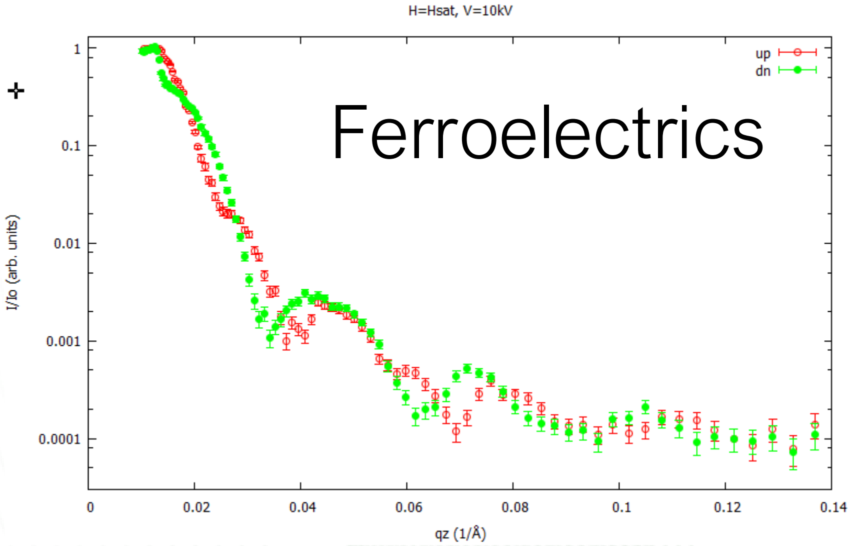


Magnetism



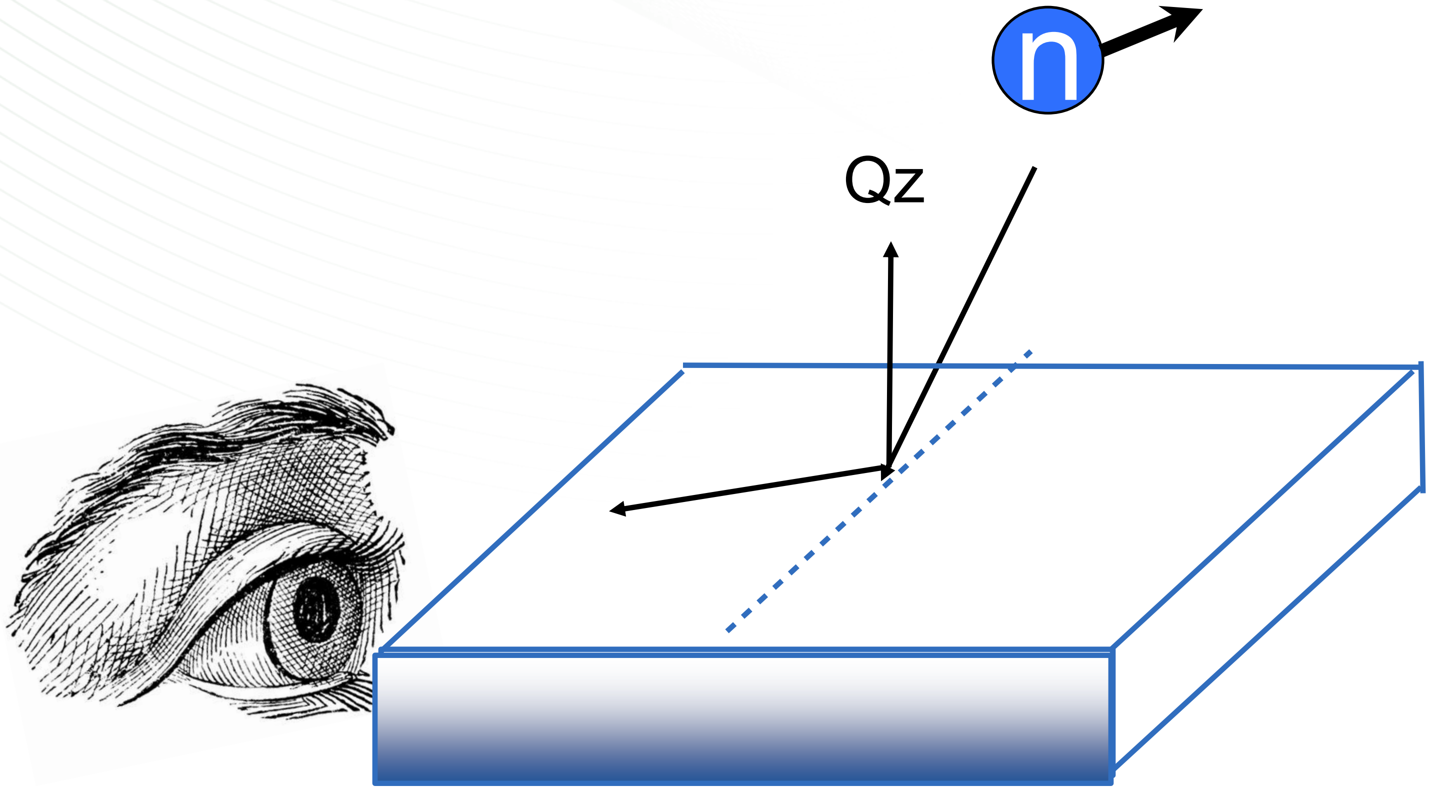
Soft Matter



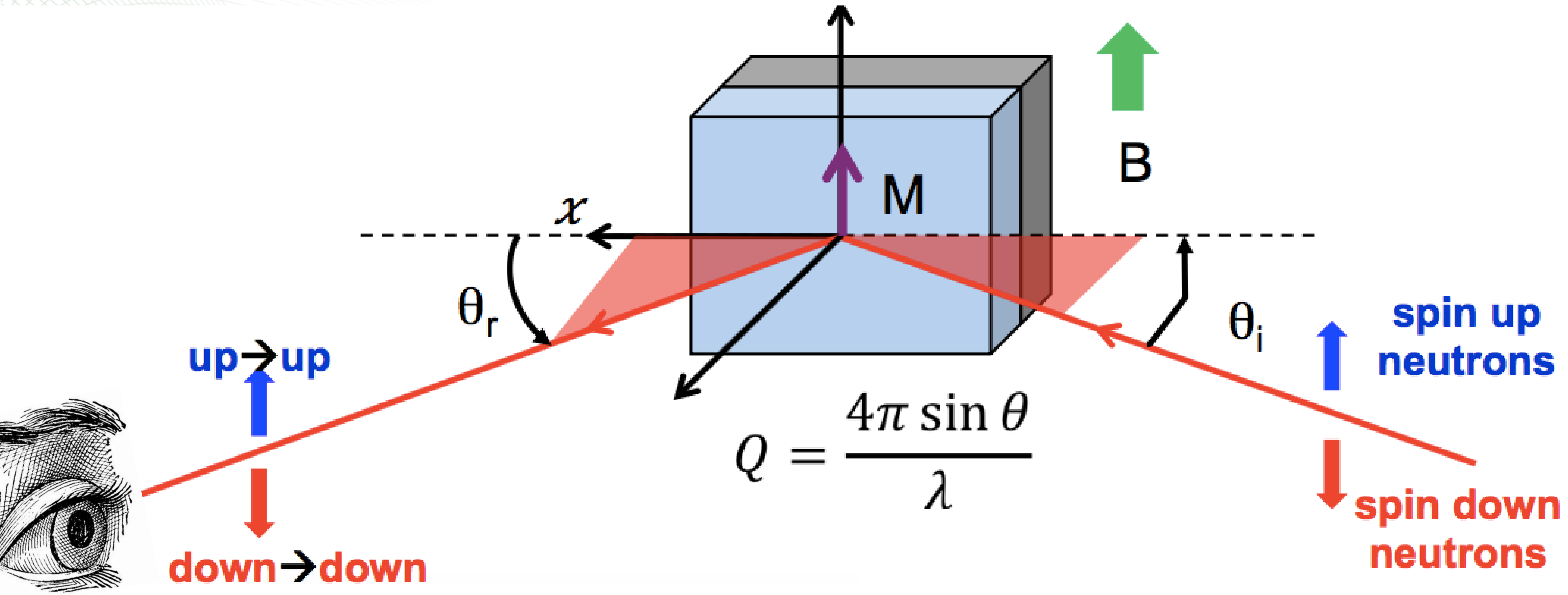


Ferroelectrics

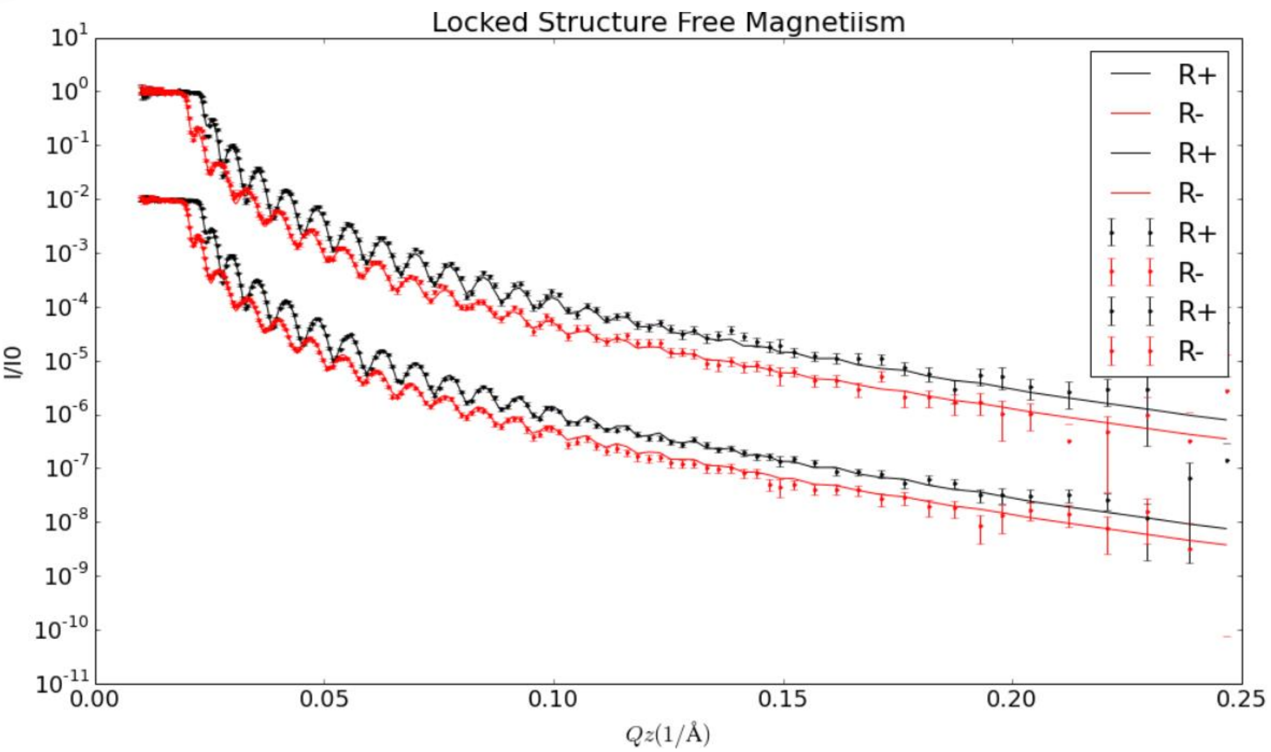
Experimental Geometry

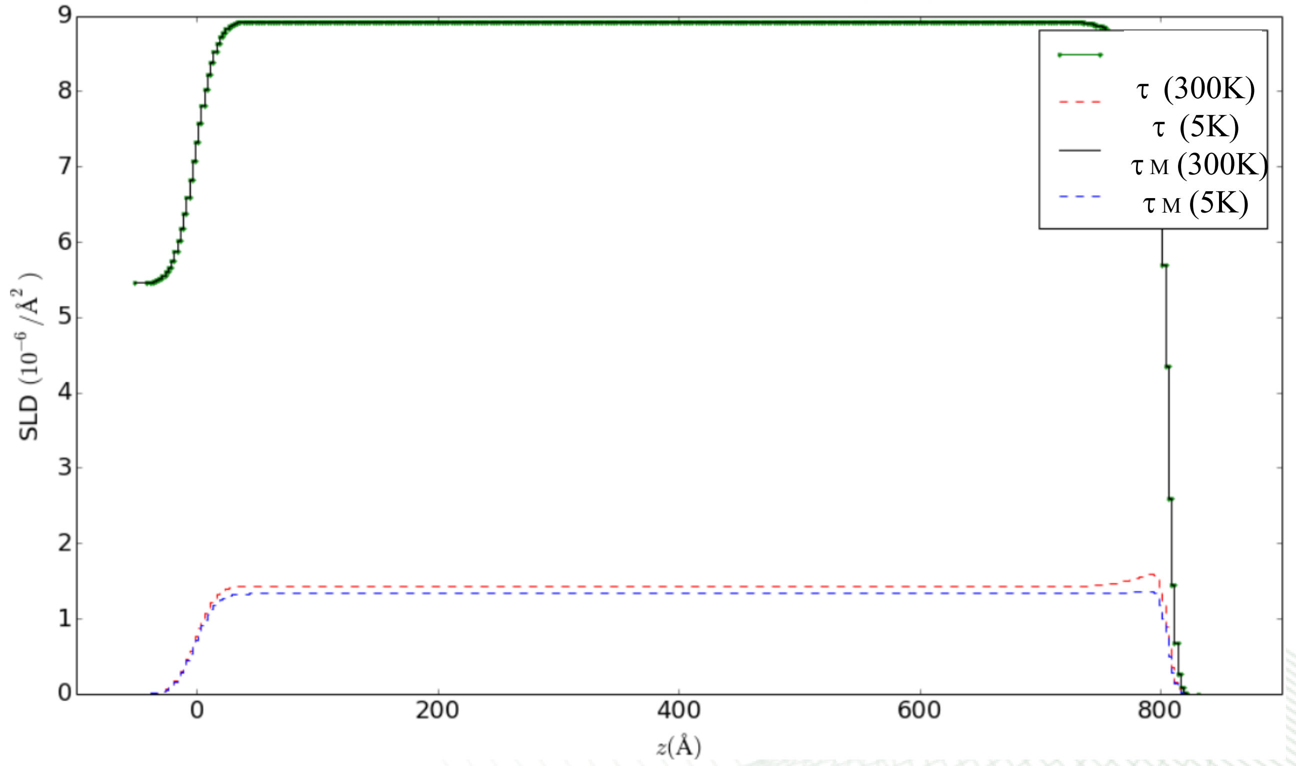


Experimental Geometry



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



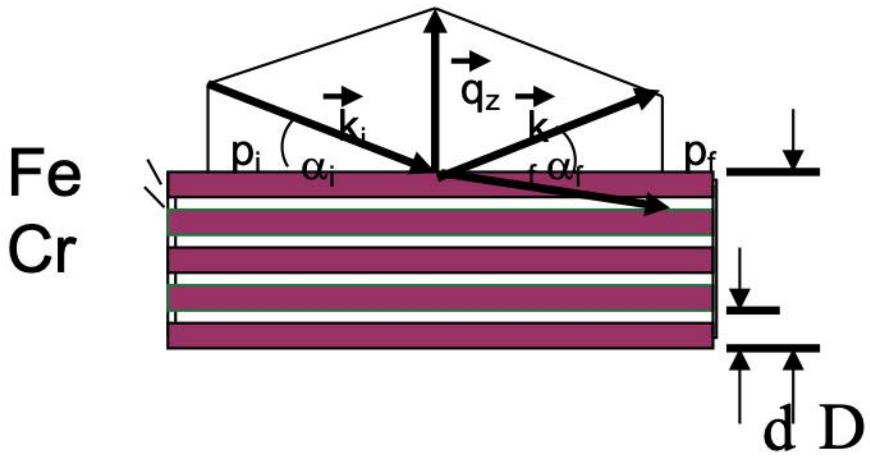


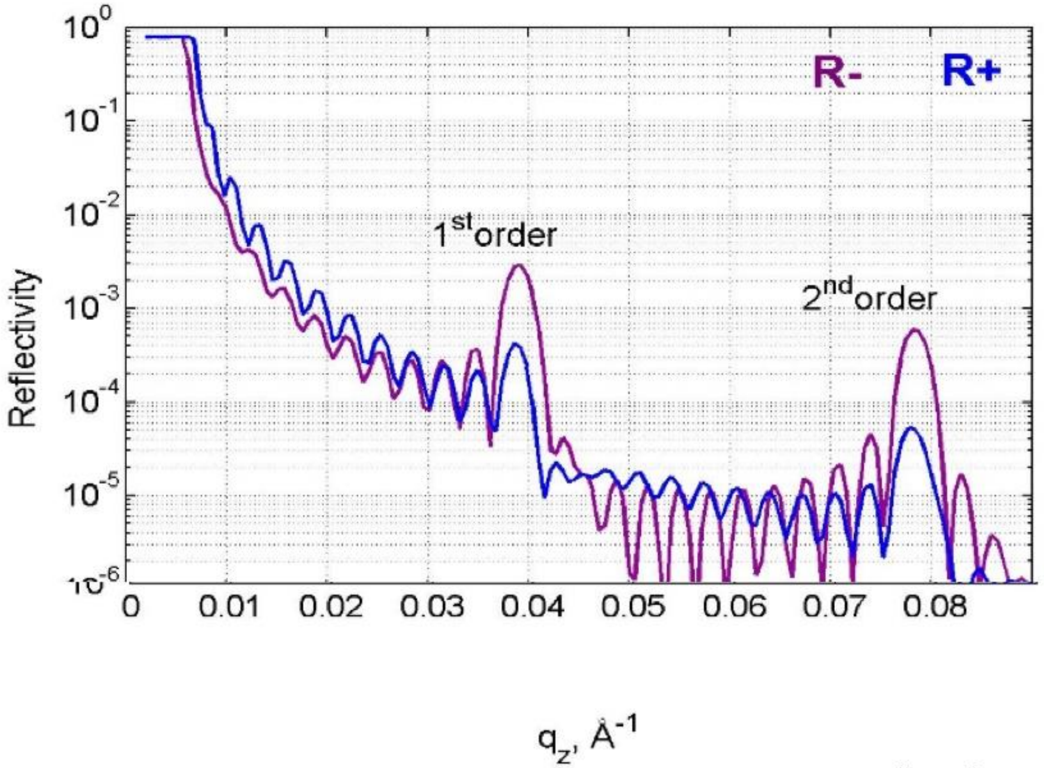
What we get from reflectometry

- Magnetic & chemical profile along the thickness (z).
- Great at uncovering non-uniform distributions in density and magnetization near interfaces.

How do we get it

$$V(z) = \frac{\hbar N b(z)}{2\pi m} - \mu \cdot B_{\perp}(z) \quad [\mathring{A}^{-2}]$$

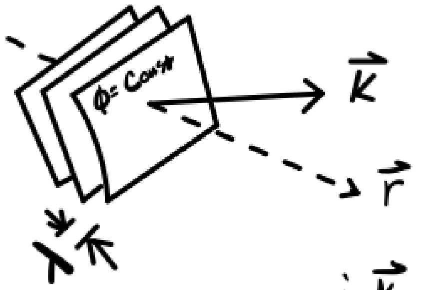




- Solve Schrodinger's eq. for a guessed potential V(z) and compare with the measured data

Reminder: solving Schrodinger's Eq.

