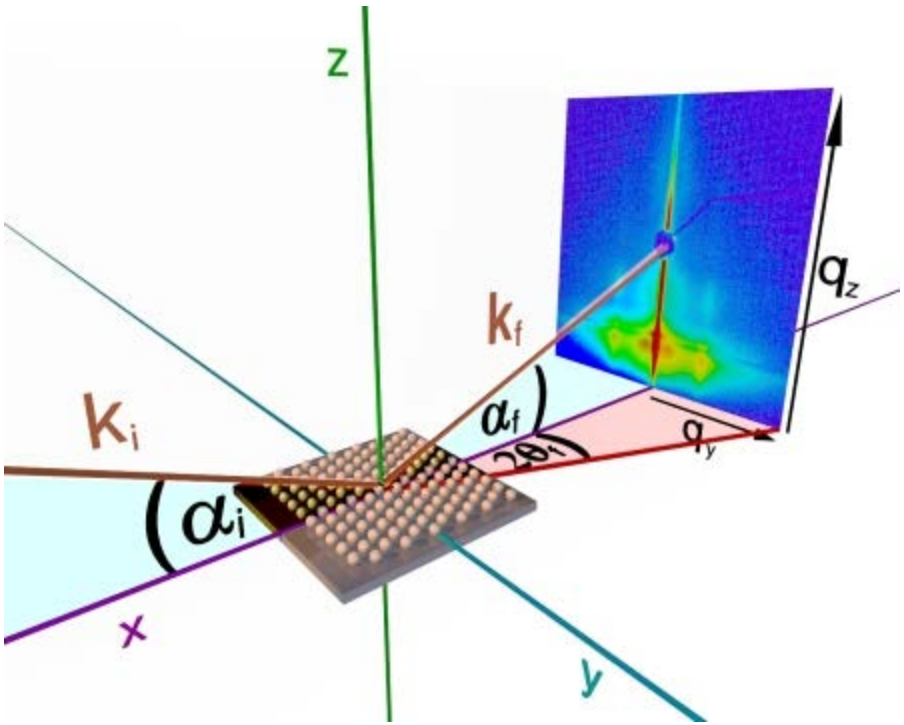
GISAXS Software Overview

"Beyond Rg" SAS Short Course, 2013.10.30

GIXS: what is it?

- Means of studying electron density contrast variations at surfaces and interfaces
- Mostly studies lateral structure, parallel to plane of sample
- X-rays incident at grazing incidence
  - Limited penetration into sample means enhanced surface sensitivity
- Scattered x-rays observed with an area detector



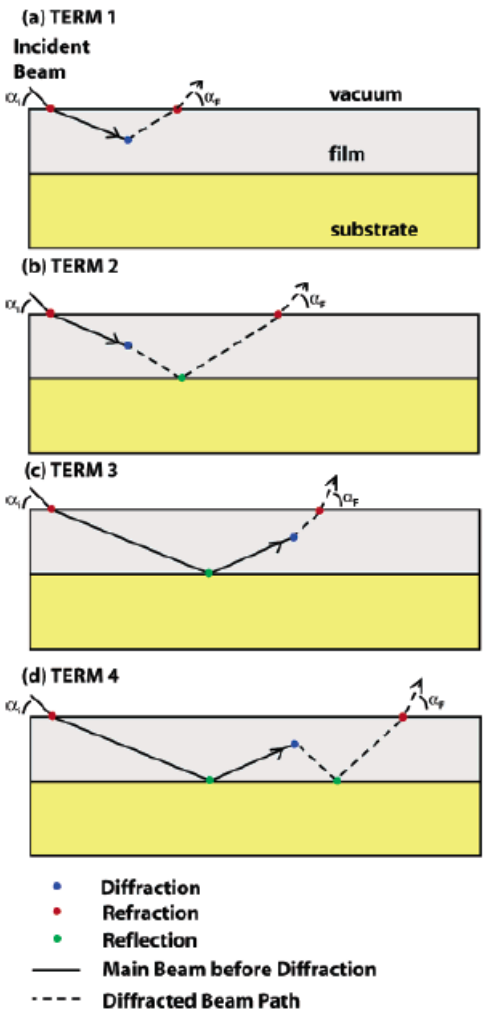
$$q_{x,y,z} = \frac{2\pi}{\lambda}\begin{bmatrix} \cos(\alpha_f)\cos(2\theta_f) - \cos(\alpha_i) \\ \cos(\alpha_f)\sin(2\theta_f) \\ \sin(\alpha_f) + \sin(\alpha_i) \end{bmatrix}$$

Images:
Prof. Andreas Meyer, U. Hamburg, www.gisaxs.de

GIXS: Why is it hard to calculate?

Total external reflection near critical angle

Distorted Wave Born Approximation (DWBA) leads to 4 scattering channels



GISAXS Software: Data Visualization and Reduction

Package	Application	Platform	Source	Available
GIXSGUI	Data reduction & Visualization	MATLAB	Zhang Jiang (APS)	http://www.aps.anl.gov/Sectors/Sector8/Operations/GIXSGUI.html
WxDiff	Data reduction & Visualization	Python (Windows)	S. Mannsfeld (SSRL), Adv. Mater. 23: 127-131 (2011)	From author
GISAXSshop	Data reduction & Visualization	Igor Pro	Byeongdu Lee (APS)	From author

