GIXSGUI FAQ: Is there a way to get a reciprocal space plot (q_z against q_r with the black wedge in it) in GIXSGUI? (And is it right that it should be in this format before doing any line cuts etc?)

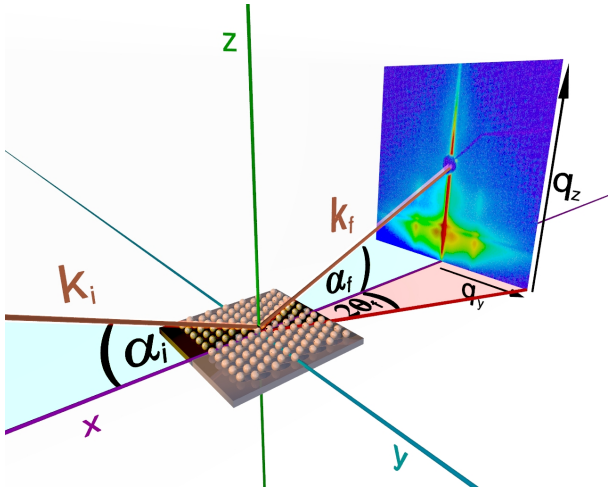
Joe Strzalka

2021.04.06

Q: How do I show GIWAXS data with the missing wedge along q_z?

- Only one point in GIWAXS 2D data satisfies the specular condition, $\alpha_f = \alpha_i$, $q_x = q_y = 0$. For all other points, $q_r = \sqrt{q_x^2 + q_y^2} \neq 0$
- Data along the qz axis is not observed, leaving a wedge-shaped blind-spot
- References:

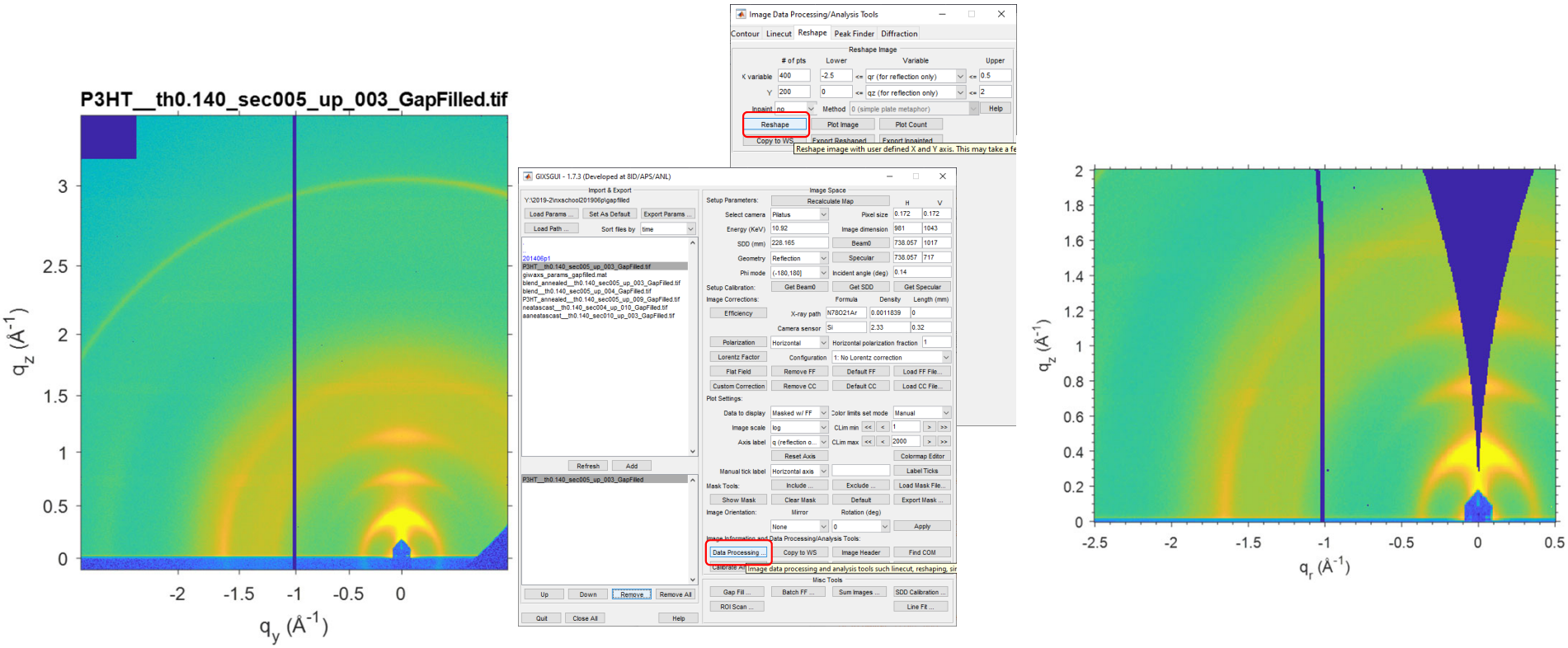
- Baker et al, Langmuir 26 9146-9151 (2010)
- Rivnay et al, Chem Rev 112, 5488-5519 (2012)