Potential Scattering



$$\Psi \propto e^{i\vec{k}\cdot\vec{r}}$$

$|\Psi|^2 \propto$ Probability of finding the neutron @ $(\vec{k},\vec{r})$

Assume:

Elastic Interactions

Total E = KE + PE = Constant

$$E\Psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\Psi$$

Vacuum $E_0 = KE = \dfrac{\hbar^2 k_0^2}{2m}$

material $E = KE + PE = \dfrac{\hbar^2 K^2}{2m} + \dfrac{2\pi\hbar^2}{m}\rho$

Conservation of energy → $E_0 = E$

$K^2 = K_0^2 - 4\pi\rho$ & $[\nabla^2 + K^2]\Psi = 0$

Define refractive Index $n = K/K_0 = \sqrt{1 - \frac{4\pi\rho}{K^2}}$

From wave eq. $\Rightarrow r(Q) = \dfrac{4\pi}{iQ}\displaystyle\int_{-\infty}^{\infty}\psi(z)\rho(z)e^{iK_{0z}z}dz$; $\psi = ?$

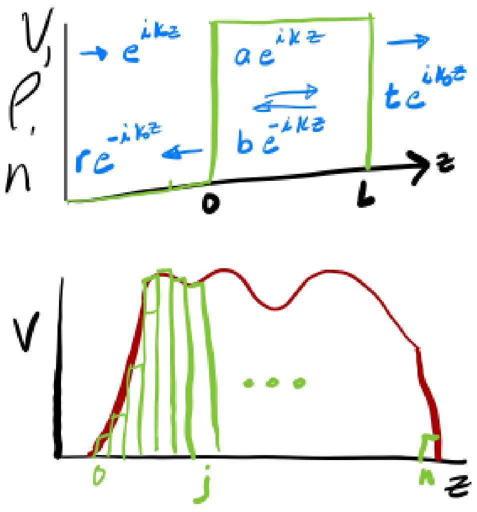
How to represent $V(\vec{r})$

For a "uniform" material ⇒ $V = \dfrac{2\pi\hbar^2}{m}\sum_n N_n b_n = \dfrac{2\pi\hbar^2}{m}\rho$

Re(b) - Scattering

Im(b) - absorption

$\uparrow$ SLD



Units & magnetic SLD

$\rho = \rho_n \pm \rho_m \left[\frac{1}{\text{Å}^2}\right]$

$\rho_m = C\sum N\mu = C'm$

μ = magnetic moment / FU

m = magnetization density

Conversion factors "C"

2.645×10^{-5} Å$/\mu_B$

$2.9109 \times 10^{-5}/4\pi$ Å^{-2} T^{-1}

2.853×10^{-9} Å^{-2} cm^3/emu

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} a_0 & b_0 \\ c_0 & d_0 \end{pmatrix}\begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix}\cdots\begin{pmatrix} a_j & b_j \\ c_j & d_j \end{pmatrix}\cdots$$

$$\begin{pmatrix} a_j & b_j \\ c_j & d_j \end{pmatrix} = \begin{pmatrix} \cos K_j\Delta_j & \frac{1}{K_j}\sin K_j\Delta_j \\ -K_j\sin K_j\Delta_j & \cos K_j\Delta_j \end{pmatrix}$$

Conservation of momentum & Particle #

$\Rightarrow \partial\psi/\partial z$ & $\psi(z)$ must be continuous @ boundary $z=0$ & $z=L$

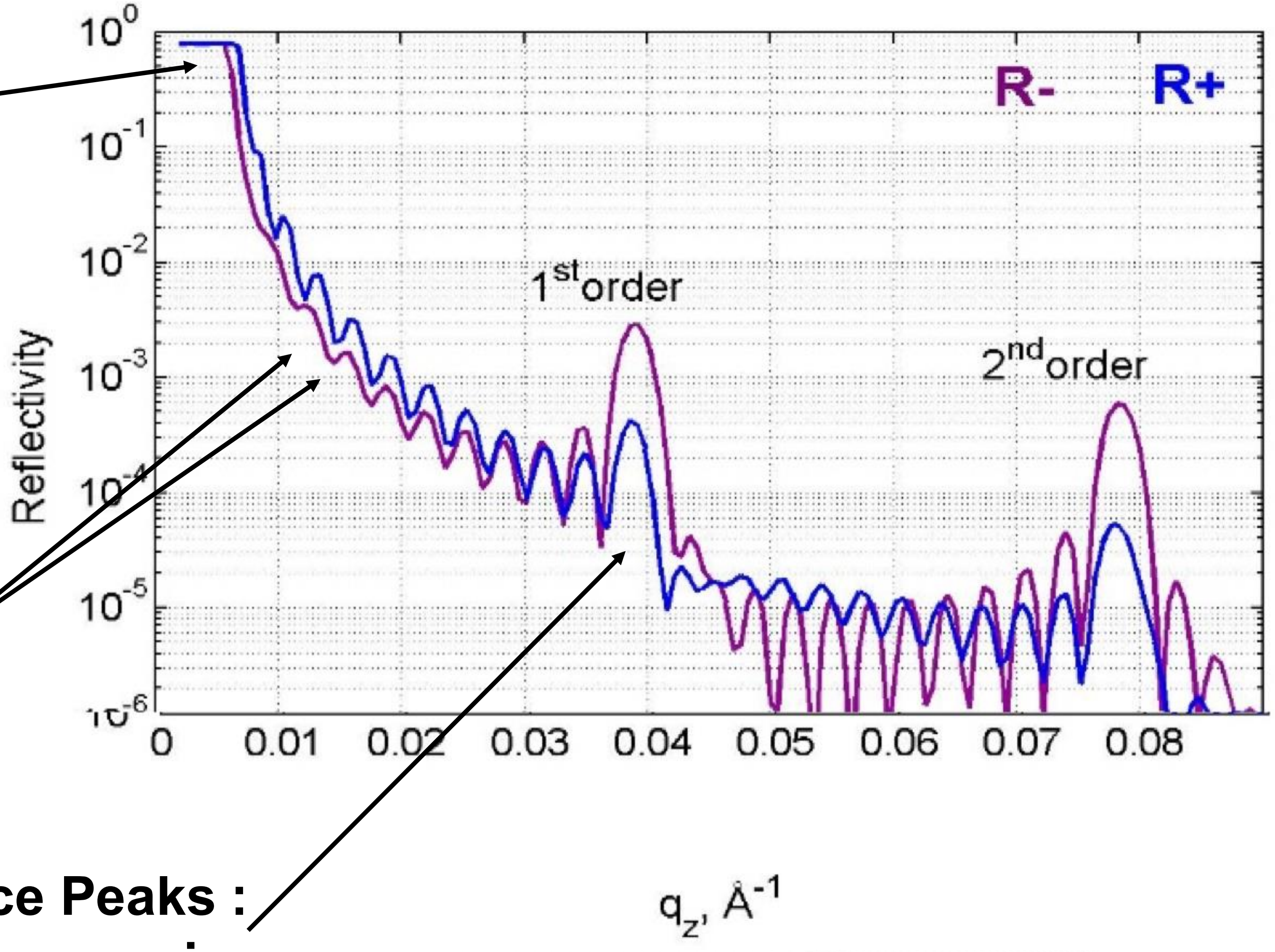
$$\begin{pmatrix} t \\ it \end{pmatrix} e^{iK_0L} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}\begin{pmatrix} 1+r \\ i(1-r) \end{pmatrix}$$

Born Approx. $\psi \rightarrow e^{iK_{0z}}$ (incident wave fn)

$r(Q) = \dfrac{4\pi}{iQ}\displaystyle\int \rho(z)e^{iQz}dz$ (Fourier Transform)

Note: this fails at Low Q → ψ must be "distorted" in the material

How to Read a Specular Reflectivity Curve



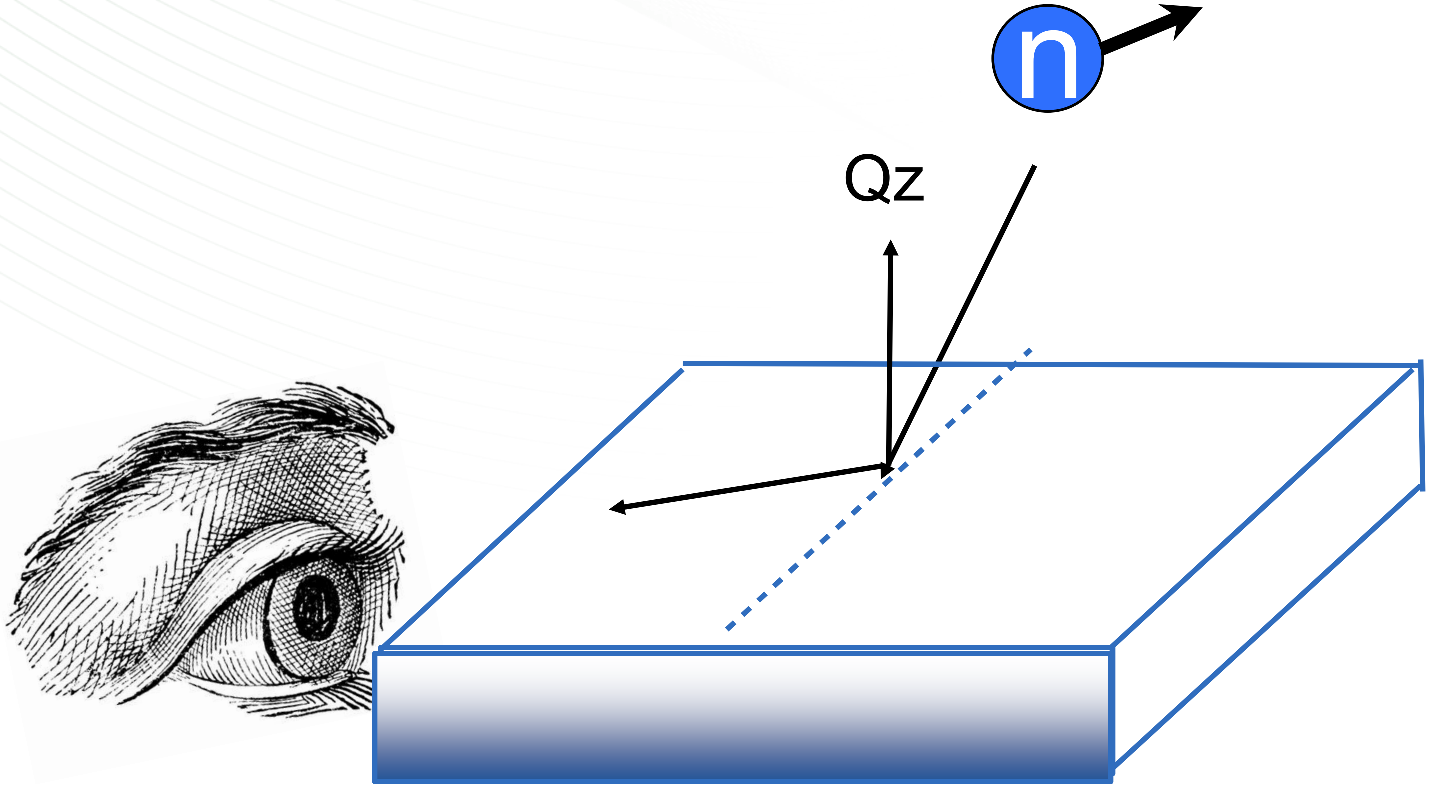
Total reflection region:
Ability to normalize
to a common scale.

Position of the turn over:
average chemical and
magnetic composition

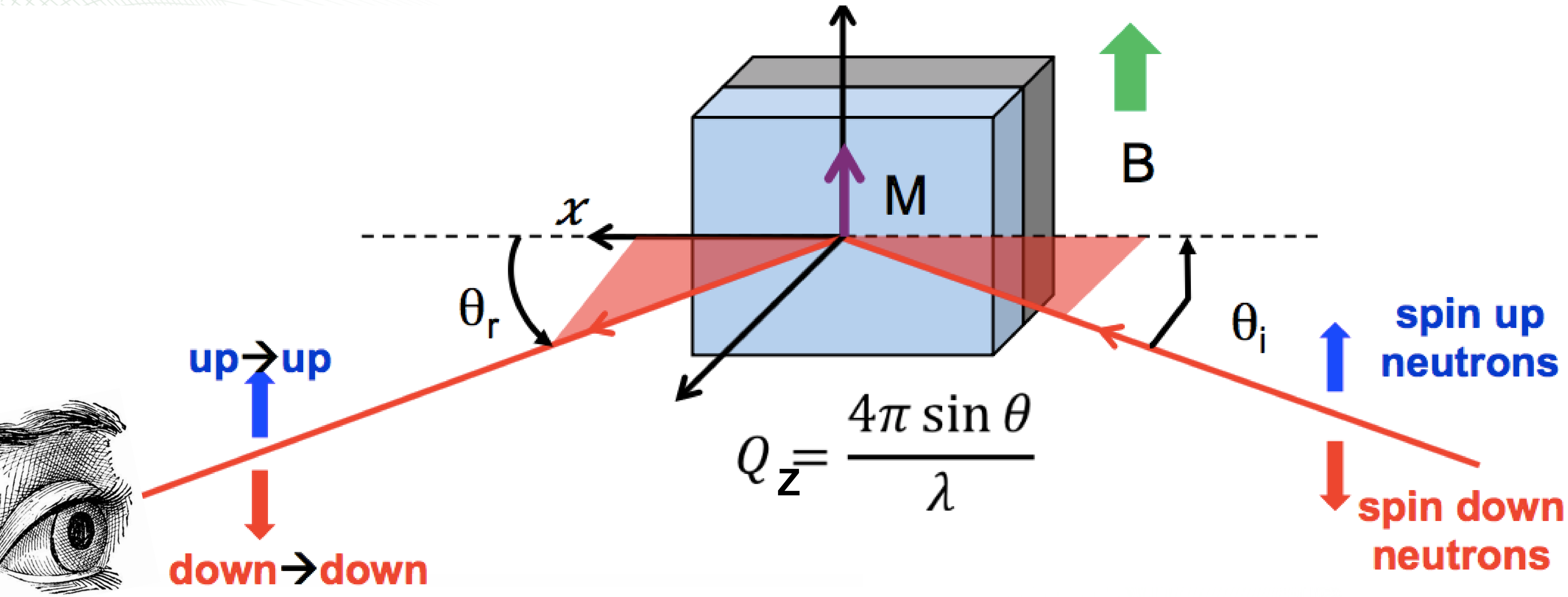
Spacing is related
to the total film thickness

Superlattice Peaks :
Superlattice spacing.
Ratio of peak intensities
can be related to roughness
in the layers.

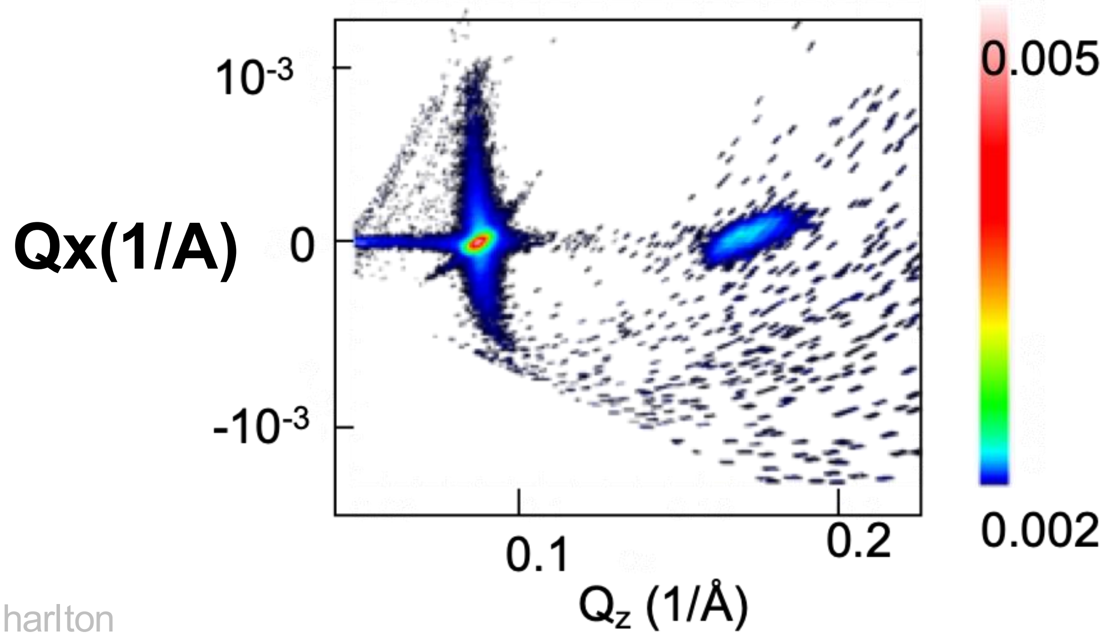
Experimental Geometry



Experimental Geometry



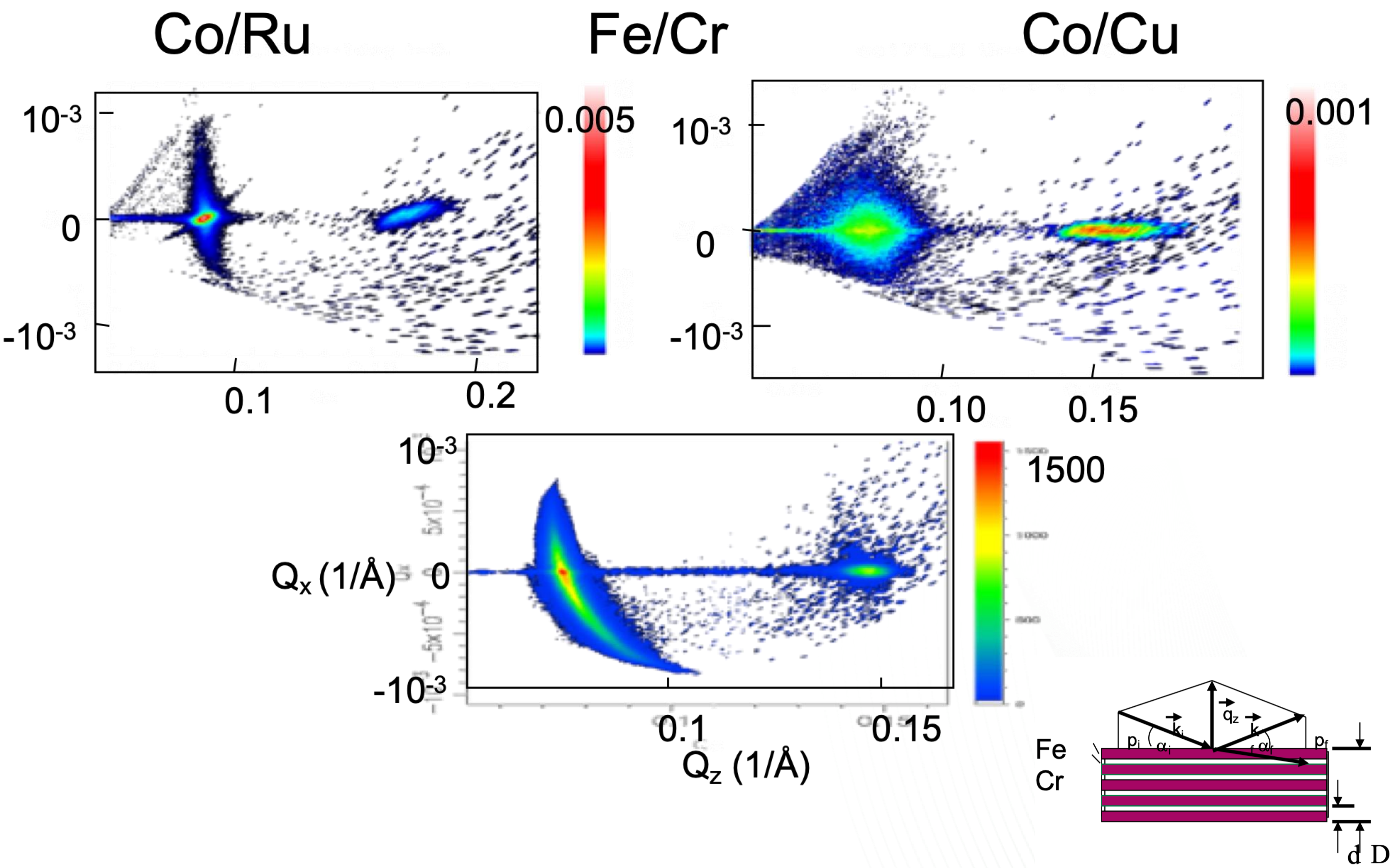
$$Q_z = \frac{4\pi \sin\theta}{\lambda}$$



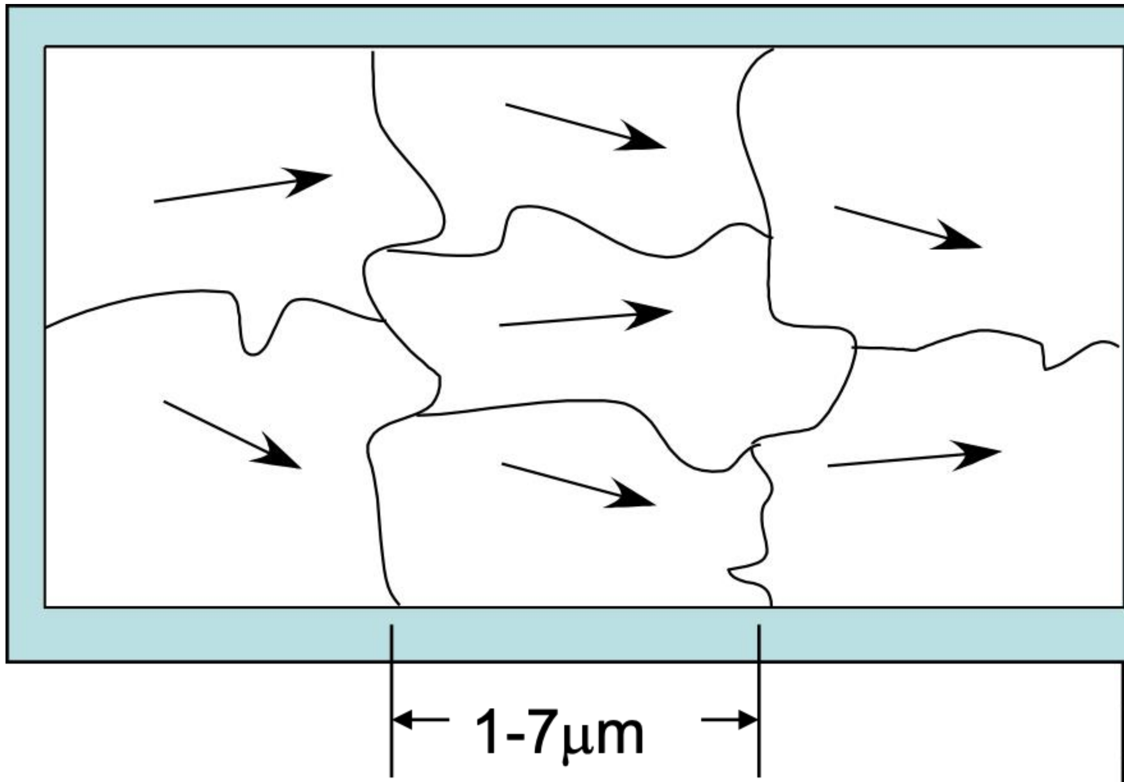
$$Qx = \frac{2\,\pi}{\lambda}(\cos\theta r - \cos\theta i)$$