GIXS Data Reduction Packages

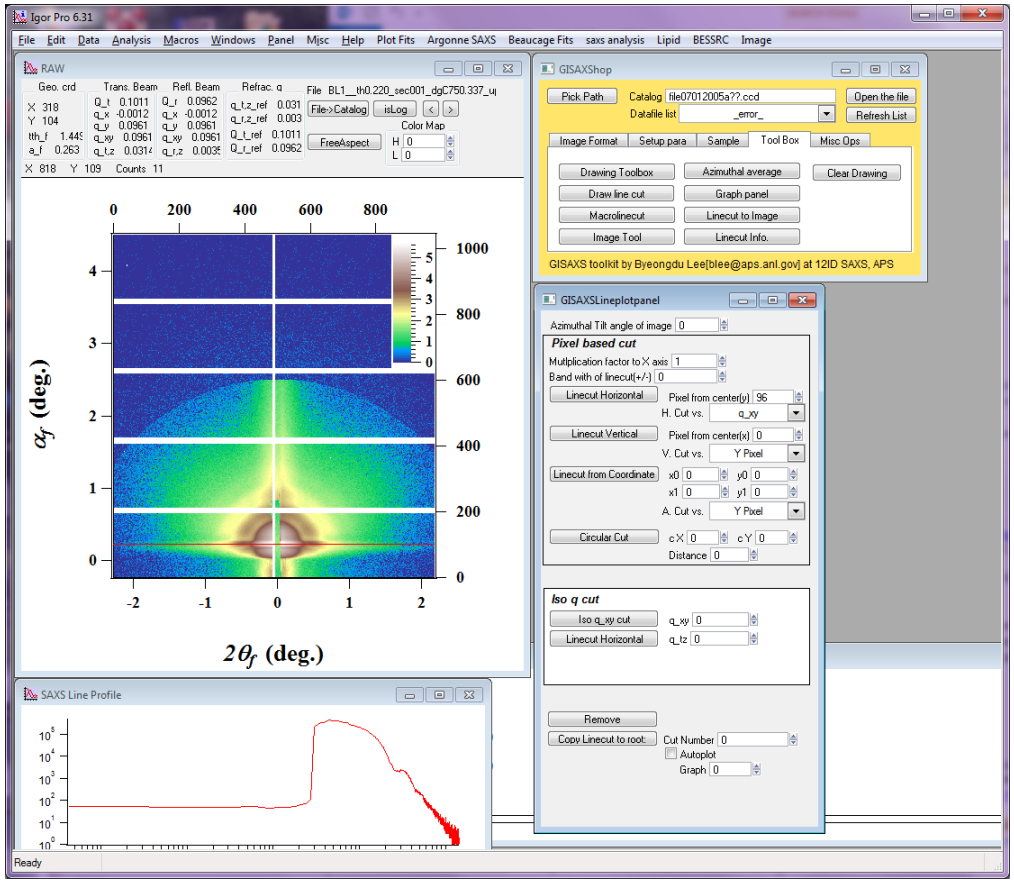
Common features of GIXSGUI, GISAXSshop & WxDiff

- GUI for displaying data
- Calibration from standard sample
- Support for Small- and Wide-Angle Regimes
- Integrations/Linecuts

GIXS Data Analysis

For users interested in qualitative analysis (peak positions, orientation, morphology) these packages may be sufficient.

GISAXS Data Reduction: GISAXSshop

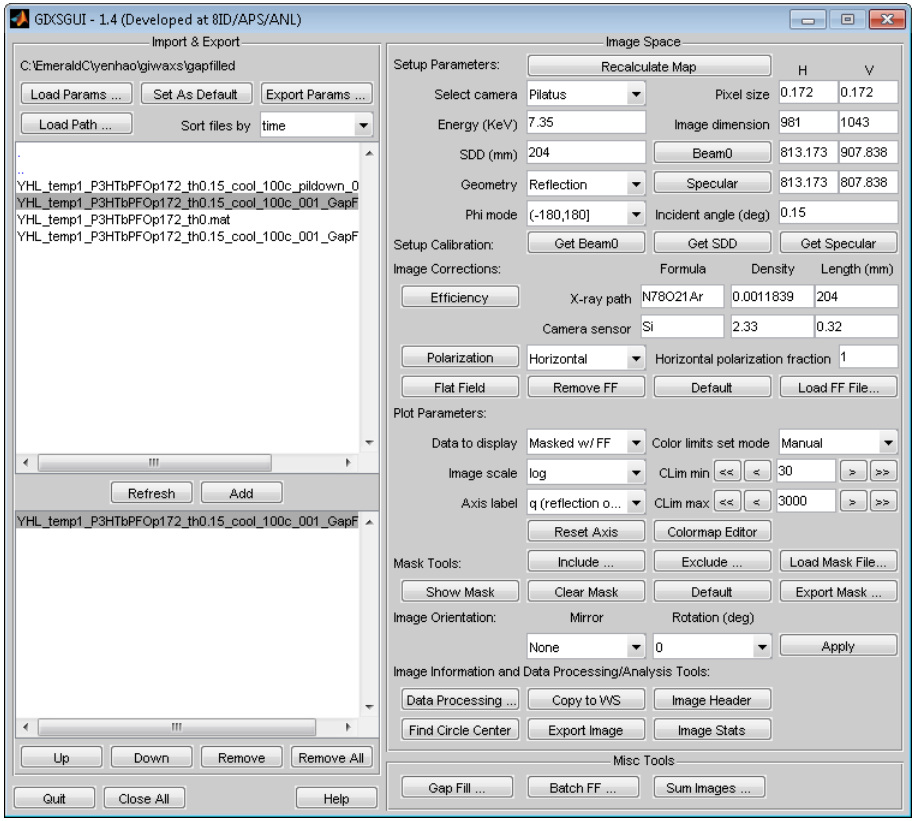


Igor Pro package

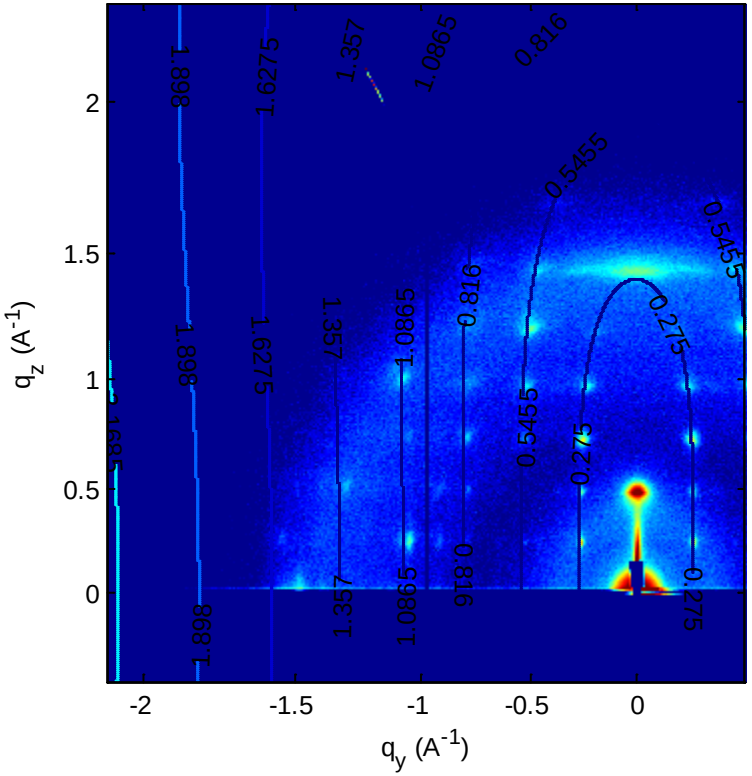
Byeongdu Lee (APS)