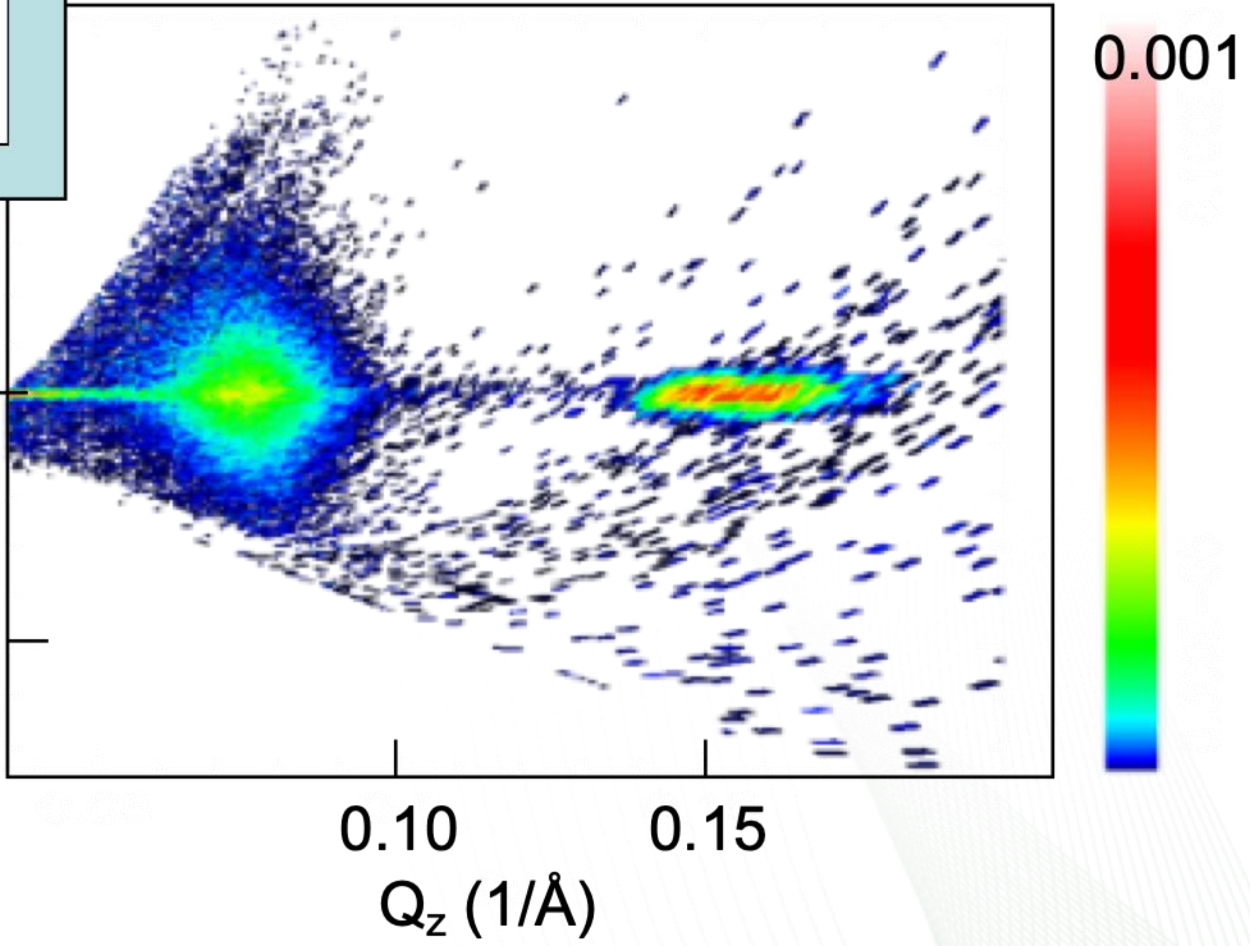
$$Qz = \frac{2\,\pi}{\lambda}(\sin\theta r + \sin\theta i)$$

How to read the tea leaves.



Co/Cu

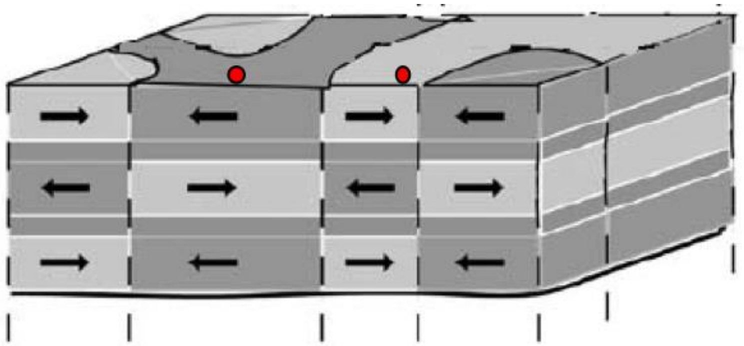




Little or no anisotropy

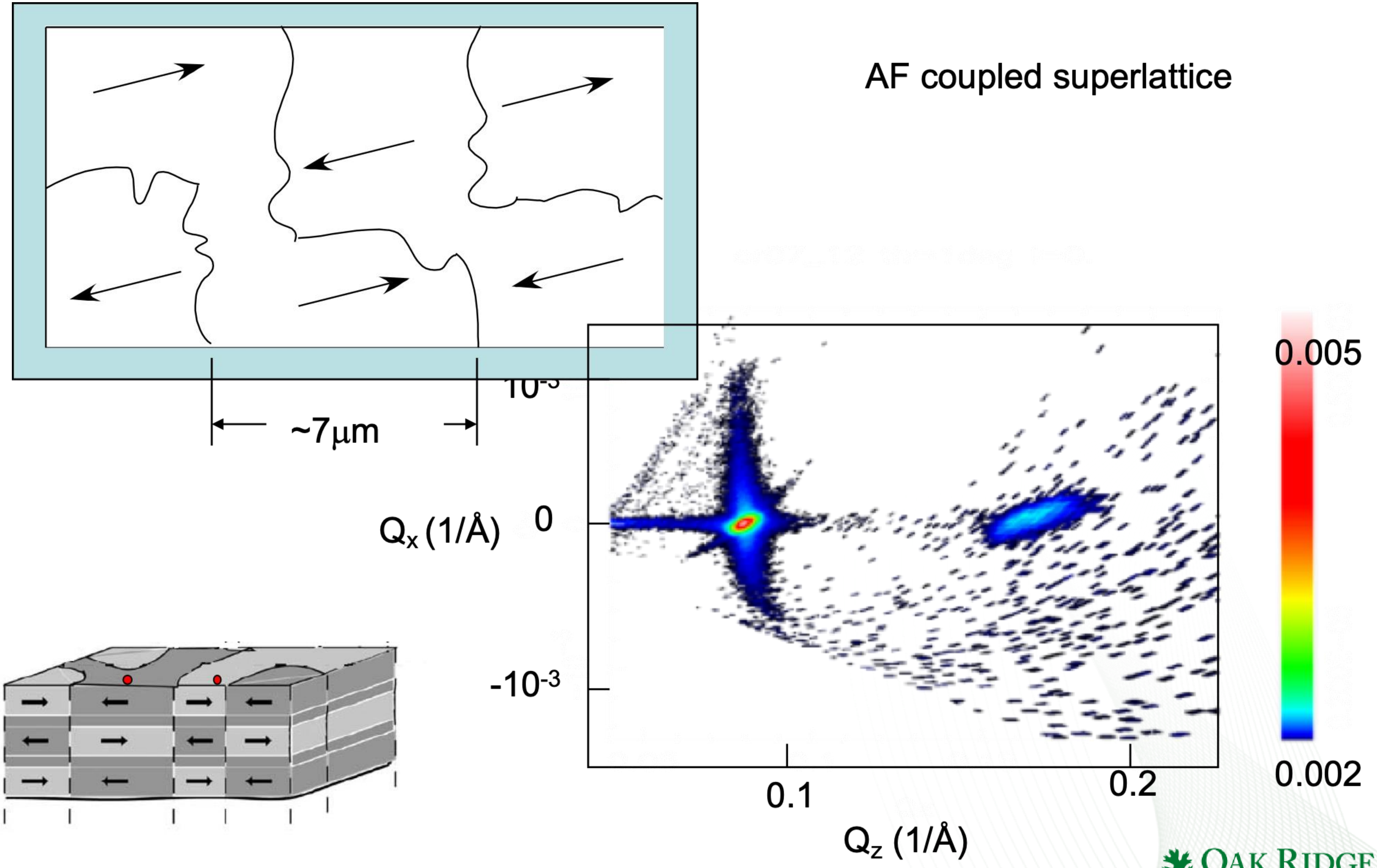
AF coupled superlattice

Angular spread : ± 30°

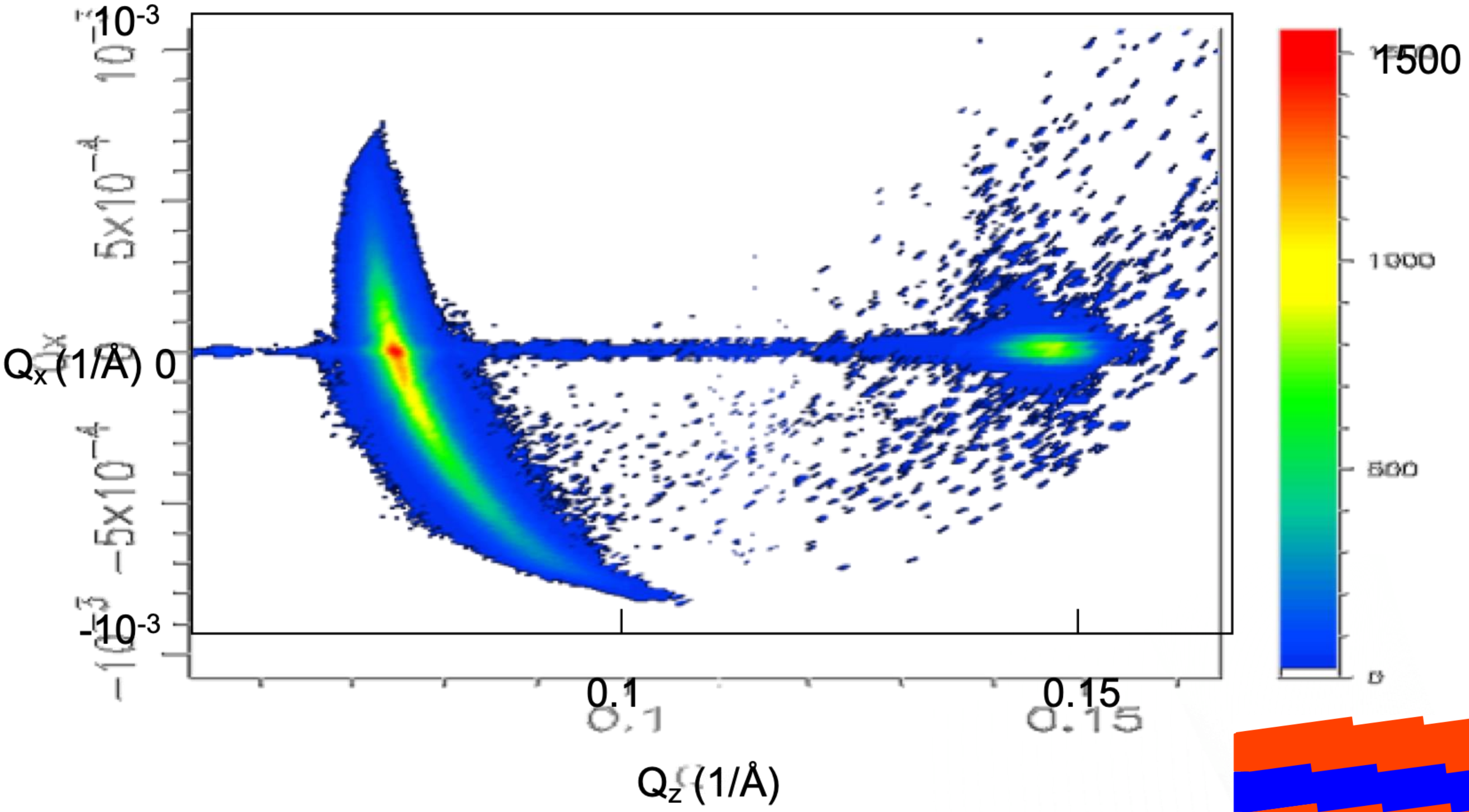


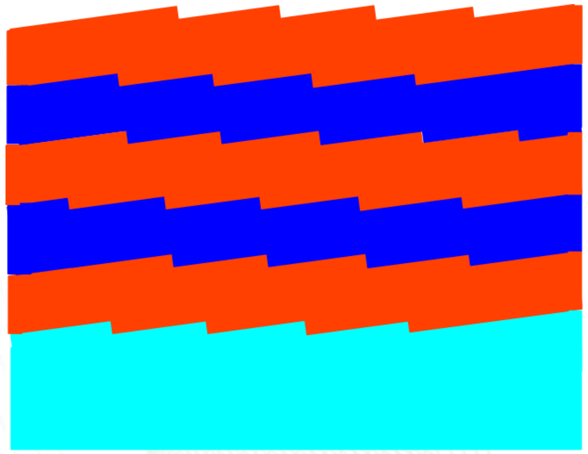
Co/Ru

AF coupled superlattice

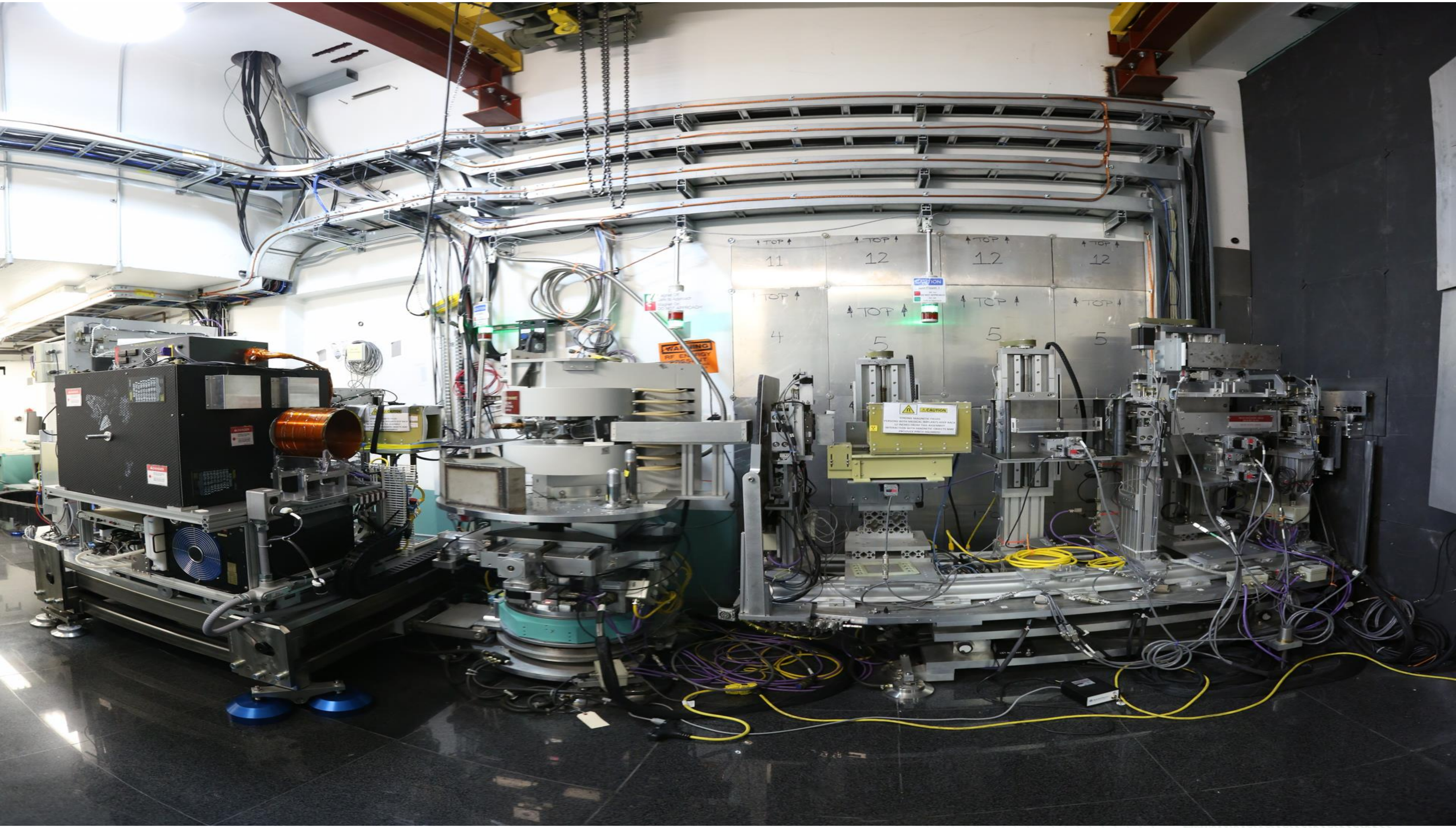


Fe/Cr on a jagged substrate

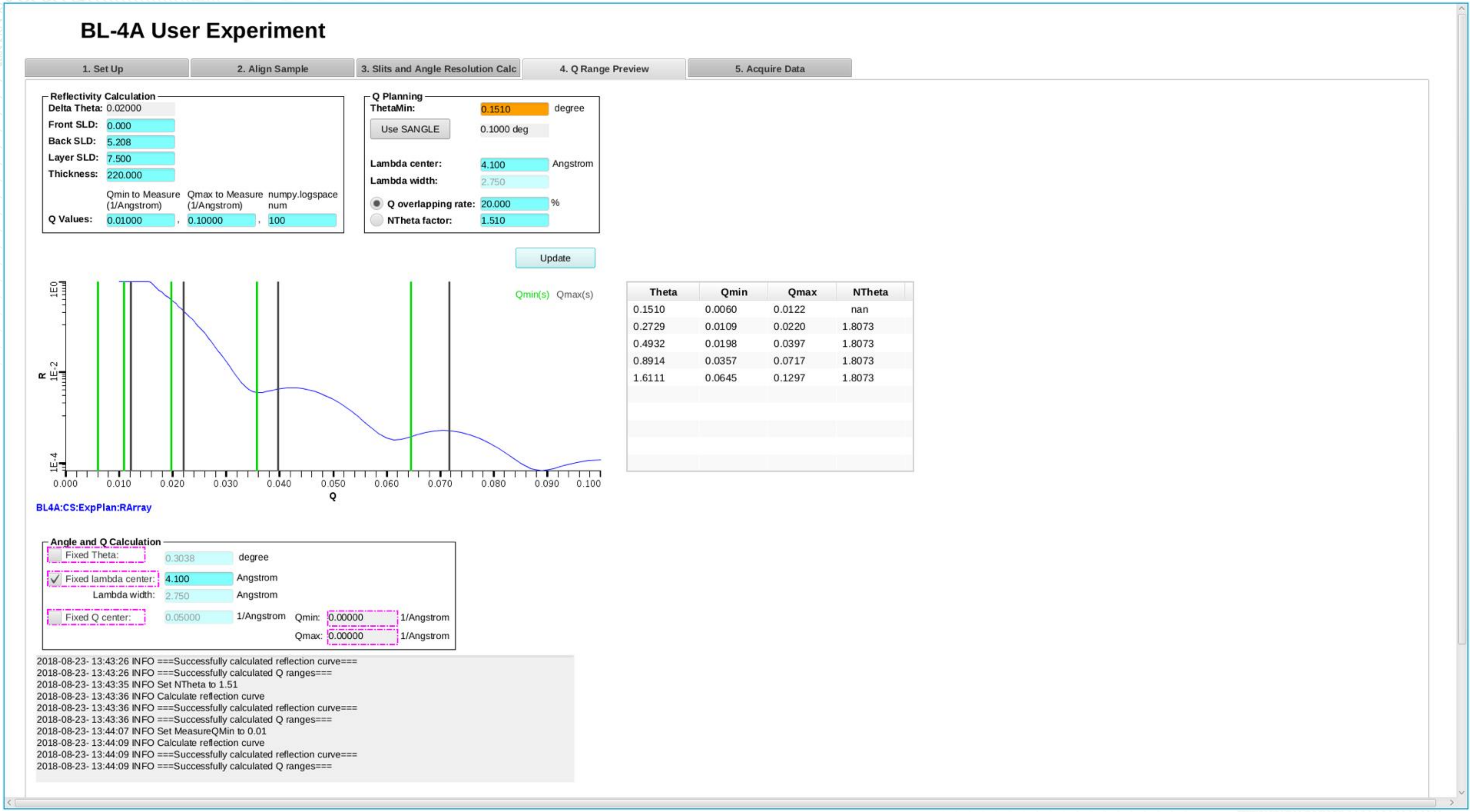




Instrument: BL4A RefM



Driving the instrument



BL-4A User Experiment

Reflectivity Calculation

Delta Theta: 0.02000
Front SLD: 0.000
Back SLD: 5.208
Layer SLD: 7.500
Thickness: 220.000