https://sites.google.com/site/byeongdu/software

GISAXS Data Reduction: GIXSGUI



Matlab package

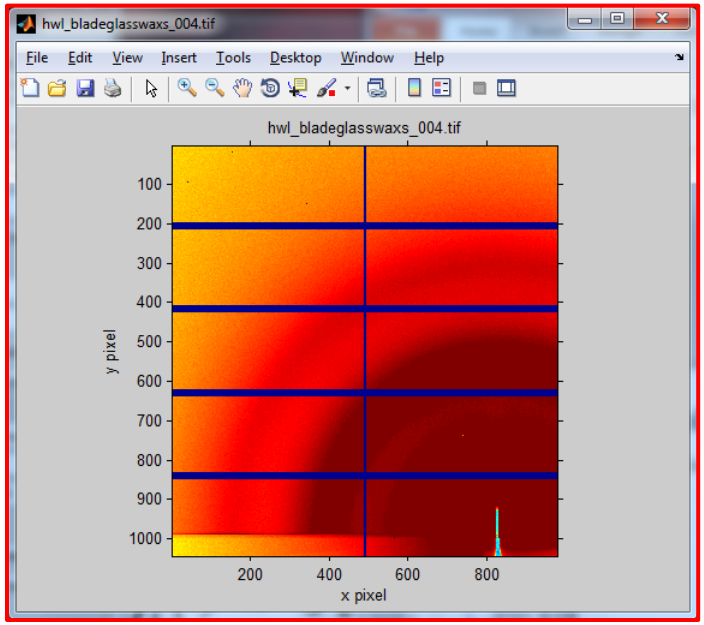


Zhang Jiang (APS)

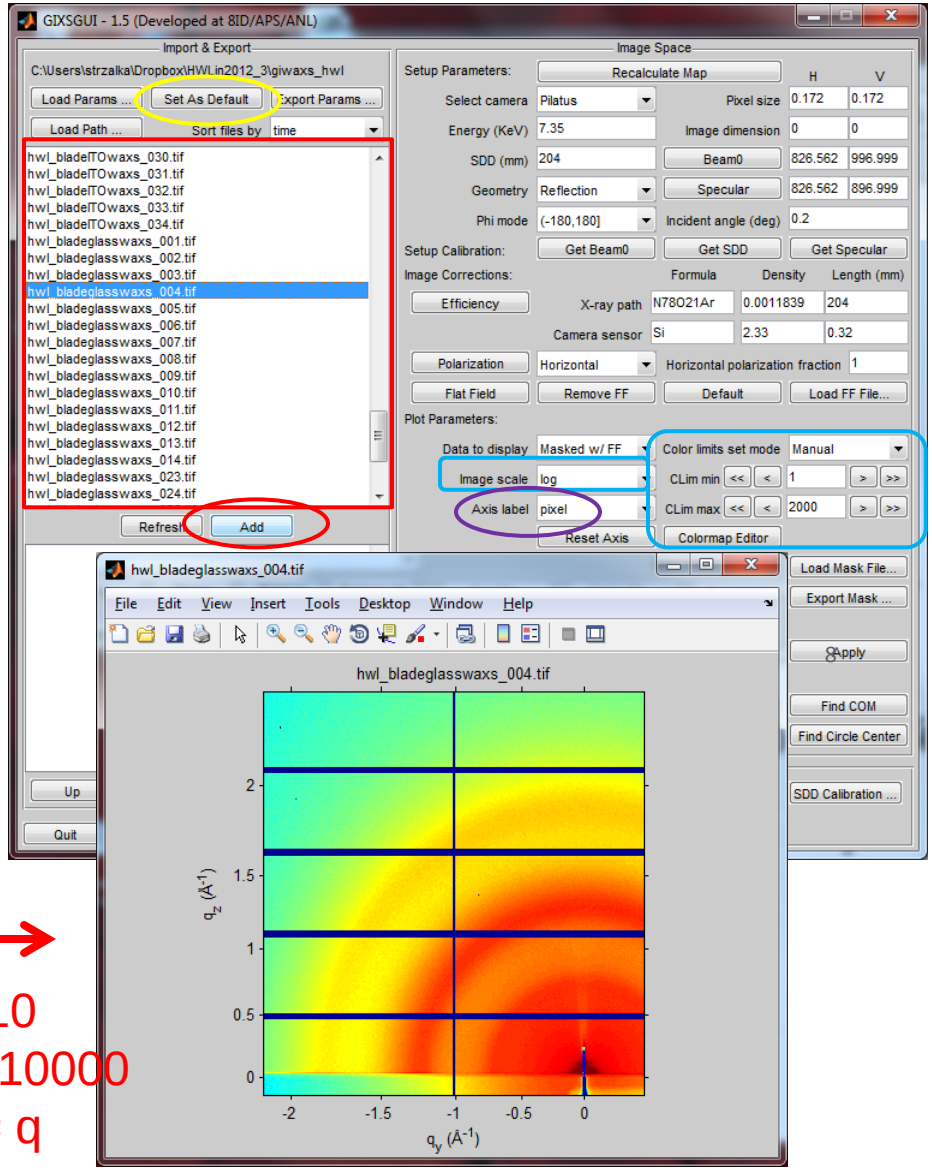
http://www.aps.anl.gov/Sectors/Sector8/Operations/GIXSGUI.html

Displaying 2-D data in GIXSGUI

- Select a file in the path list box
  - Double click on the filename OR
  - Click the Add button
  - Image appears
  - Adjust color scale with controls
  - Control axes with Axis label menu
  - Make new settings default with Set as Default button

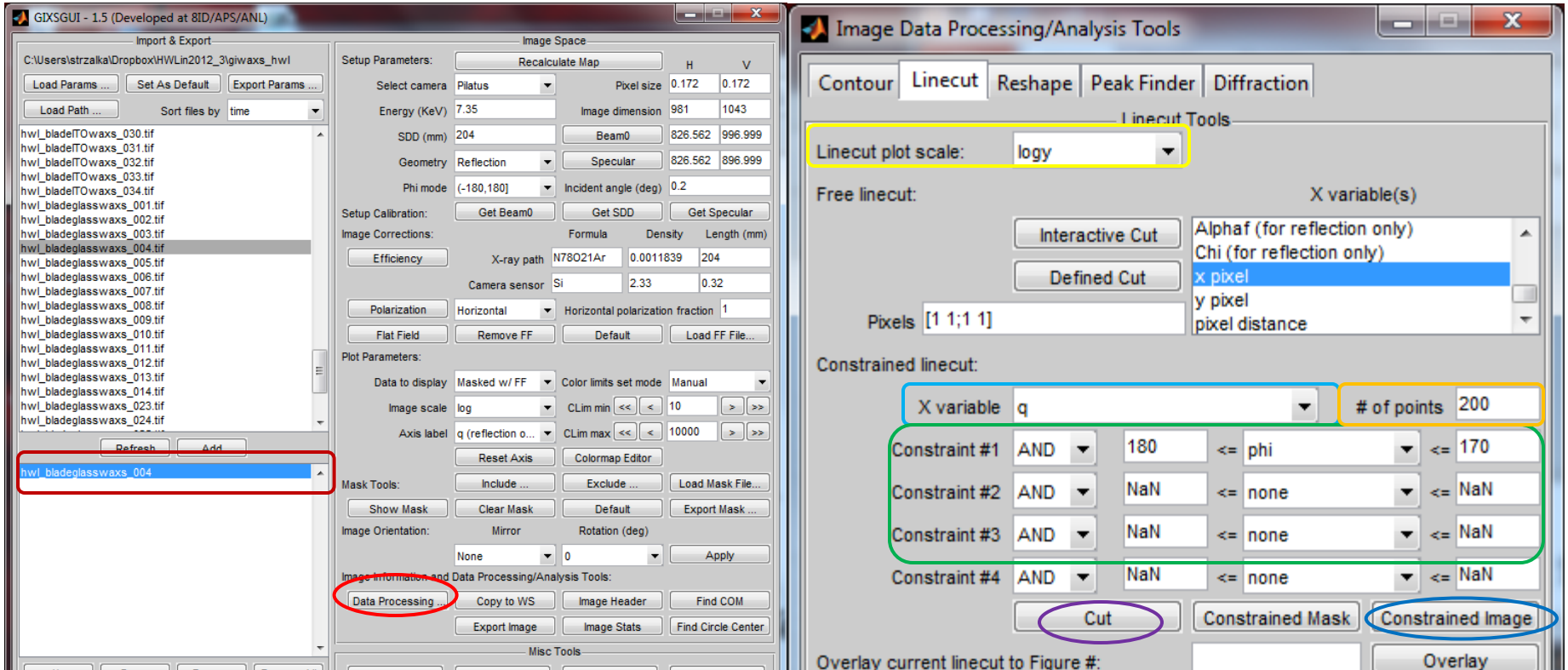


Clim min = 10
Clim max = 10000
Axis label = q



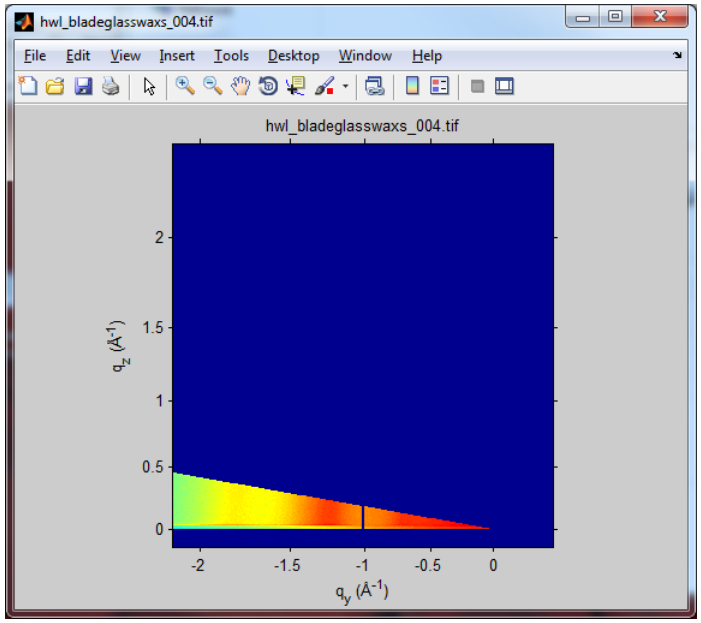
GIXSGUI: Applying simple linecuts

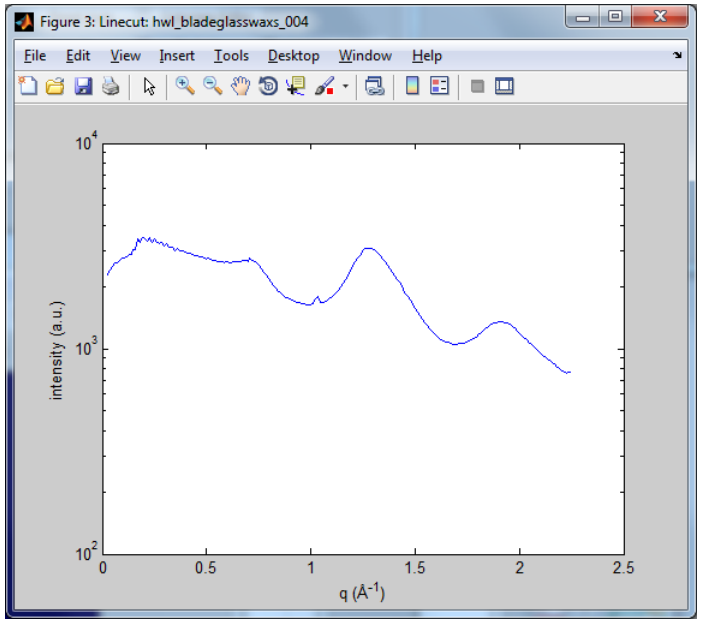
- Data processing button calls up new window
- For Constrained linecut, set X variable, Constraints, enter # of points in the result and set the Linecut plot scale
- Click Constrained Image to see the region included in the integration
- Click Cut to produce the linecut
- Note: linecut is performed on whichever image is selected in the list box.



GIXSGUI: Example Linecut

- Settings on previous slide produce the Constrained Image (left) and the linecut (right) below.





GISAXS Software: Particle Analysis

Package	Application	Platform	Source	Available
IsGISAXS	Nanostructures (Islands) on surfaces	Fortran90 Windows	R. Lazzari, (U. Curie) J. Appl. Cryst. 35:406-21 (2002)	http://ln-www.insp.upmc.fr/axe4/Oxydes/IsGISAXS/isgisaxs.htm
FitGISAXS	(Buried) Nanostructures	Igor Pro	D. Babboneau (U. Poitiers) *J. Appl. Cryst.* ***43*** *929-936 (2010)*	http://www.pprime.fr/?q=fr/nanoparticules-nanostructures
BornAgain	(Buried) Nanostructures	Python	C. Durniak et al, (JCNS MLZ)	http://apps.jcns.fz-juelich.de/doku/sc/bornagain:start