	Qmin to Measure (1/Angstrom)	Qmax to Measure (1/Angstrom)	numpy.logspace num
Q Values:	0.01000	0.10000	100

Q Planning

ThetaMin: 0.1510 degree
0.1000 deg
Lambda center: 4.100 Angstrom
Lambda width: 2.750
● Q overlapping rate: 20.000 %
○ NTheta factor: 1.510

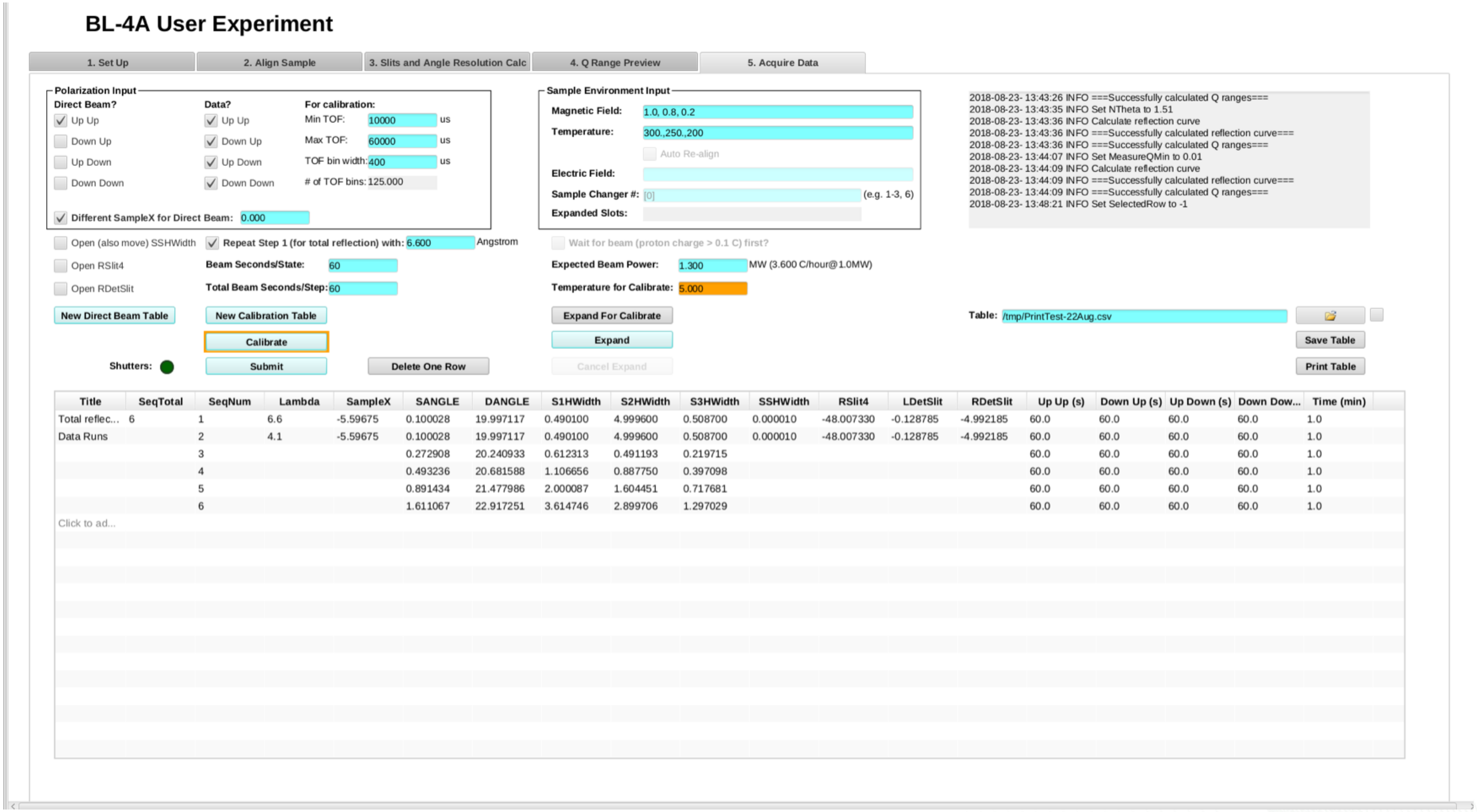
Theta	Qmin	Qmax	NTheta
0.1510	0.0060	0.0122	nan
0.2729	0.0109	0.0220	1.8073
0.4932	0.0198	0.0397	1.8073
0.8914	0.0357	0.0717	1.8073
1.6111	0.0645	0.1297	1.8073

Angle and Q Calculation

☐ Fixed Theta: 0.3038 degree
☑ Fixed lambda center: 4.100 Angstrom
Lambda width: 2.750 Angstrom
☐ Fixed Q center: 0.05000 1/Angstrom
Qmin: 0.00000 1/Angstrom
Qmax: 0.00000 1/Angstrom

```
2018-08-23- 13:43:26 INFO ===Successfully calculated reflection curve===
2018-08-23- 13:43:26 INFO ===Successfully calculated Q ranges===
2018-08-23- 13:43:35 INFO Set NTheta to 1.51
2018-08-23- 13:43:36 INFO Calculate reflection curve
2018-08-23- 13:43:36 INFO ===Successfully calculated reflection curve===
2018-08-23- 13:43:36 INFO ===Successfully calculated Q ranges===
2018-08-23- 13:44:07 INFO Set MeasureQMin to 0.01
2018-08-23- 13:44:09 INFO Calculate reflection curve
2018-08-23- 13:44:09 INFO ===Successfully calculated reflection curve===
2018-08-23- 13:44:09 INFO ===Successfully calculated Q ranges===
```

Driving the instrument



BL-4A User Experiment

Polarization Input

Direct Beam?
☑ Up Up
☐ Down Up
☐ Up Down
☐ Down Down

Data?
☑ Up Up
☑ Down Up
☑ Up Down
☑ Down Down

For calibration:
Min TOF: 10000 us
Max TOF: 60000 us
TOF bin width: 400 us
# of TOF bins: 125.000

☑ **Different SampleX for Direct Beam:** 0.000

☐ Open (also move) SSHWidth
☑ **Repeat Step 1 (for total reflection) with:** 6.600 Angstrom
☐ Open RSlit4
Beam Seconds/State: 60
☐ Open RDetSlit
Total Beam Seconds/Step: 60

Shutters: ●

Sample Environment Input

Magnetic Field: 1.0, 0.8, 0.2
Temperature: 300.,250.,200
☐ Auto Re-align
Electric Field:
Sample Changer #: [0] (e.g. 1-3, 6)
Expanded Slots:

☐ Wait for beam (proton charge > 0.1 C) first?
Expected Beam Power: 1.300 MW (3.600 C/hour@1.0MW)
Temperature for Calibrate: 5.000

```
2018-08-23- 13:43:26 INFO ===Successfully calculated Q ranges===
2018-08-23- 13:43:35 INFO Set NTheta to 1.51
2018-08-23- 13:43:36 INFO Calculate reflection curve
2018-08-23- 13:43:36 INFO ===Successfully calculated reflection curve===
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2018-08-23- 13:44:07 INFO Set MeasureQMin to 0.01
2018-08-23- 13:44:09 INFO Calculate reflection curve
2018-08-23- 13:44:09 INFO ===Successfully calculated reflection curve===
2018-08-23- 13:44:09 INFO ===Successfully calculated Q ranges===
2018-08-23- 13:48:21 INFO Set SelectedRow to -1
```

Table: /tmp/PrintTest-22Aug.csv

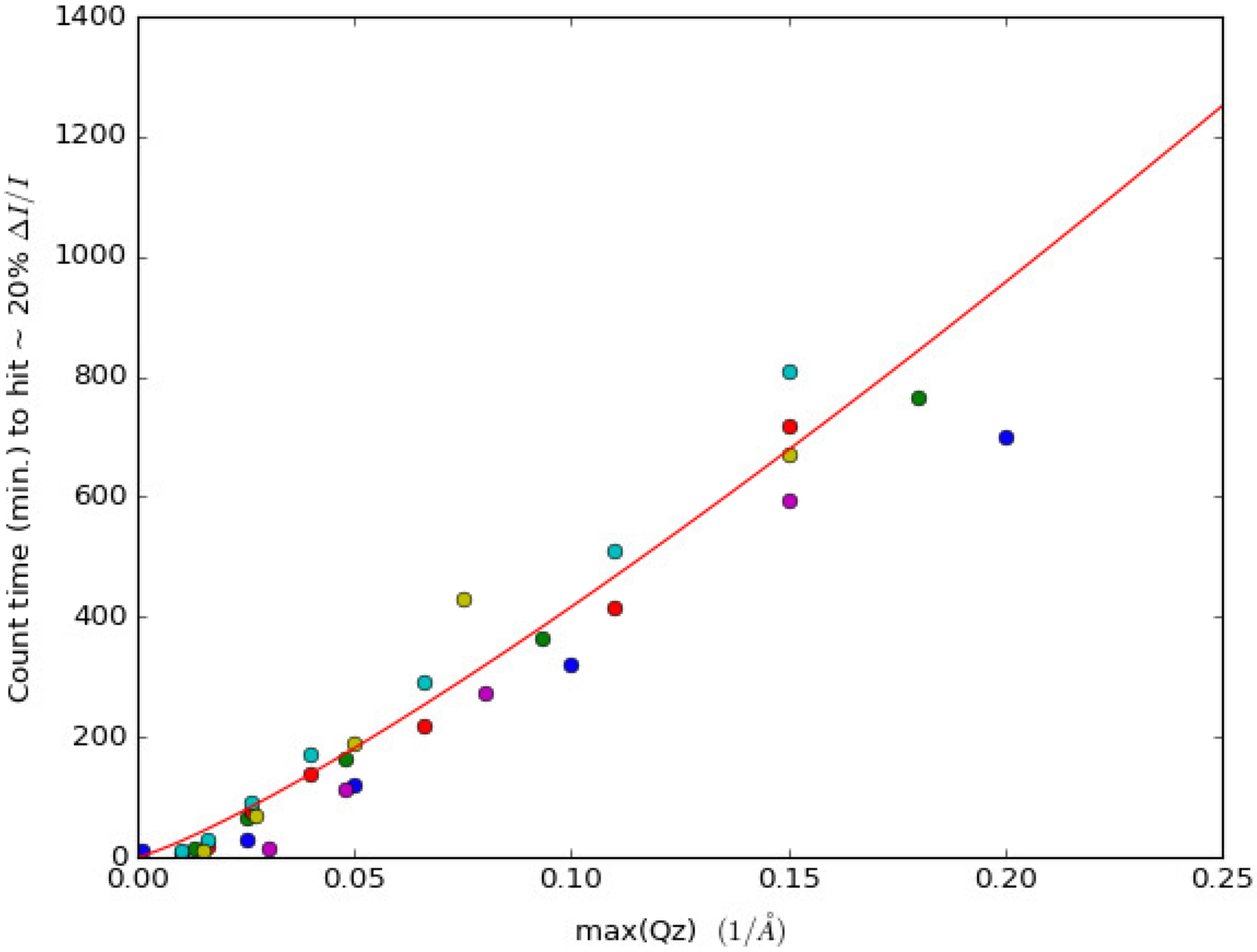
Title	SeqTotal	SeqNum	Lambda	SampleX	SANGLE	DANGLE	S1HWidth	S2HWidth	S3HWidth	SSHWidth	RSlit4	LDetSlit	RDetSlit	Up Up (s)	Down Up (s)	Up Down (s)	Down Dow...	Time (min)
Total reflec...	6	1	6.6	-5.59675	0.100028	19.997117	0.490100	4.999600	0.508700	0.000010	-48.007330	-0.128785	-4.992185	60.0	60.0	60.0	60.0	1.0
Data Runs		2	4.1	-5.59675	0.100028	19.997117	0.490100	4.999600	0.508700	0.000010	-48.007330	-0.128785	-4.992185	60.0	60.0	60.0	60.0	1.0
		3			0.272908	20.240933	0.612313	0.491193	0.219715					60.0	60.0	60.0	60.0	1.0
		4			0.493236	20.681588	1.106656	0.887750	0.397098					60.0	60.0	60.0	60.0	1.0
		5			0.891434	21.477986	2.000087	1.604451	0.717681					60.0	60.0	60.0	60.0	1.0
		6			1.611067	22.917251	3.614746	2.899706	1.297029					60.0	60.0	60.0	60.0	1.0
Click to ad...																		

Experiment length estimate

- Polarized Beam
- No Polarization Analysis
- Sample size: 1cm x 1cm
- Errorbar at Q max: ΔI/I ~ 20%
- No rebinning
- Normalized Slit Settings

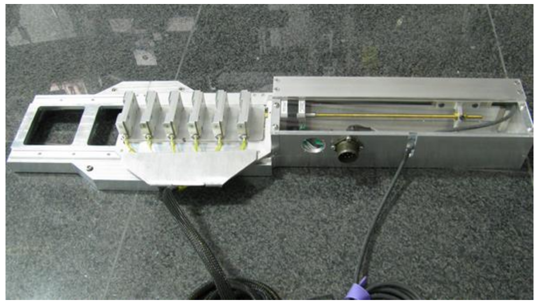
$$t = 6000\, Q_{z\_max}^{1.2}$$

where *t* is time in min. and *Qz_max* is in 1/Å

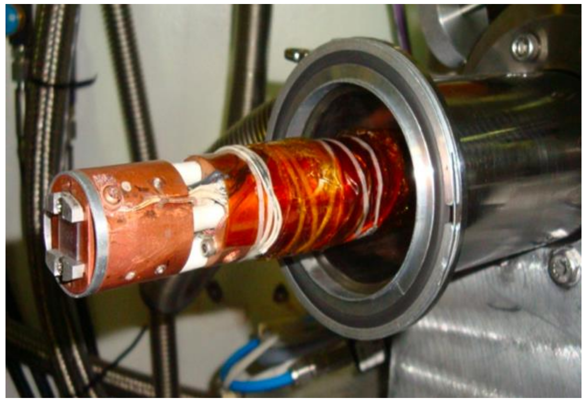


Sample environment & polarization handling

Sample Environments



Room temperature sample changer

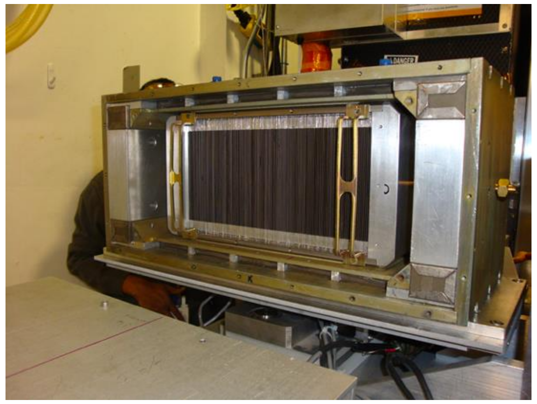


Displex: 5K to 750K, E-field +/- 200V, 360 axial rotation

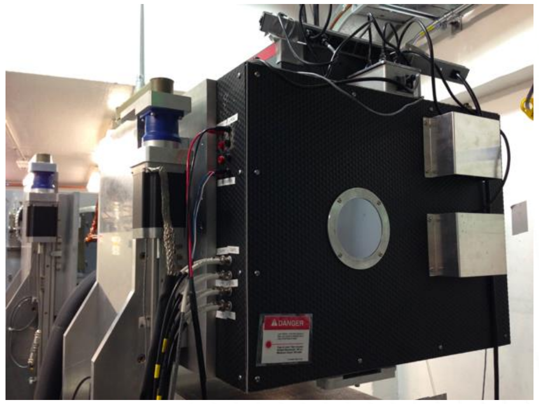
Electromagnet: 50mm gap, Hmax=1.15T

Polarization Capability

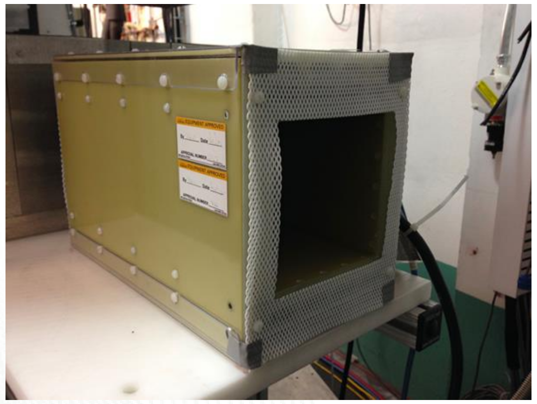
Incident polarizer: reflection or transmission V-Cavity



Fan analyzer



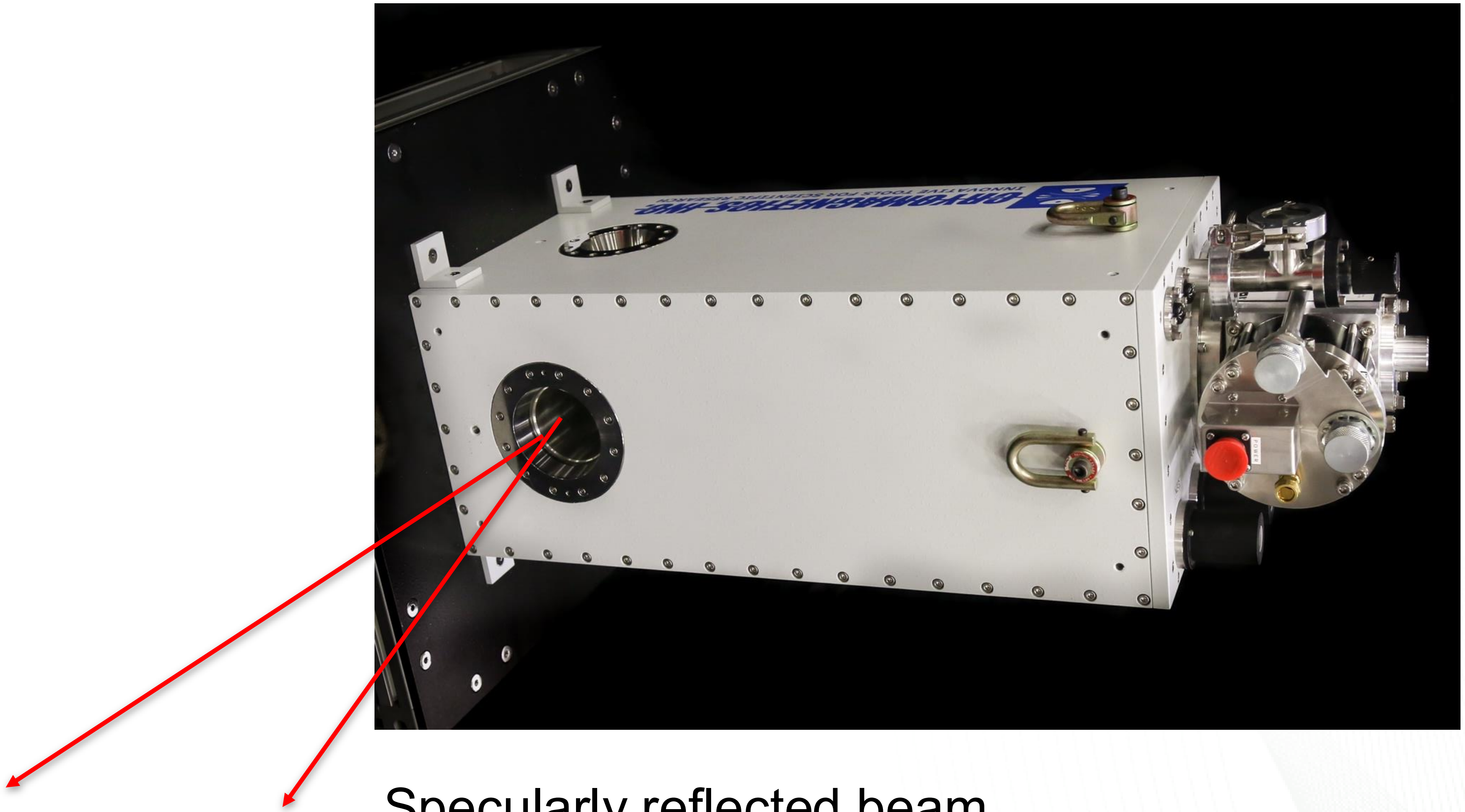
In situ 3He Analyzer



RF Flipper

MAG-H is part of the solution! (We have this part already.)

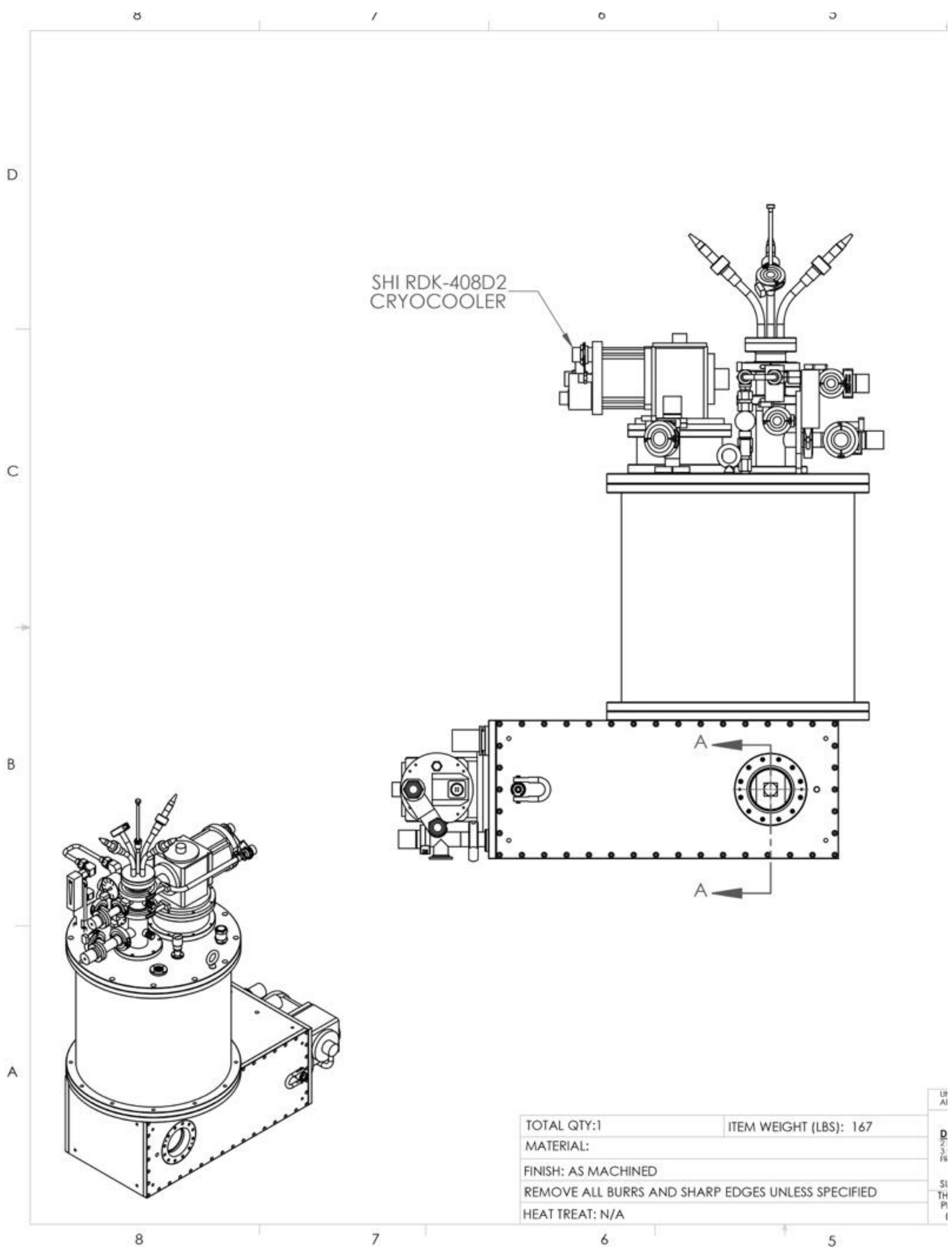
Two open (hollow) bores. Magnet does not produce scattering.



Specularly reflected beam

Transmitted beam

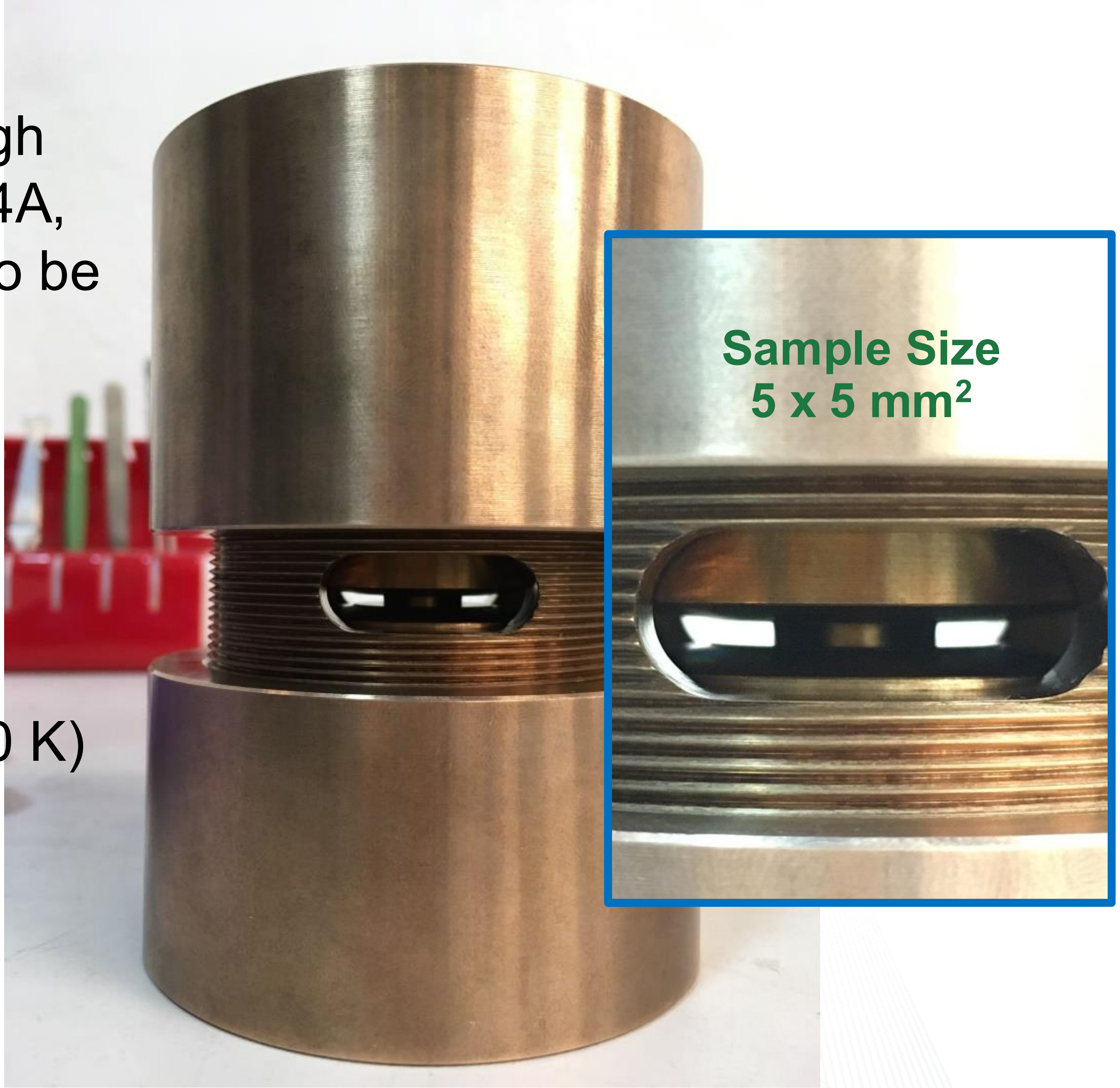
Top Loading Cryostat



Ultra large volume pressure cell

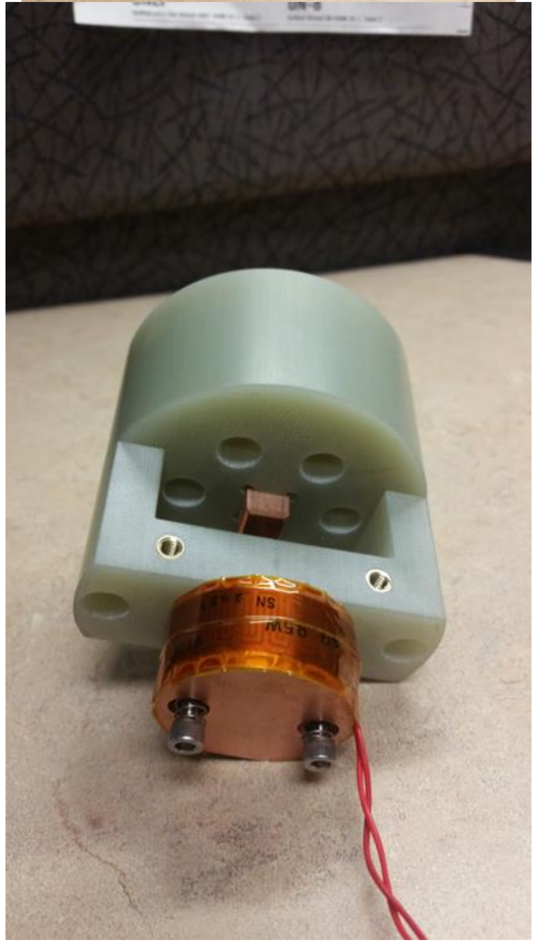
To achieve the goal of performing high pressure reflectometry on beamline 4A, certain engineering constraints had to be considered.

- Capability of reaching ≥ 2 GPa
- Low neutron absorption
- Low thermal contraction
- Good thermal conduction
- Accessible temperatures (20-400 K)
- Polarized neutron compatible

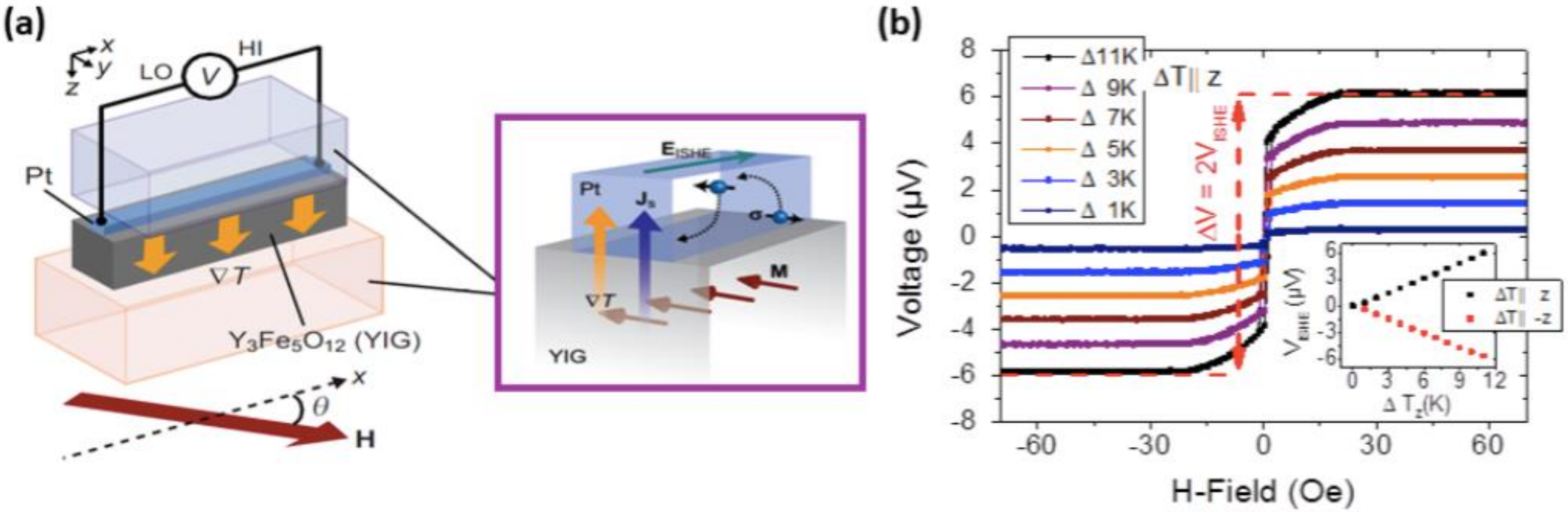


Copper Beryllium

Thermal Gradient Cell

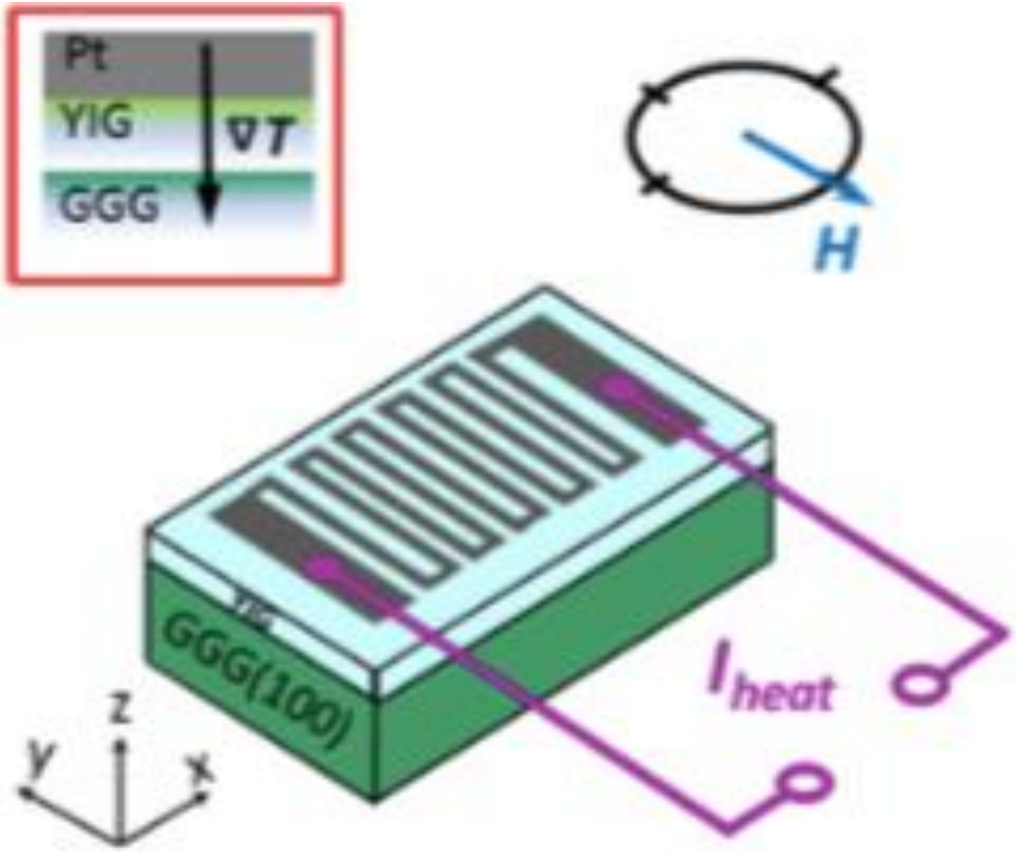


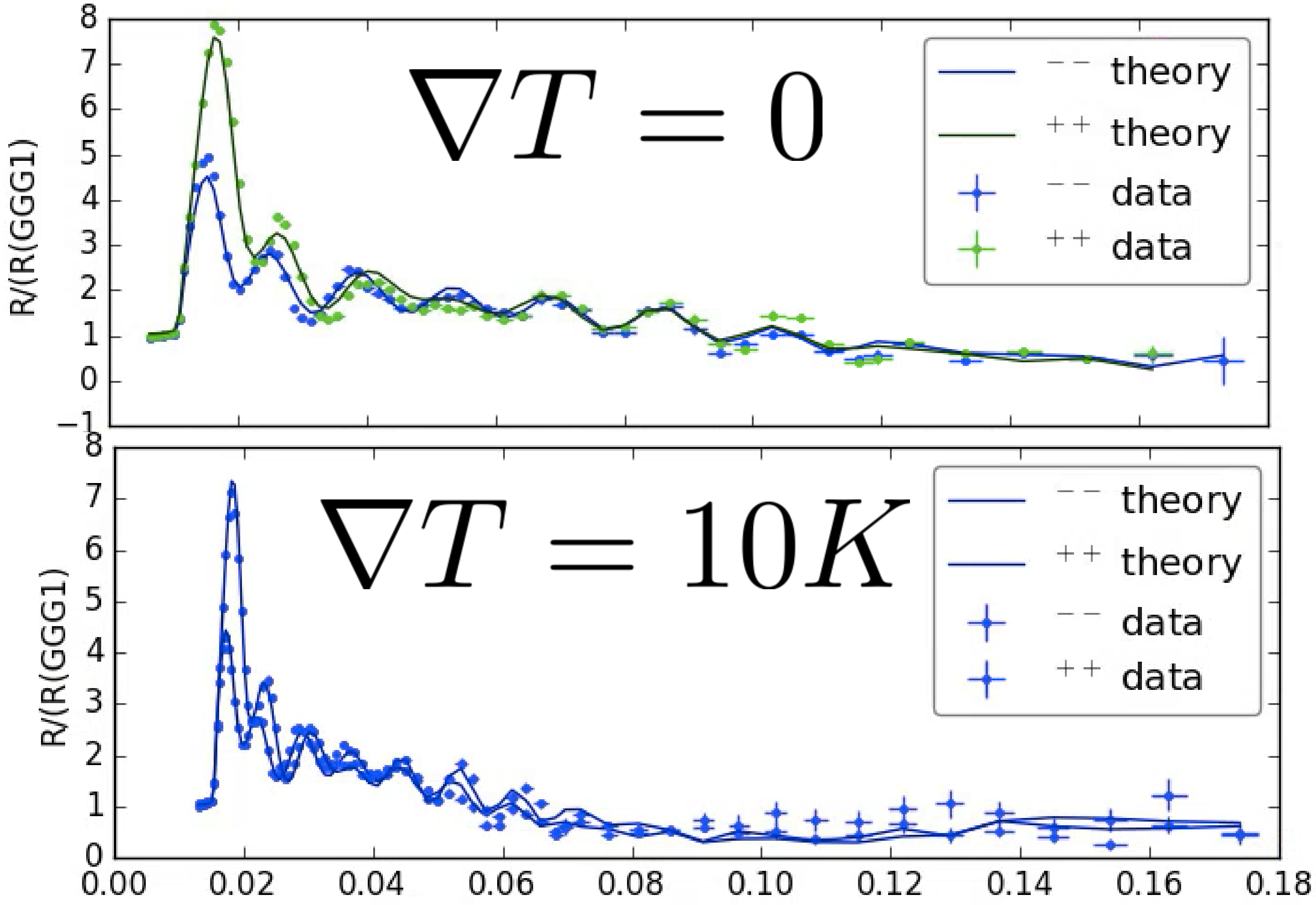
E. J. Guo,[1] A. Herklotz,[2] Y. H. Liu,[1] H. N. Lee,[2] and M. R. Fitzsimmons[1]

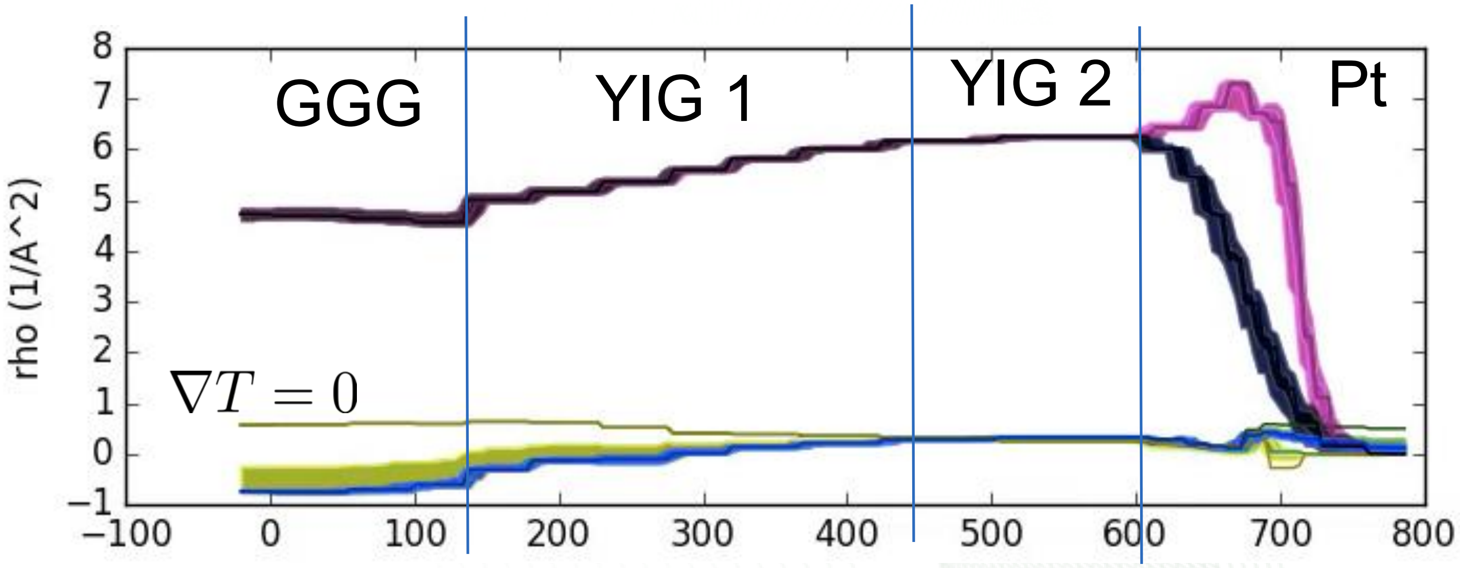


Prep work before the PNR experiment

Spin Seebeck Effect







Fitting Options

Refl1d. (NIST, DANSE. project). reflectometry.org

SimulReflec: http://www-llb.cea.fr/prism/programs/programs.html

Parratt: http://www.hmi.de/bensc/instrumentation/instrumente/v6/refl/parratt_en.htm