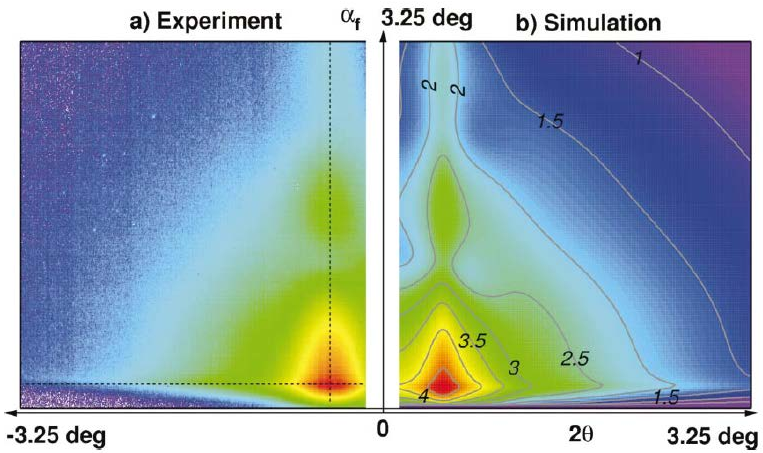
GISAXS Particle Analysis: IsGISAXS

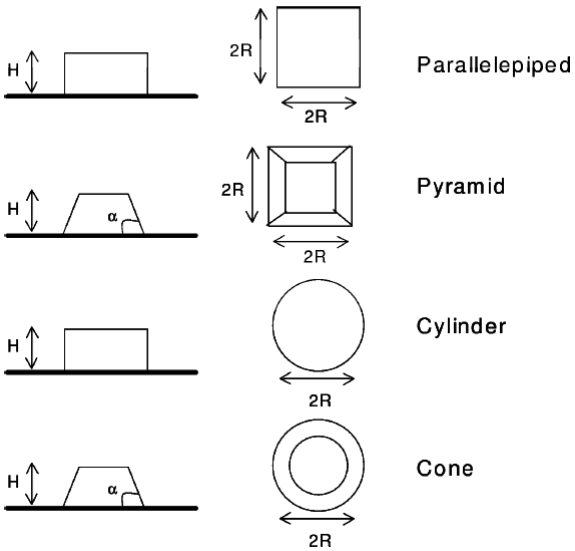
Calculates simulated intensity for islands – discrete nanostructures on surfaces

-No support for buried structures

-Limited to regularly shaped structures

-Command-line driven



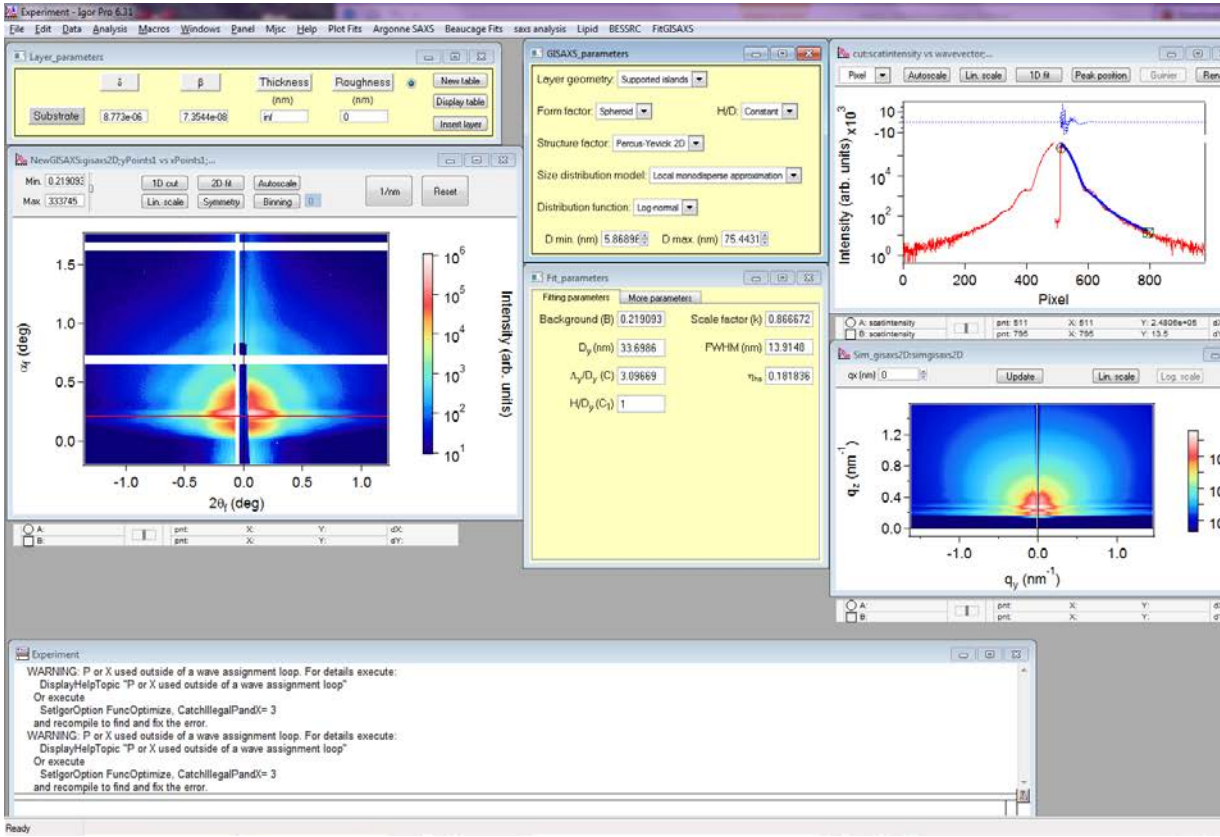


R. Lazzari, (U. Curie) J. Appl. Cryst. 35:406-21 (2002)
http://ln-www.insp.upmc.fr/axe4/Oxydes/IsGISAXS/isgisaxs.htm

GISAXS Particle Analysis: FitGISAXS

- IGOR Pro user-friendly package implements all of IsGISAXS
  - + Supports DWBA
  - + Buried nanostructures