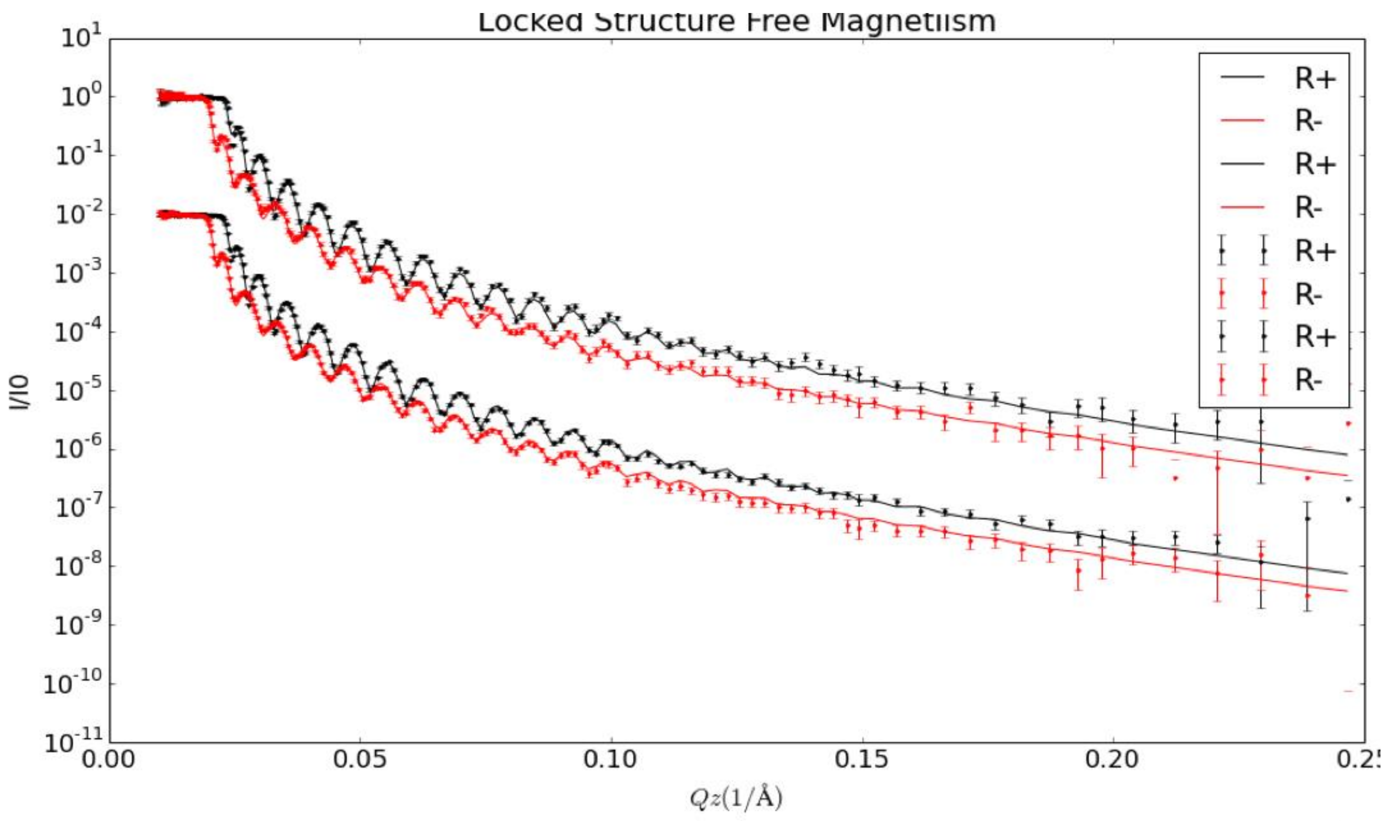
IMD: http://www.rxollc.com/idl/

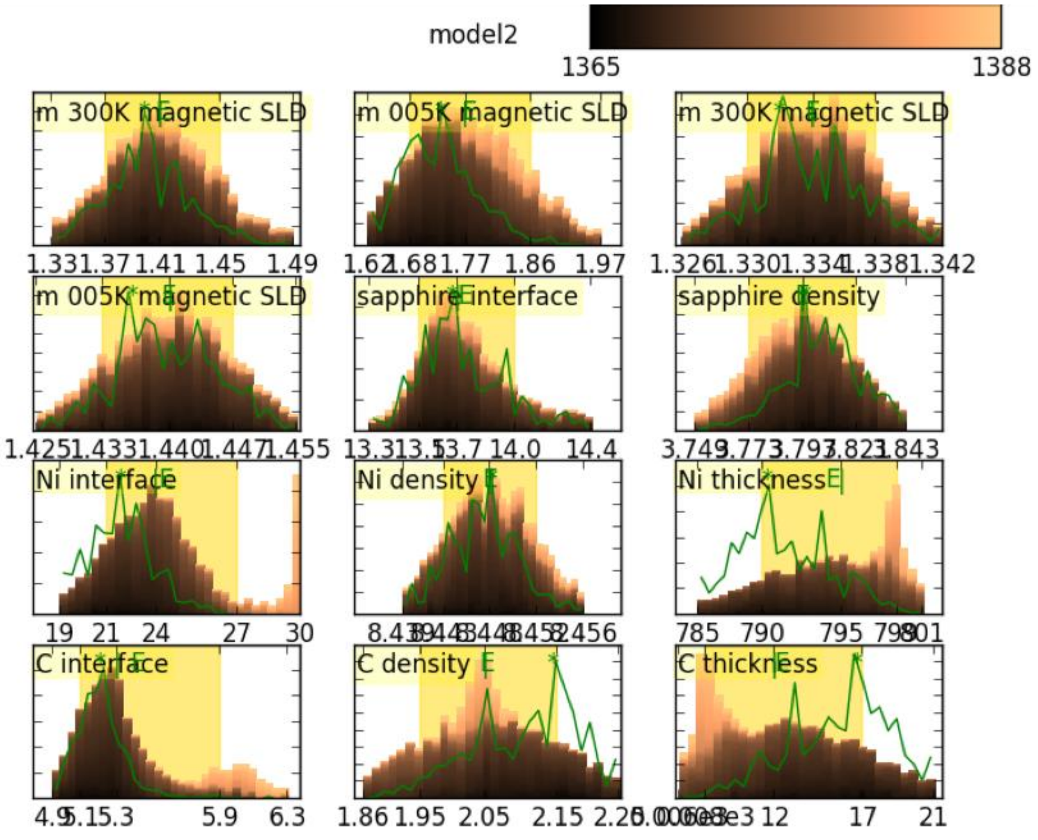
BornAgain: http://bornagainproject.org

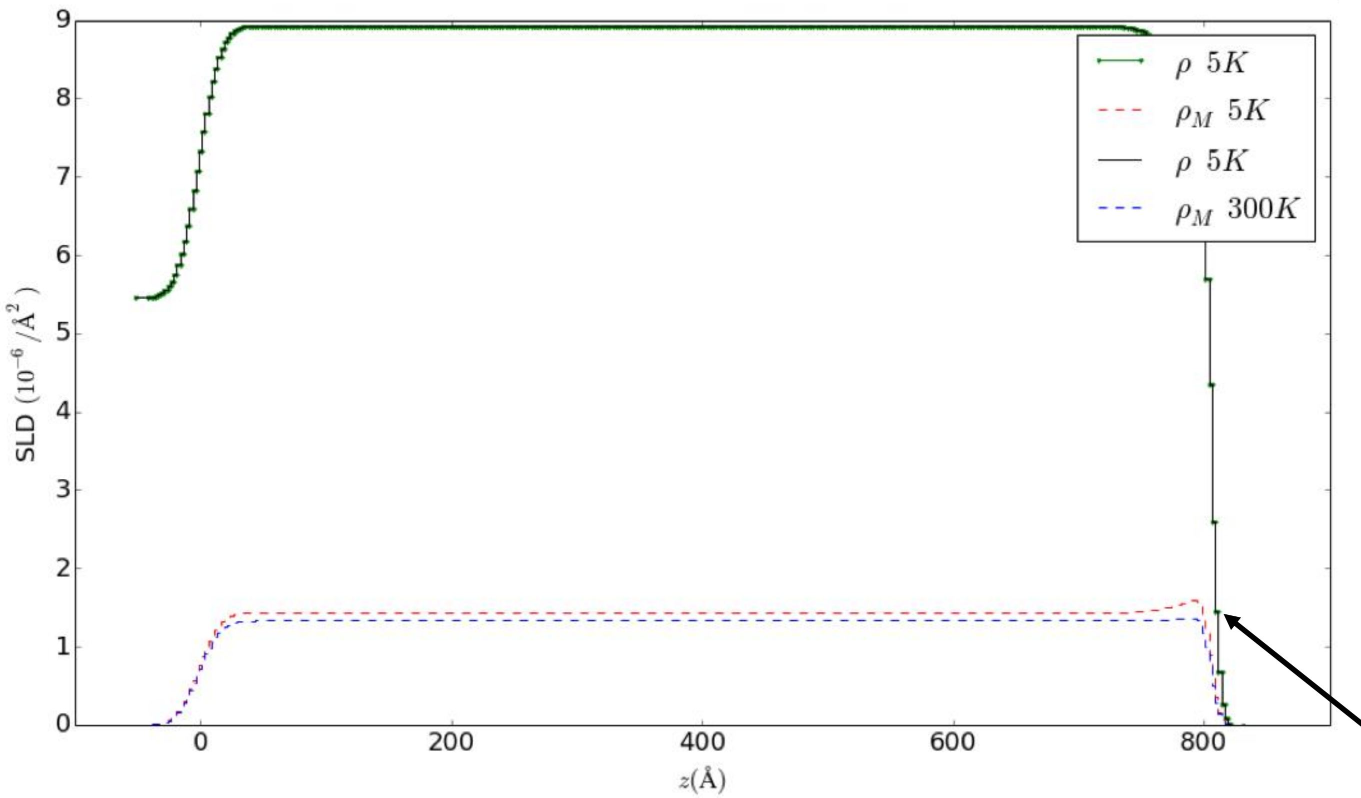
MotoFit: http://motofit.sourceforge.net/wiki/index.php/Main_Page

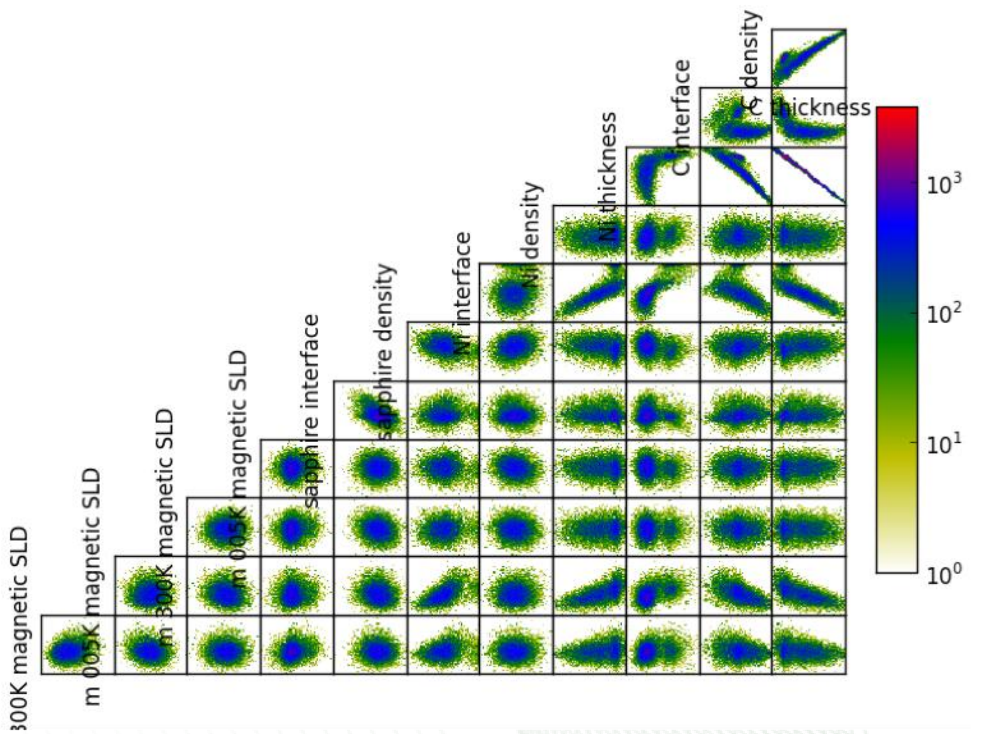
GenX: http://genx.sourceforge.net/

Simple fitting example Al2O3/Ni/Gr/Air







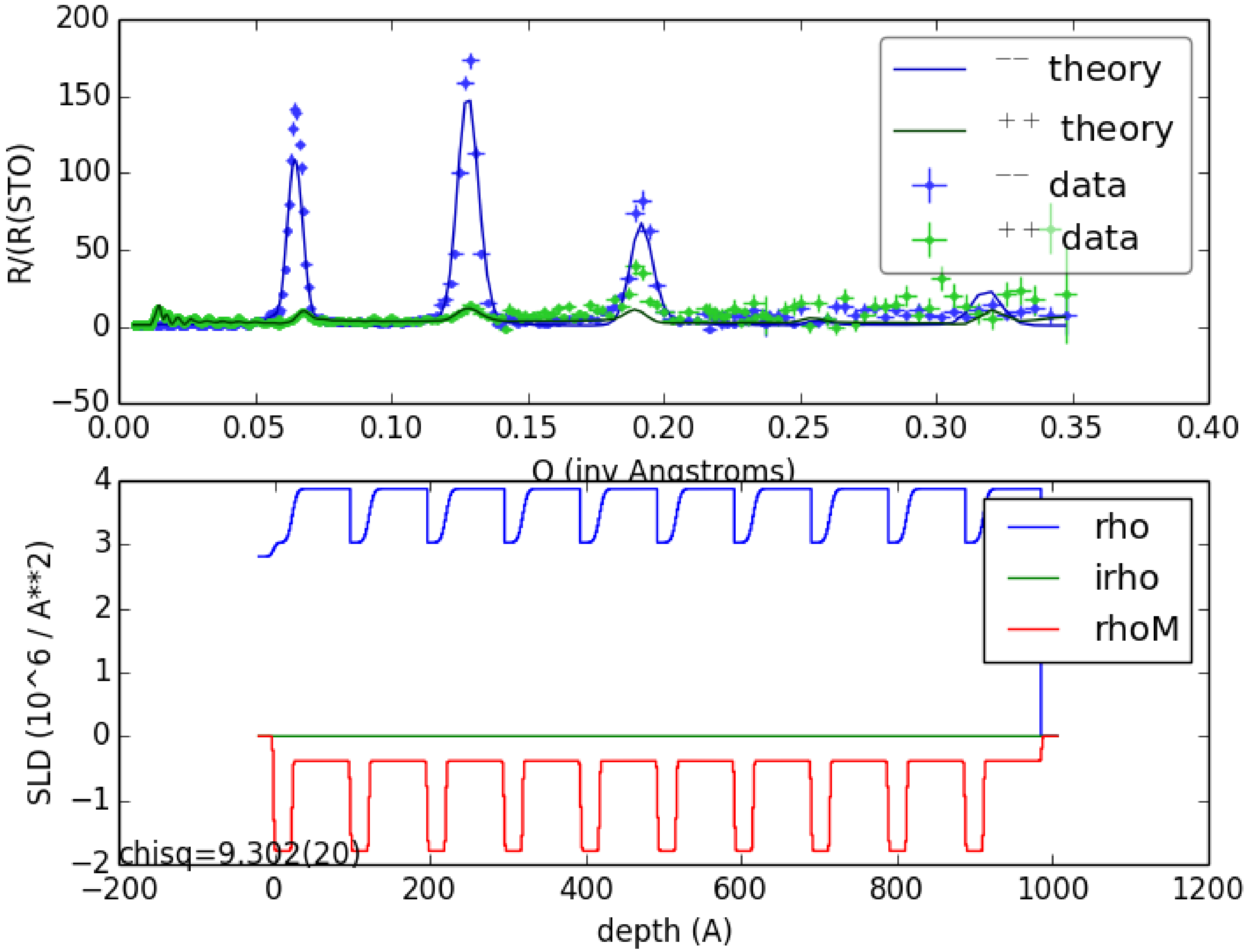


Refl1D (reflectometry.org)

70 emu/cc

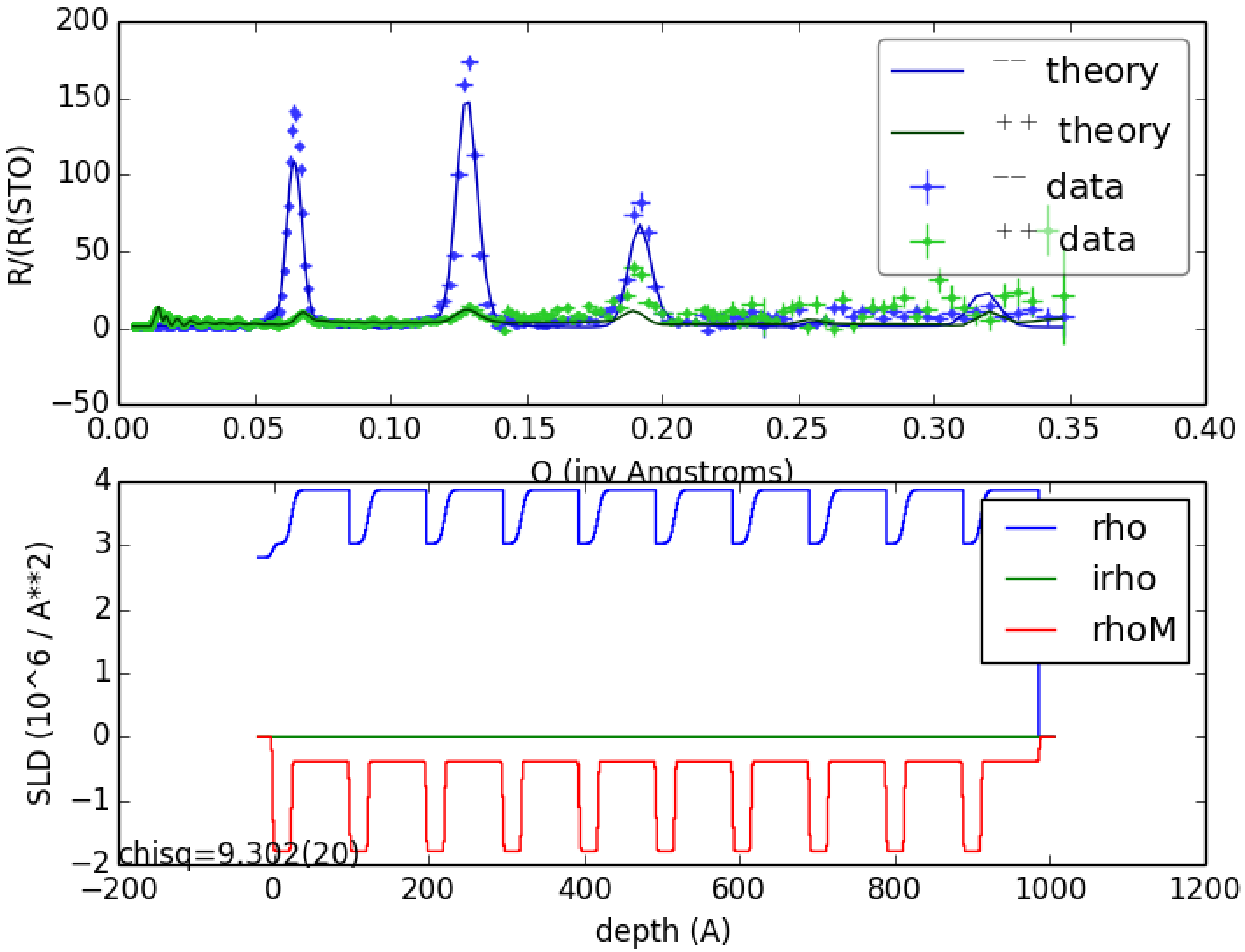
Fitting process: Defining the layered structure

```
# Materials
BFO  = SLD(name='BFO' , rho=4.400, irho=0.0)
LSMO = SLD(name='LSMO', rho=3.400, irho=0.0)
STO  = SLD(name='STO' , rho=3.54, irho=0.0)

bilayer =(LSMO(16.0,1,magnetism=Magnetism(rhoM=0.1,
                     thetaM=90, interface_above=1,
                                   interface_below=1)) |
        BFO(83.0,1,magnetism=Magnetism(rhoM=0.6,
                     thetaM=90,interface_above=1,
                                 interface_below=1)) )
sample = (STO(0,5)
                 |bilayer
                 |bilayer
                 |bilayer
                 |bilayer
                 |bilayer
                 |bilayer
                 |bilayer
                 |bilayer
                 |bilayer
                 |bilayer
                 |  air)
```

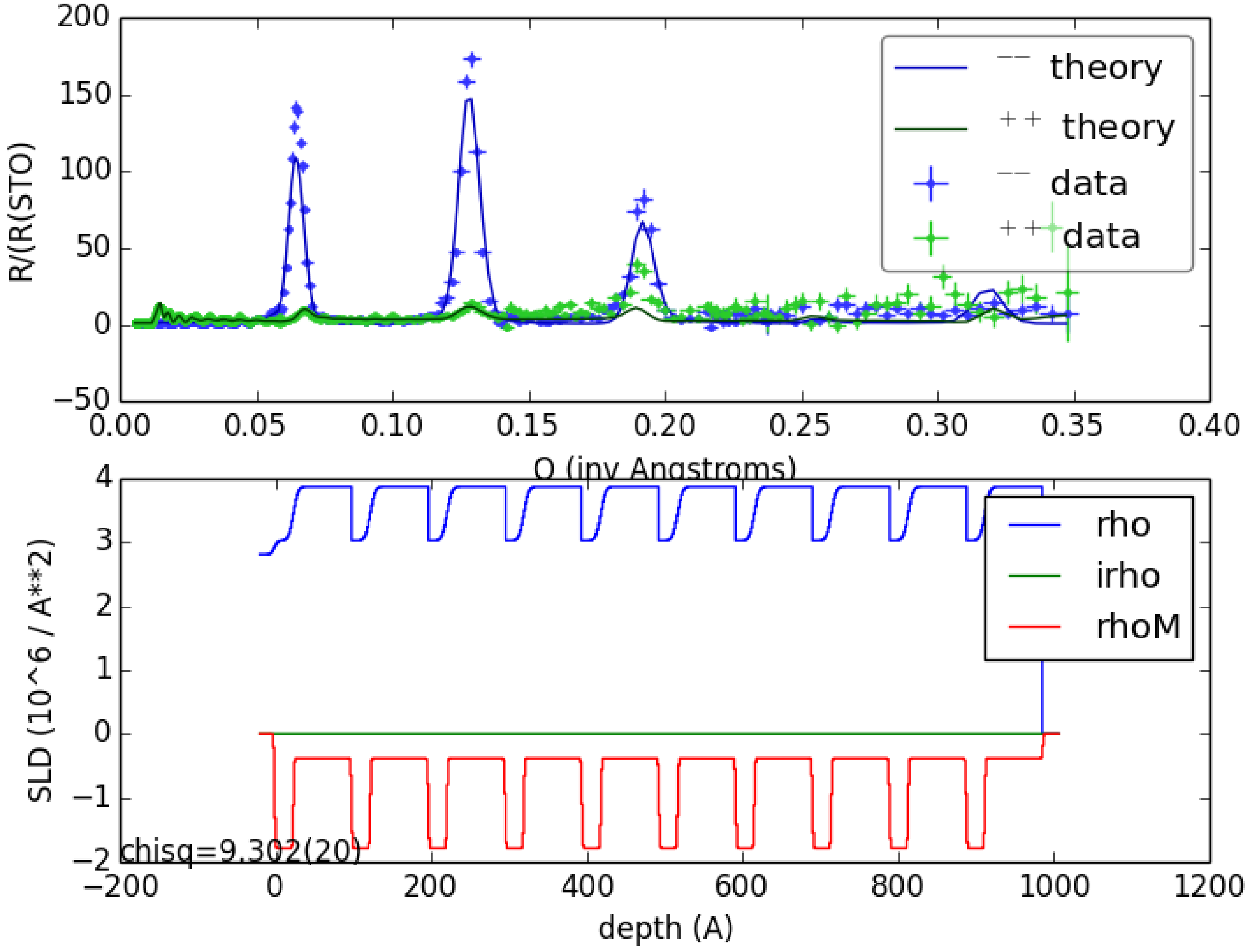


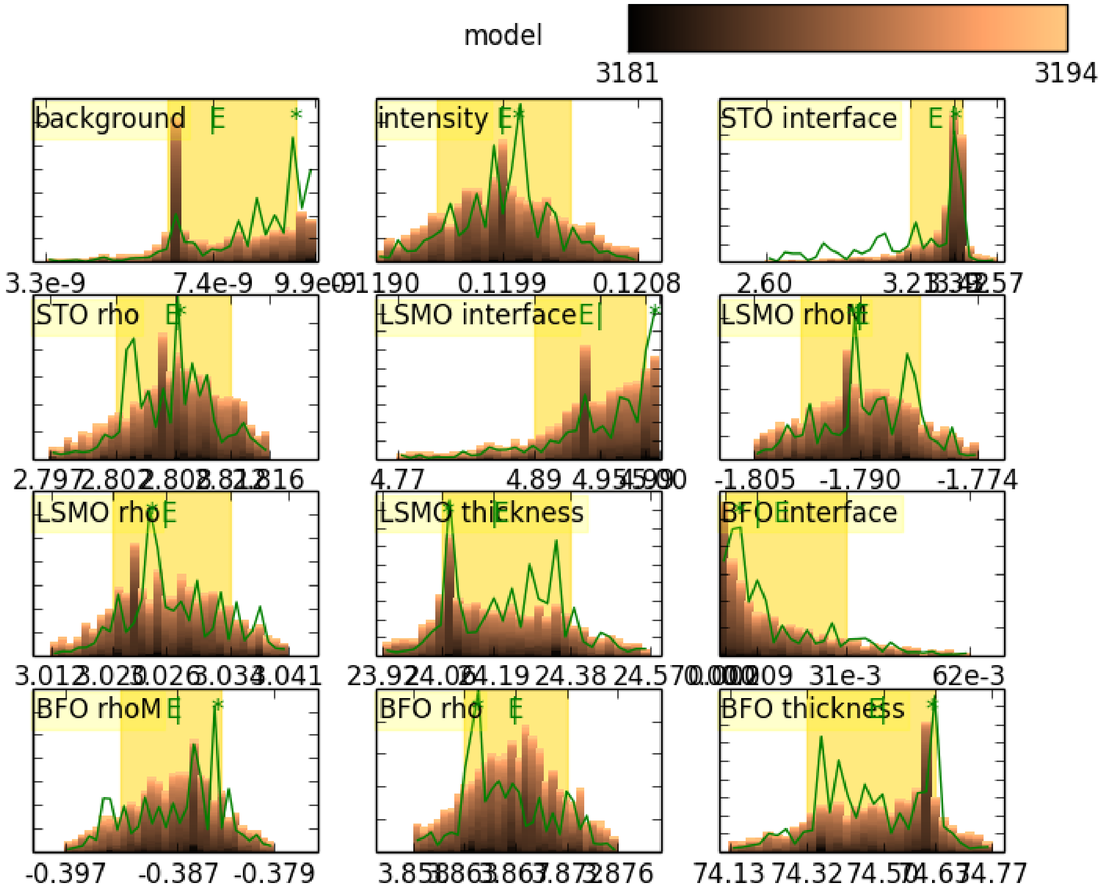
Fitting process: Adding fitting parameters

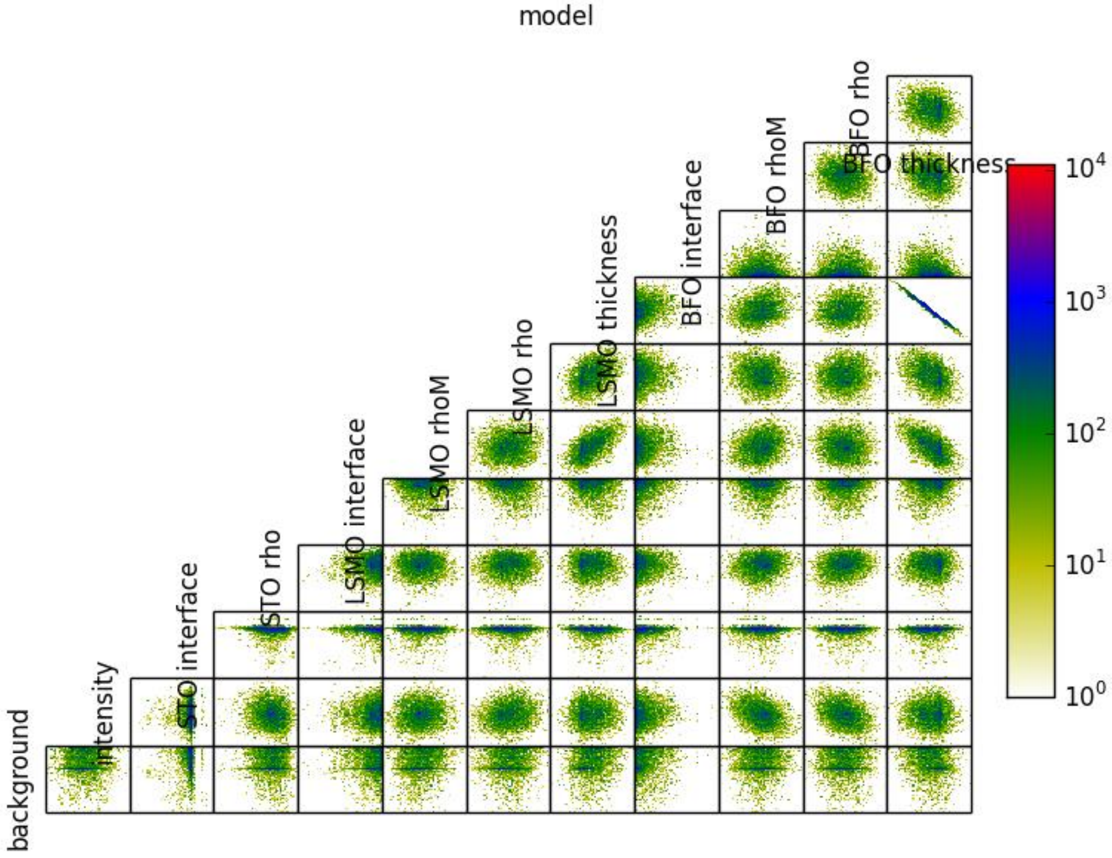
```
# Fitting parameters
sample['LSMO'].thickness.range(0,100)  #
sample['BFO'].thickness.range(0,200)  #

sample['STO'].interface.range(0,30)#
sample['LSMO'].interface.range(0,5)
sample['BFO'].interface.range(0,5)#

sample['STO'].material.rho.range(0,9)#
sample['LSMO'].material.rho.range(0,9)#
sample['BFO'].material.rho.range(0,10)#

sample['LSMO'].magnetism.rhoM.range(-10.1,10.6) #
sample['BFO'].magnetism.rhoM.range(-10.1,10.5) #
```



Fitting process: The results



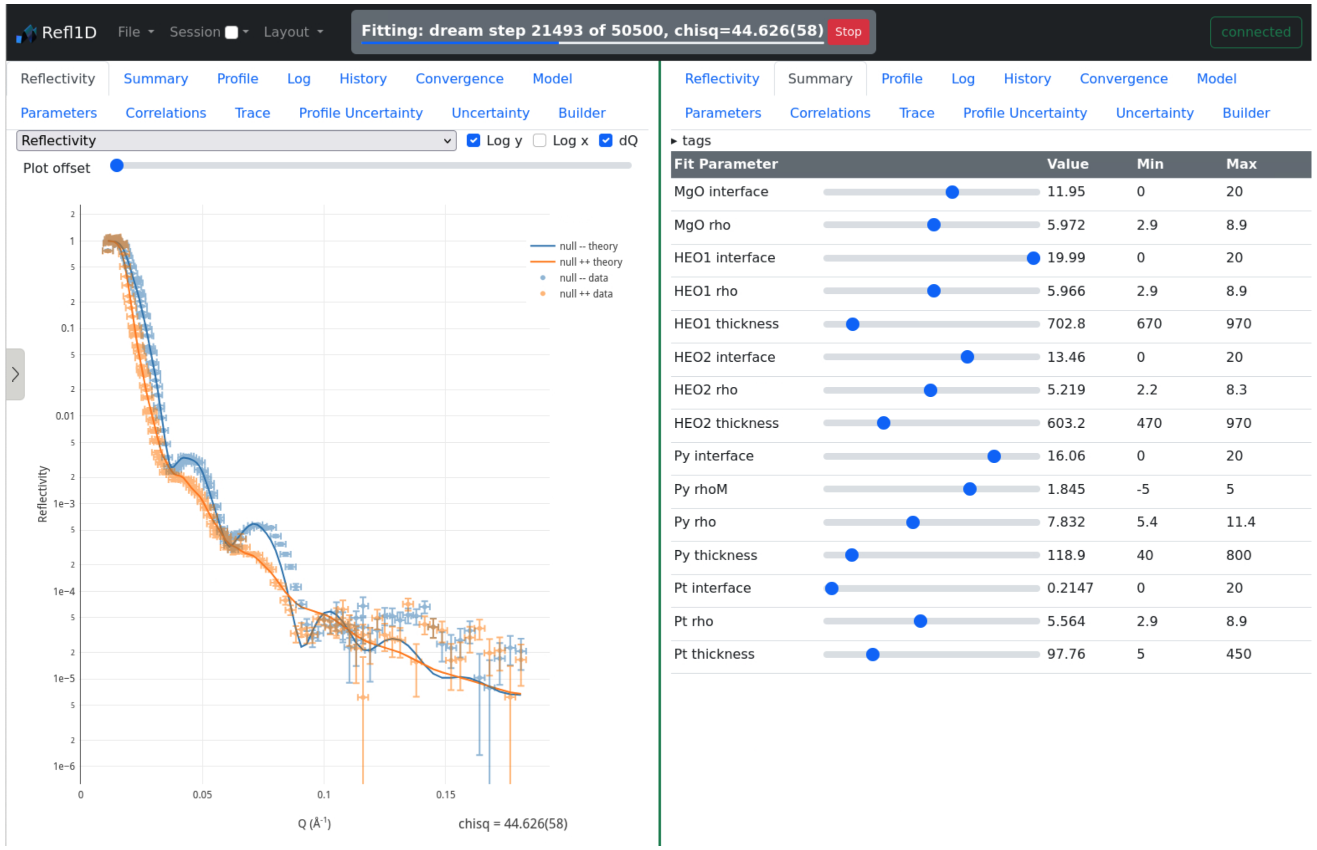




Summary

- Basics of Neutron Reflectivity
  - Origins in Schrodinger's Eq.
  - How to read Reflectivity Curves
- Instrument Walkthrough
  - Driving, and time estimates
  - Sample environment options
- Fitting Examples and options

Refl1d – Webview



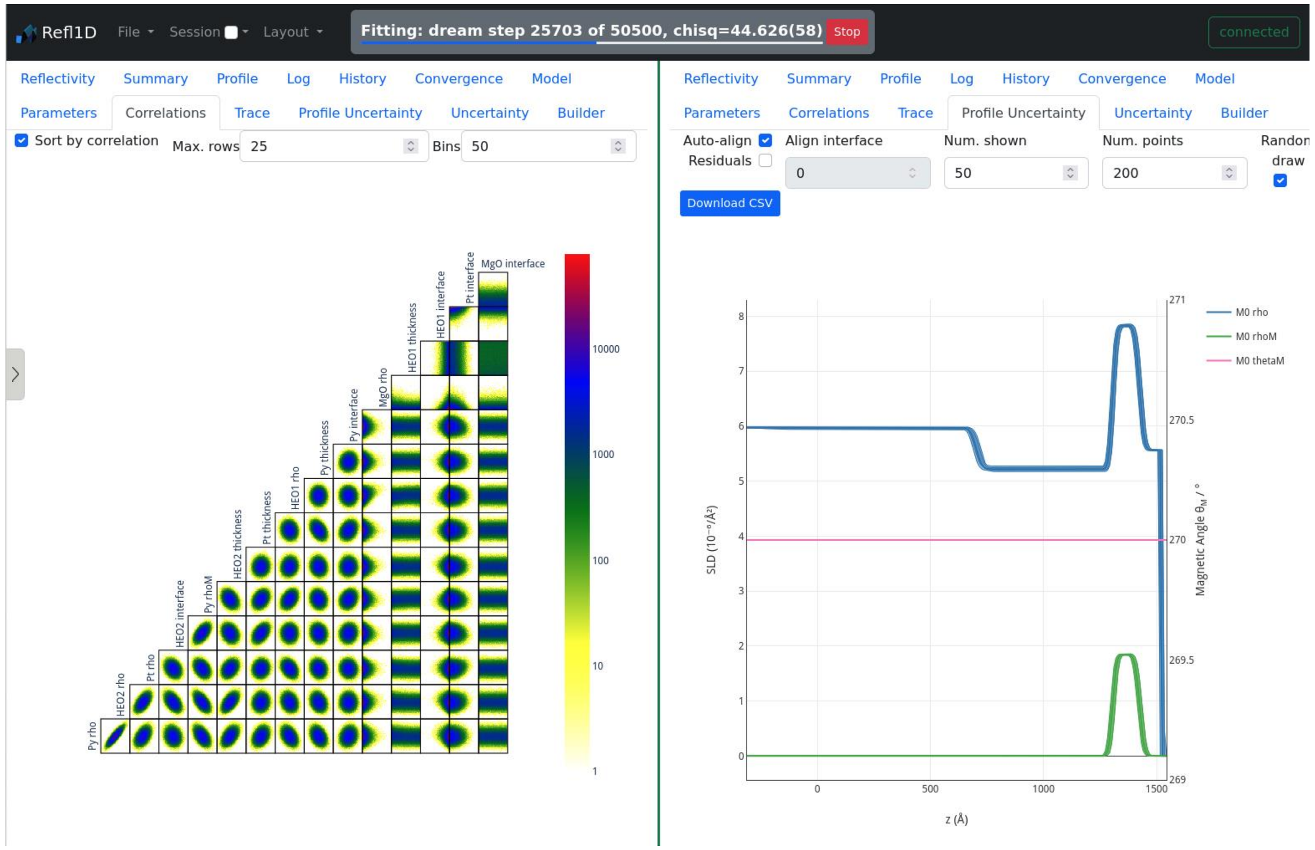
Fitting: dream step 21493 of 50500, chisq=44.626(58)

Reflectivity ☑ Log y ☐ Log x ☑ dQ

Plot offset

chisq = 44.626(58)

Fit Parameter	Value	Min	Max
MgO interface	11.95	0	20
MgO rho	5.972	2.9	8.9
HEO1 interface	19.99	0	20
HEO1 rho	5.966	2.9	8.9
HEO1 thickness	702.8	670	970
HEO2 interface	13.46	0	20
HEO2 rho	5.219	2.2	8.3
HEO2 thickness	603.2	470	970
Py interface	16.06	0	20
Py rhoM	1.845	-5	5
Py rho	7.832	5.4	11.4
Py thickness	118.9	40	800
Pt interface	0.2147	0	20
Pt rho	5.564	2.9	8.9
Pt thickness	97.76	5	450

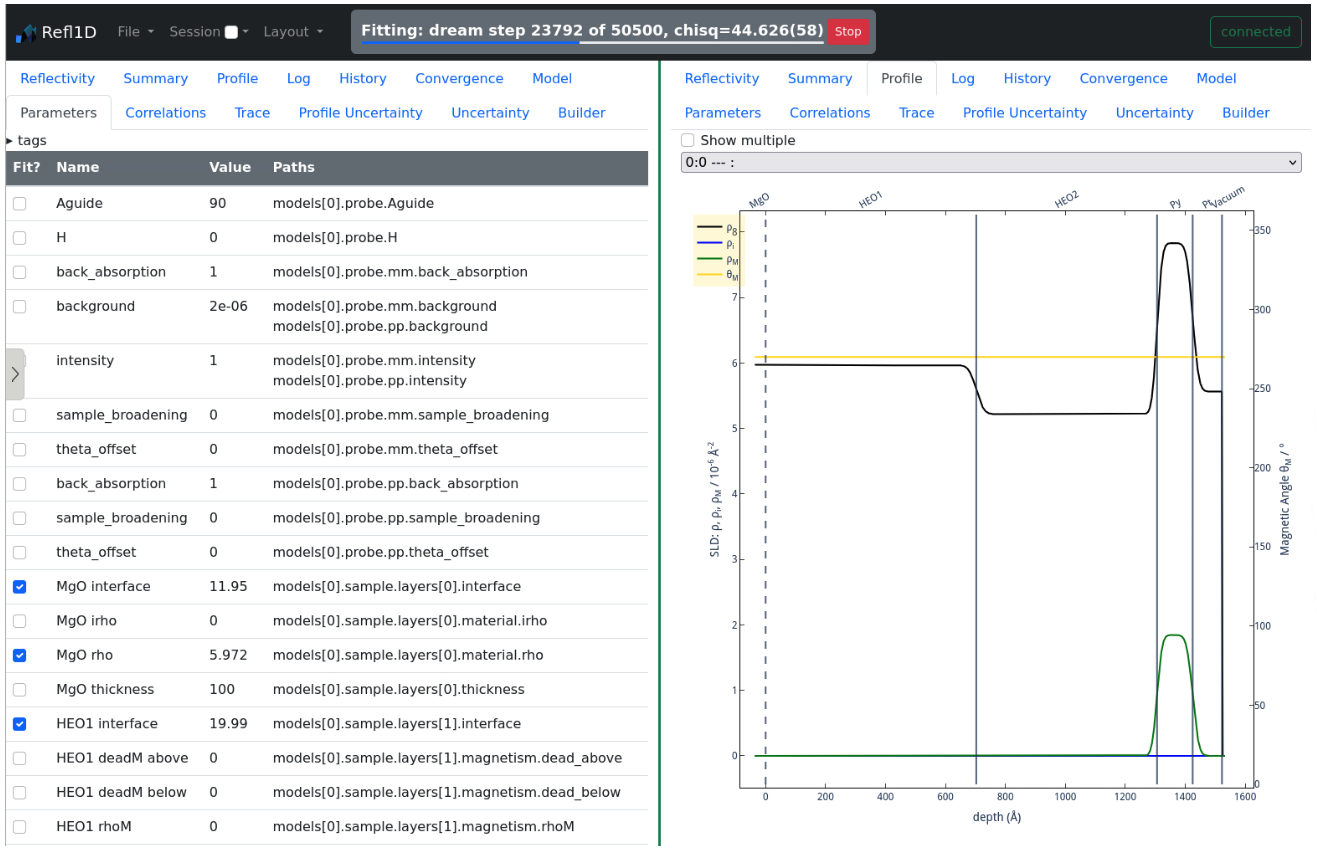


Fitting: dream step 25703 of 50500, chisq=44.626(58)