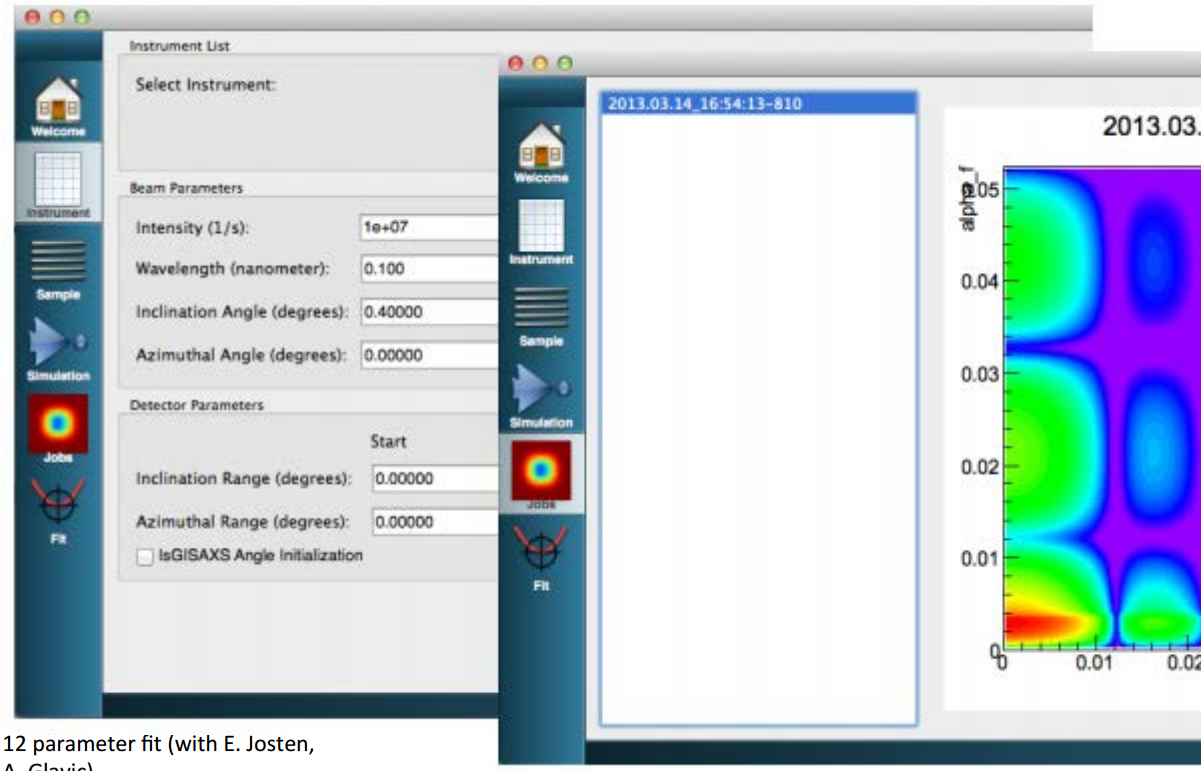
Demo: Wed PM session



D. Babboneau (U. Poitiers) J. Appl. Cryst. 43 929-936 (2010)
http://www.pprime.fr/?q=fr/nanoparticules-nanostructures

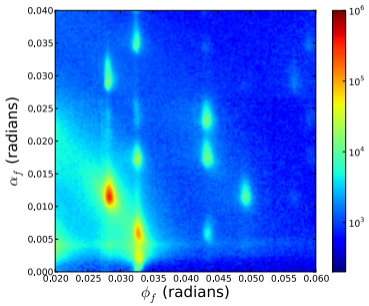
GISAXS Particle Analysis: BornAgain

- Python-based package implements all of IsGISAXS
  - Supports DWBA
  - Buried nanostructures
  - Supports GISANS (with neutron polarization)

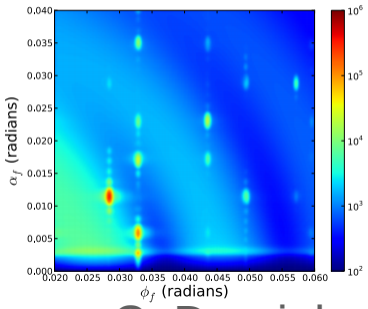


Graphical output

Real data (courtesy E. Josten)



12 parameter fit (with E. Josten, A. Glavic)



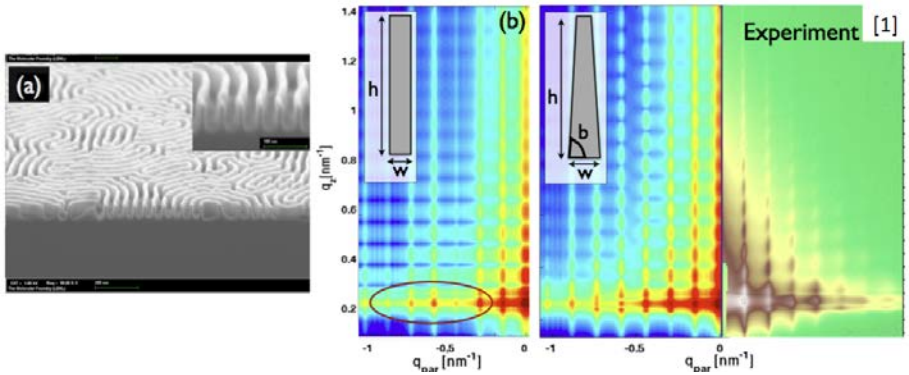
C. Durniak et al, (JCNS MLZ)
http://apps.jcns.fz-juelich.de/doku/sc/bornagain:start

GISAXS Software: Thin Film Analysis

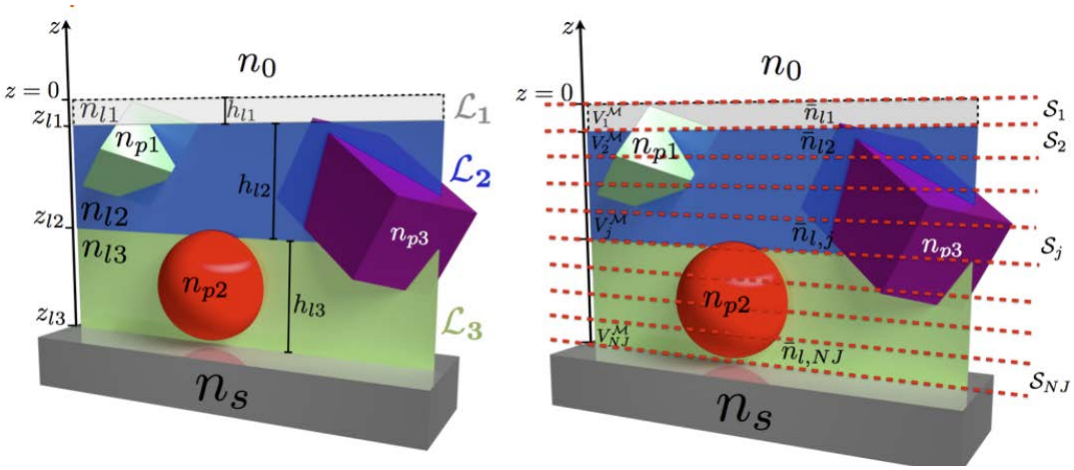
Package	Application	Platform	Source	Available
HipGISAXS	High-Performance Simulaiions	Multicore machines	A. Hexemer et al. (ALS)	http://portal.nersc.gov/project/m1285/hipgisaxs.html
SimDiffraction	Oriented powders on surfaces	?	D. Breiby (SLS), J. Appl. Cryst. **41:** 262-271 (2008)	From author
NANOCELL	Calculate locations of Bragg peaks from nanostructured thin films	Mathematica	H. Hillhouse (Washington), *J. Phys. Chem. B* **110** 9882 (2006)	From author
Multilayer DWBA	Buried nanostructures	Matlab	Z. Jiang, J. Wang. S. Sinha, S. Narayanan Phys. Rev. B 84, 075440 (2011)	Collaboration with authors

GISAXS Thin Film Analysis: HipGISAXS

- Simulation code for parrallel multicore processing



[1] Xiaodan Gu, Zuwei Liu, Ilja Gunkel, S. T. Chourou, Sung Woo Hong, Deirdre L. Olynick, and Thomas P. Russell. *Advanced Materials* (2012)



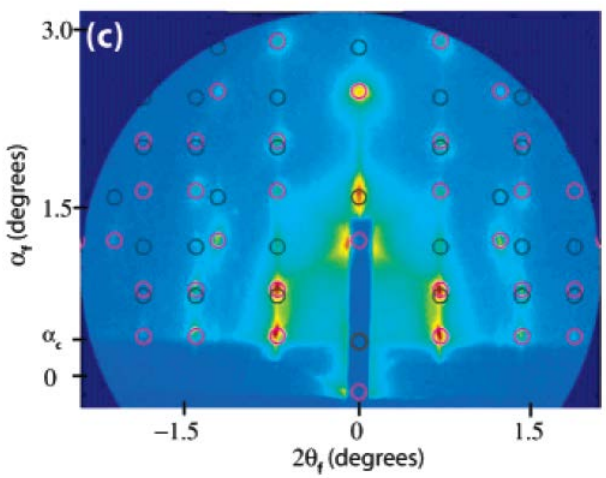
A. Hexemer et al. (ALS)
http://portal.nersc.gov/project/m1285/hipgisaxs.html

GISAXS Thin Film Analysis: NANOCELL

Predicts *positions* of Bragg reflections, does not calculate intensity

Determine space group symmetry, amount of disorder, lattice constants

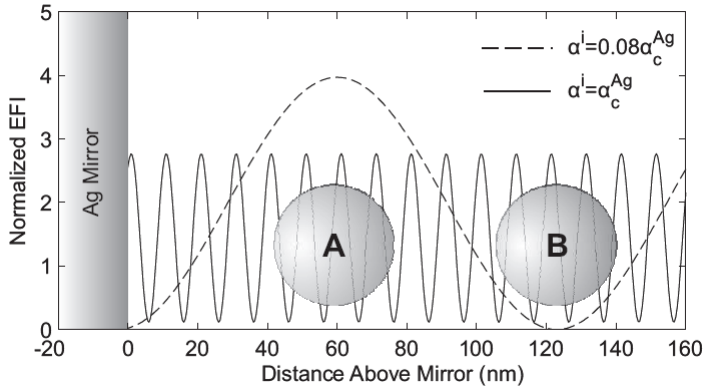
Applies from $\alpha_i > \alpha_c$, $\alpha_f > \alpha_c$, out to transmission SAXS

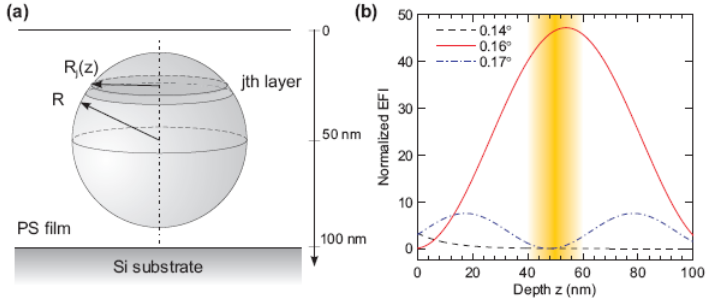


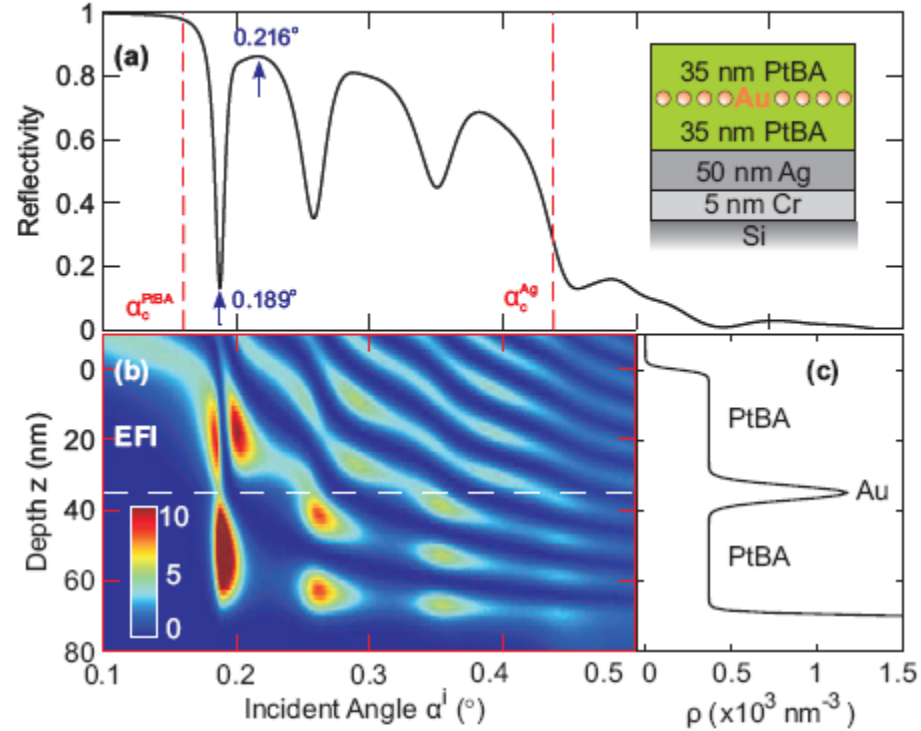
H. Hillhouse (Washington), J. Phys. Chem. B 110 9882 (2006)