☑ Sort by correlation Max. rows 25 Bins 50

Auto-align ☑ Align interface 0 Num. shown 50 Num. points 200 Random draw ☑

Residuals ☐

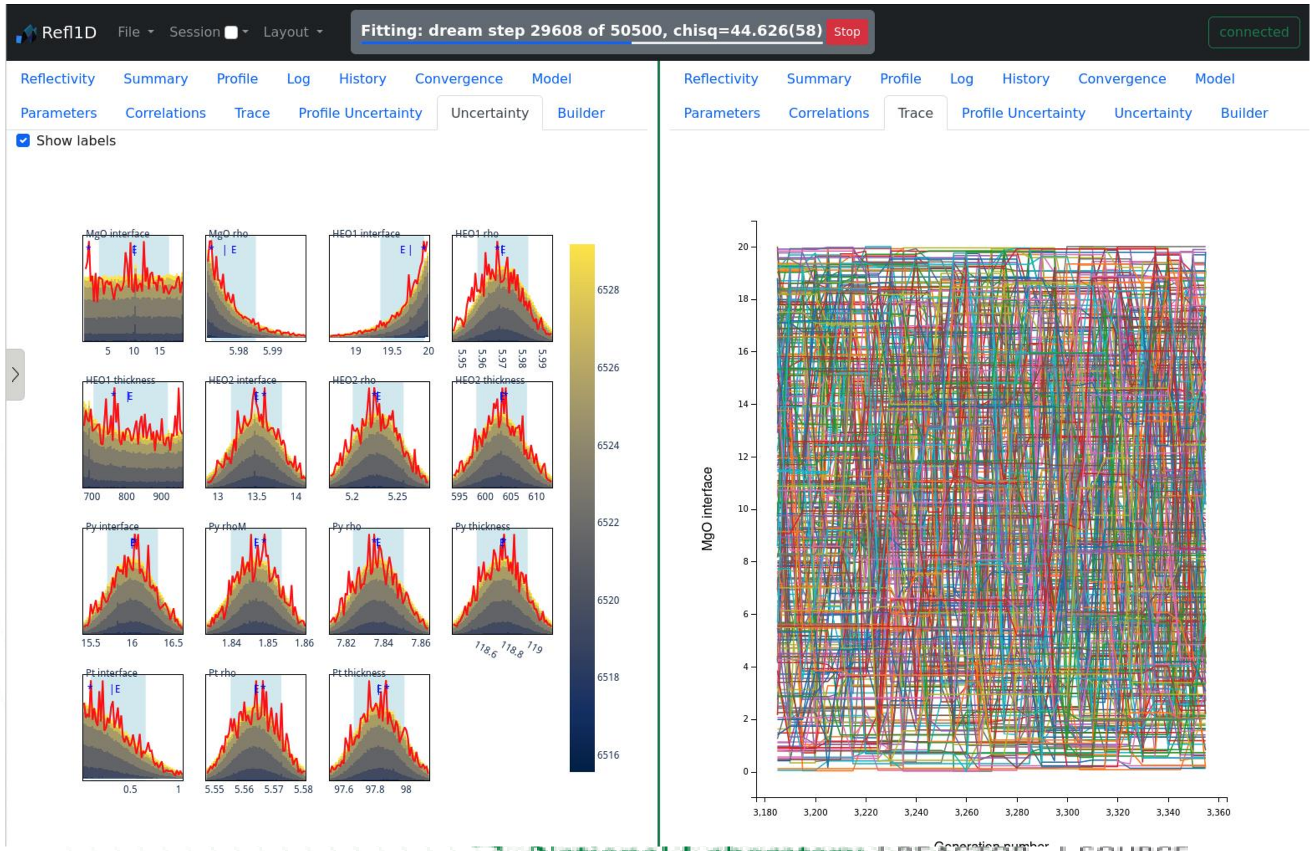


Fitting: dream step 23792 of 50500, chisq=44.626(58)

Fit?	Name	Value	Paths
☐	Aguide	90	models[0].probe.Aguide
☐	H	0	models[0].probe.H
☐	back_absorption	1	models[0].probe.mm.back_absorption
☐	background	2e-06	models[0].probe.mm.background models[0].probe.pp.background
	intensity	1	models[0].probe.mm.intensity models[0].probe.pp.intensity
☐	sample_broadening	0	models[0].probe.mm.sample_broadening
☐	theta_offset	0	models[0].probe.mm.theta_offset
☐	back_absorption	1	models[0].probe.pp.back_absorption
☐	sample_broadening	0	models[0].probe.pp.sample_broadening
☐	theta_offset	0	models[0].probe.pp.theta_offset
☑	MgO interface	11.95	models[0].sample.layers[0].interface
☐	MgO irho	0	models[0].sample.layers[0].material.irho
☑	MgO rho	5.972	models[0].sample.layers[0].material.rho
☐	MgO thickness	100	models[0].sample.layers[0].thickness
☑	HEO1 interface	19.99	models[0].sample.layers[1].interface
☐	HEO1 deadM above	0	models[0].sample.layers[1].magnetism.dead_above
☐	HEO1 deadM below	0	models[0].sample.layers[1].magnetism.dead_below
☐	HEO1 rhoM	0	models[0].sample.layers[1].magnetism.rhoM

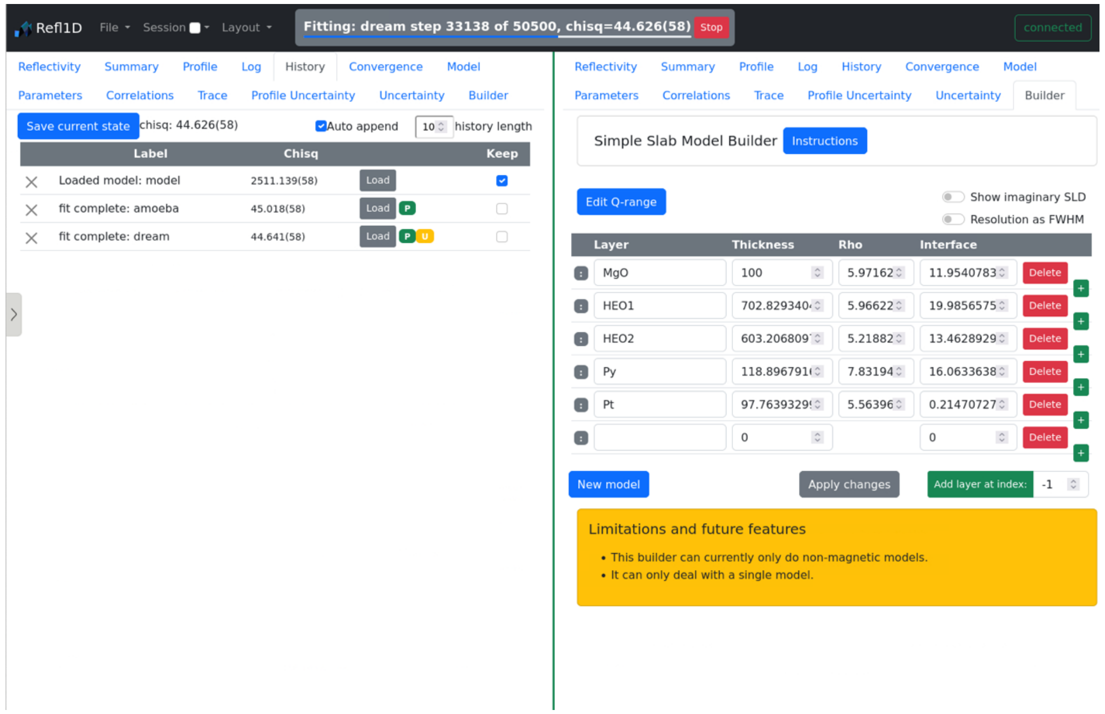
☐ Show multiple

0:0 --- :



Fitting: dream step 29608 of 50500, chisq=44.626(58)

☑ Show labels



Fitting: dream step 33138 of 50500, chisq=44.626(58)

chisq: 44.626(58) ☑ Auto append 10 history length

Label	Chisq		Keep
Loaded model: model	2511.139(58)	Load	☑
fit complete: amoeba	45.018(58)	Load P	☐
fit complete: dream	44.641(58)	Load P U	☐

Simple Slab Model Builder

○ Show imaginary SLD

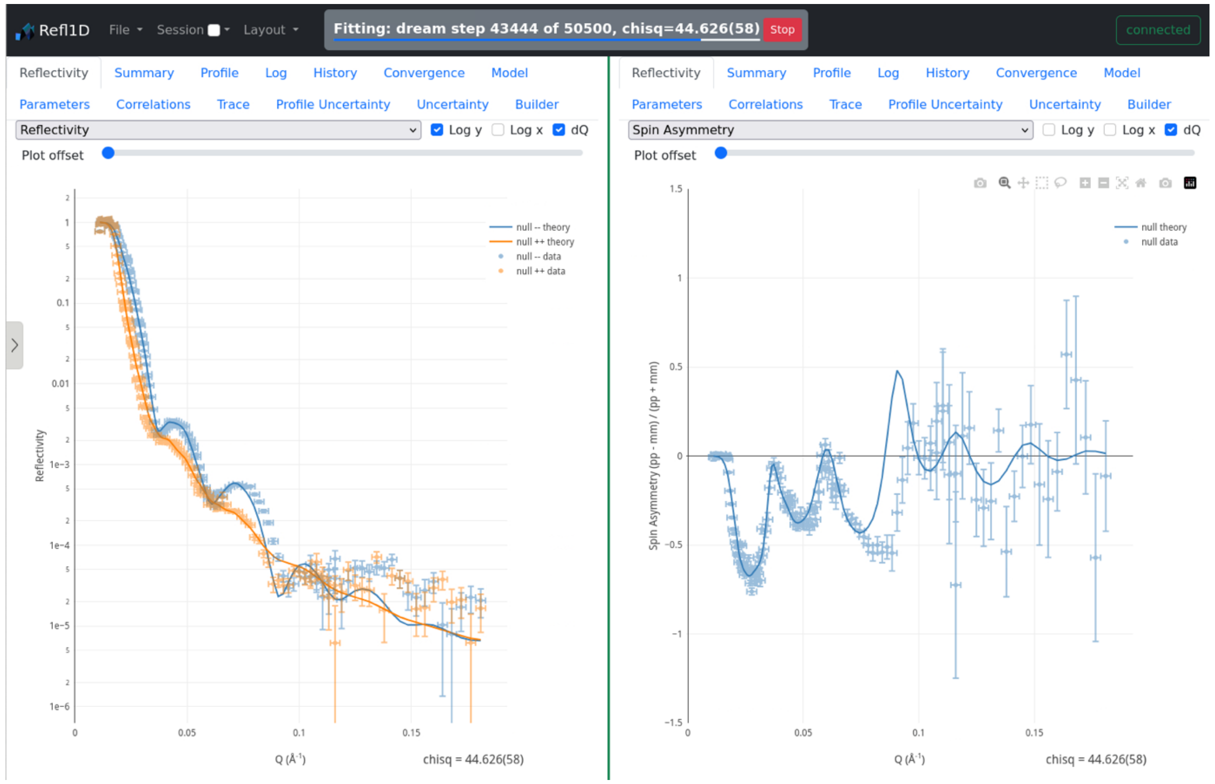
○ Resolution as FWHM

Layer	Thickness	Rho	Interface
MgO	100	5.97162	11.9540783
HEO1	702.829340	5.96622	19.9856575
HEO2	603.206809	5.21882	13.4628929
Py	118.896791	7.83194	16.0633638
Pt	97.7639329	5.56396	0.21470727
	0		0

Add layer at index: -1

Limitations and future features

- This builder can currently only do non-magnetic models.
- It can only deal with a single model.



Fitting: dream step 43444 of 50500, chisq=44.626(58)

Reflectivity ☑ Log y ☐ Log x ☑ dQ

Plot offset

chisq = 44.626(58)

Spin Asymmetry ☐ Log y ☐ Log x ☑ dQ

Plot offset

chisq = 44.626(58)

Fitting: dream step 46118 of 50500, chisq=44.626(58)

RQ^4 ☐ Log y ☐ Log x ☑ dQ

Plot offset

chisq = 44.626(58)

Fresnel (R/R_substrate) ☐ Log y ☐ Log x ☑ dQ

Plot offset

chisq = 44.626(58)

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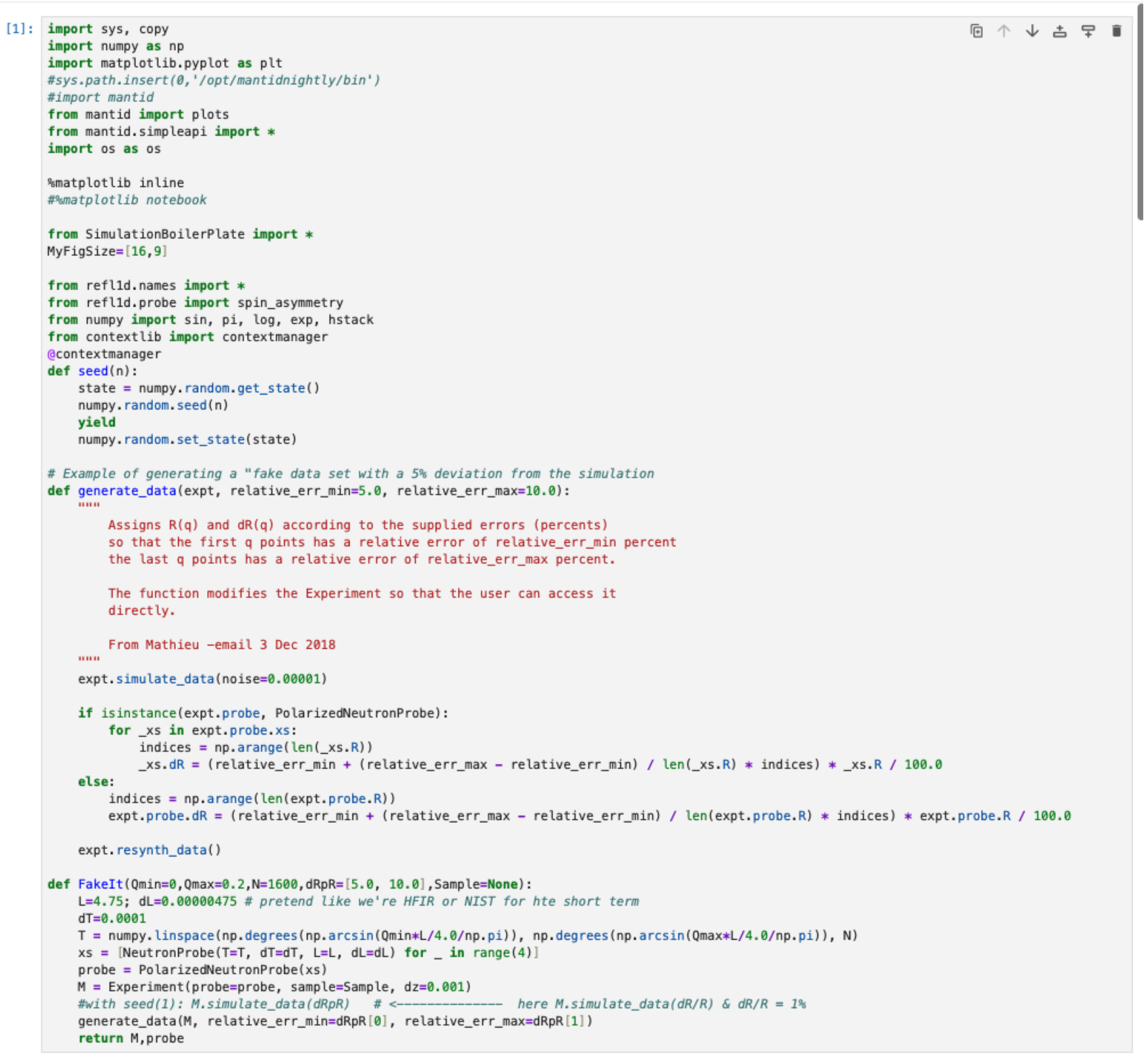
Refl1D in a python notebook



[1]:

```python
import sys, copy
import numpy as np
import matplotlib.pyplot as plt
#sys.path.insert(0,'/opt/mantidnightly/bin')
#import mantid
from mantid import plots
from mantid.simpleapi import *
import os as os

%matplotlib inline
#%matplotlib notebook

from SimulationBoilerPlate import *
MyFigSize=[16,9]

from refl1d.names import *
from refl1d.probe import spin_asymmetry
from numpy import sin, pi, log, exp, hstack
from contextlib import contextmanager
@contextmanager
def seed(n):
    state = numpy.random.get_state()
    numpy.random.seed(n)
    yield
    numpy.random.set_state(state)

# Example of generating a "fake data set with a 5% deviation from the simulation
def generate_data(expt, relative_err_min=5.0, relative_err_max=10.0):
    """
        Assigns R(q) and dR(q) according to the supplied errors (percents)
        so that the first q points has a relative error of relative_err_min percent
        the last q points has a relative error of relative_err_max percent.

        The function modifies the Experiment so that the user can access it
        directly.

        From Mathieu -email 3 Dec 2018
    """
    expt.simulate_data(noise=0.00001)

    if isinstance(expt.probe, PolarizedNeutronProbe):
        for _xs in expt.probe.xs:
            indices = np.arange(len(_xs.R))
            _xs.dR = (relative_err_min + (relative_err_max - relative_err_min) / len(_xs.R) * indices) * _xs.R / 100.0
    else:
        indices = np.arange(len(expt.probe.R))
        expt.probe.dR = (relative_err_min + (relative_err_max - relative_err_min) / len(expt.probe.R) * indices) * expt.probe.R / 100.0

    expt.resynth_data()

def FakeIt(Qmin=0,Qmax=0.2,N=1600,dRpR=[5.0, 10.0],Sample=None):
    L=4.75; dL=0.00000475 # pretend like we're HFIR or NIST for hte short term
    dT=0.0001
    T = numpy.linspace(np.degrees(np.arcsin(Qmin*L/4.0/np.pi)), np.degrees(np.arcsin(Qmax*L/4.0/np.pi)), N)
    xs = [NeutronProbe(T=T, dT=dT, L=L, dL=dL) for _ in range(4)]
    probe = PolarizedNeutronProbe(xs)
    M = Experiment(probe=probe, sample=Sample, dz=0.001)
    #with seed(1): M.simulate_data(dRpR)   # <-------------  here M.simulate_data(dR/R) & dR/R = 1%
    generate_data(M, relative_err_min=dRpR[0], relative_err_max=dRpR[1])
    return M,probe
```

[56]:

```python
def MakeSample(d1,d2):
    Sub     = SLD(name="Sub",     rho=1.4,  irho=0.0)
    Layer1  = SLD(name="Layer1",  rho=1.7,  irho=0.0)
    Layer2  = SLD(name="Layer2",  rho=1.0, irho=0.0)

    sample= (
        Sub(0,3)|
        Layer1(600,1)|
        air
        )

    return sample
#----------------------------------------------------------------------
er=0.0000001
sample=MakeSample(d1=250,d2=250)
M1,probe1 = FakeIt(Qmin=0.001,Qmax=0.5,N=2000,dRpR=[er,er],Sample=sample)
#MakeReport(M1, probe1,Title="".format(),salim=[-1.2, 1.2],forcefigsize=MyFigSize)
# ---------------------------------------------------------------------
#You can also extract the simulated curves and plot them using matplotlib/numpy like this.
smm, smp, spm, spp = M1.reflectivity() # UU, UD, DU, DD This is the simulation results.
sQ, sSA,sdSA = spin_asymmetry(spp[0], spp[1], None, smm[0], smm[1], None)

plt.figure(figsize=MyFigSize)
#plt.errorbar(probe1.pp.Q, probe1.pp.R, xerr=probe1.pp.dQ, yerr=probe1.pp.dR,fmt='b-',alpha=0.5)
#plt.errorbar(probe1.mm.Q, probe1.mm.R, xerr=probe1.mm.dQ, yerr=probe1.mm.dR,fmt='g-',alpha=0.5)
plt.subplot(2,1,1)
plt.plot(spp[0],spp[1],'r-'); plt.plot(smm[0],smm[1],'b-')
plt.xlim([0.001,0.5])
plt.yscale('log'); plt.xscale('linear')
plt.ylabel('$Reflectivity\ (Arb. Units)$')
plt.xlabel('$Q_z$')
plt.title('');

plt.subplot(2,1,2)
z,rho,irho = M1.smooth_profile()
plt.plot(z,rho,'b-')
```

[56]:

```
Text(0, 0.5, '$SLD (10^{-6} \\AA^{-2})$')
```