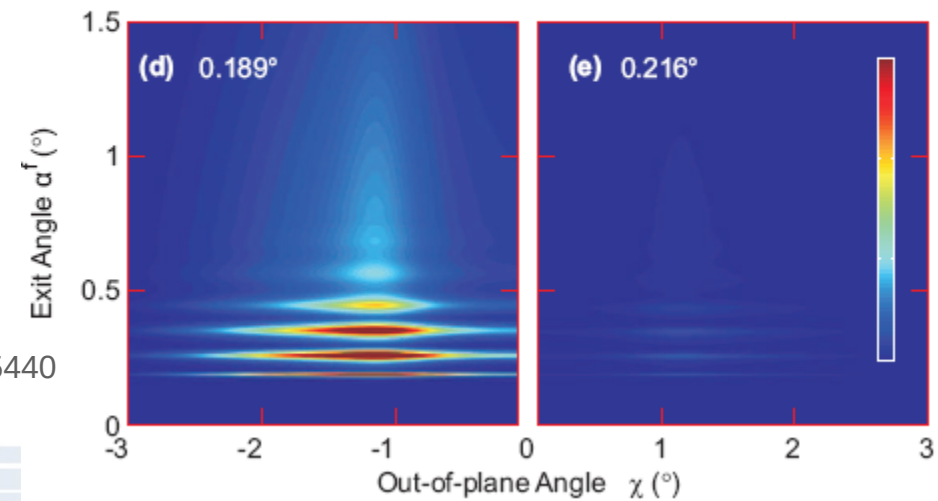
GISAXS Thin Film Analysis: Multilayer DWBA

Rigorously compute electric field intensity across thin film and treat buried structures properly







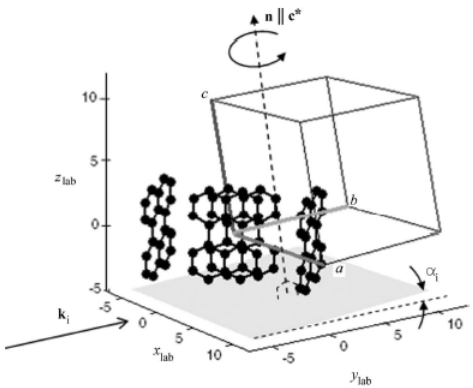


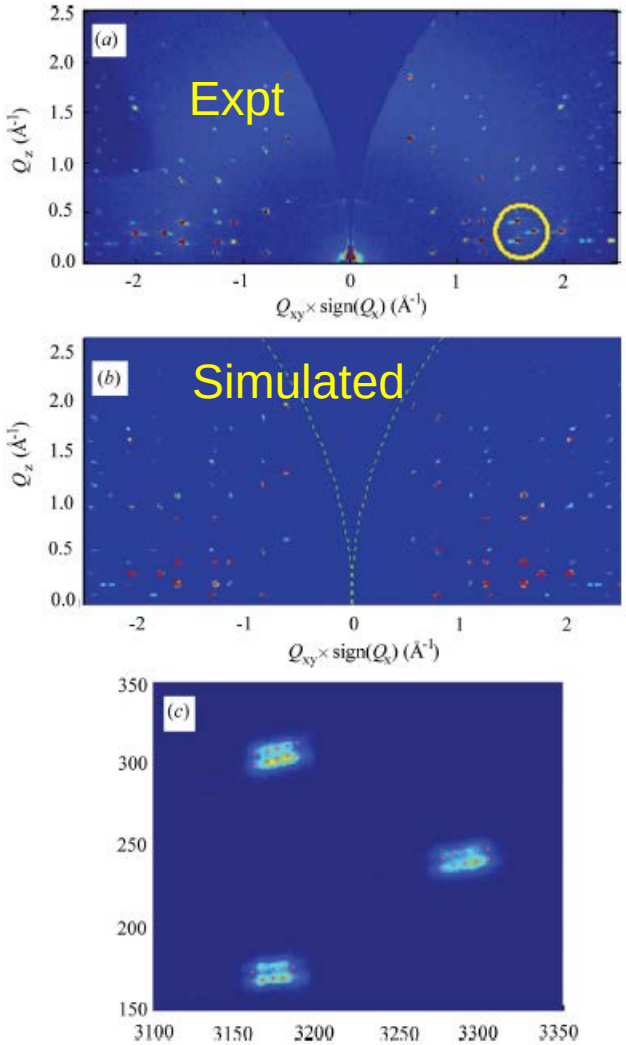
Z. Jiang, J. Wang. S. Sinha, S. Narayanan Phys. Rev. B 84, 075440 (2011)

GIWAXS Thin Film Analysis: SimDiffraction

Simulate scattering from oriented powders

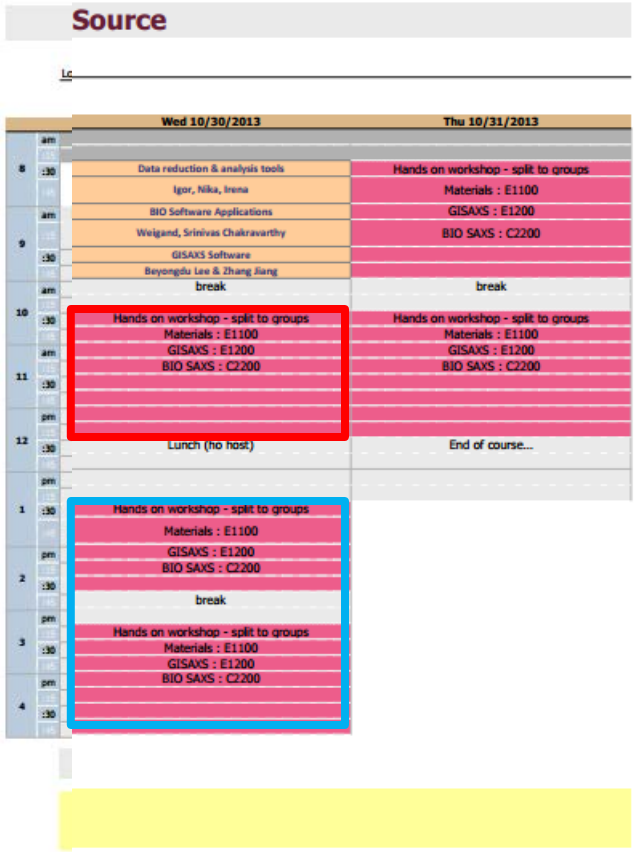
Input molecular model of small molecule unit cell.





D. Breiby (SLS), J. Appl. Cryst. 41: 262-271 (2008)

GISAXS Software Hands-On Schedule



Wed, 10:30-12:30
Thin Film Data Analysis with GIXSGUI (Matlab)

Wed 1:30-2:45, 3:15-4:30
Particle Data Analysis with GISAXSshop, FitGISAXS (Igor Pro) and Matlab code

Thurs:
No formal program, available for questions