$$q_{x,y,z} = \frac{2\pi}{\lambda}\begin{bmatrix}\cos(\alpha_f)\cos(2\theta_f) - \cos(\alpha_i)\\ \cos(\alpha_f)\sin(2\theta_f)\\ \sin(\alpha_f) + \sin(\alpha_i)\end{bmatrix} \quad (1)$$

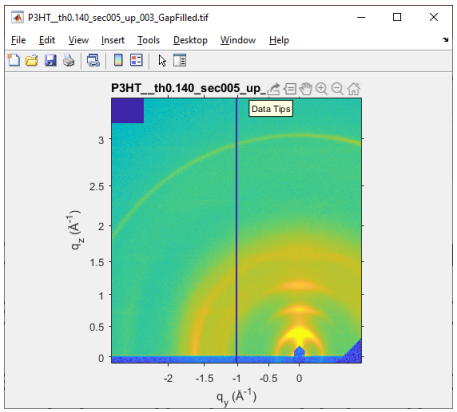
"A. Meyer, Institute of Physical Chemistry, University of Hamburg, http://www.gisaxs.de"

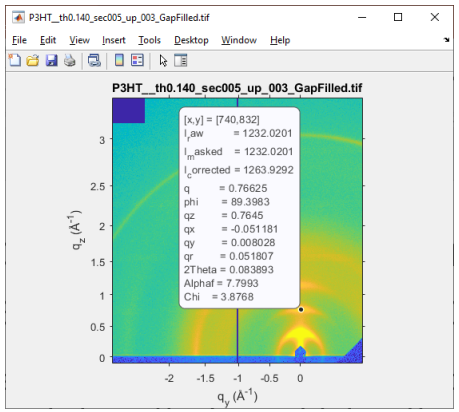
Q: How do I show GIWAXS data with the missing wedge along q_z?

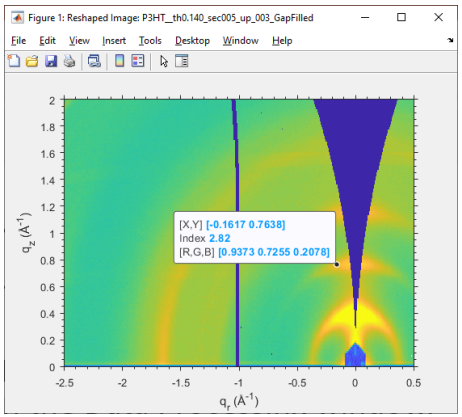


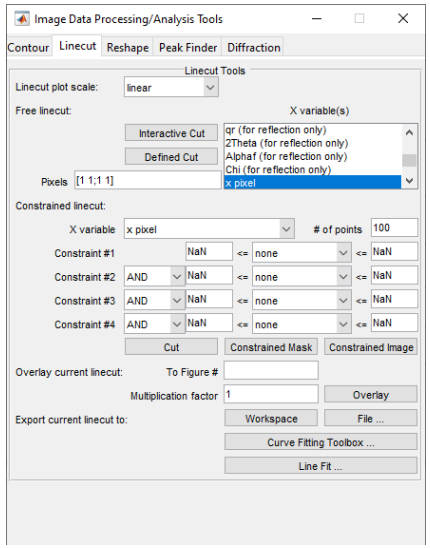
Q: should the 2D data be in the qz vs. qr format before doing any line cuts etc?

- A: No. The reshaping is only for display purposes. All linecuts are handled properly from the Linecut tab in the Data Processing window. The data cursor shows that GIXSGUI has mapped the values of several variables onto the 2D data. The reshaped data does not retain this information.



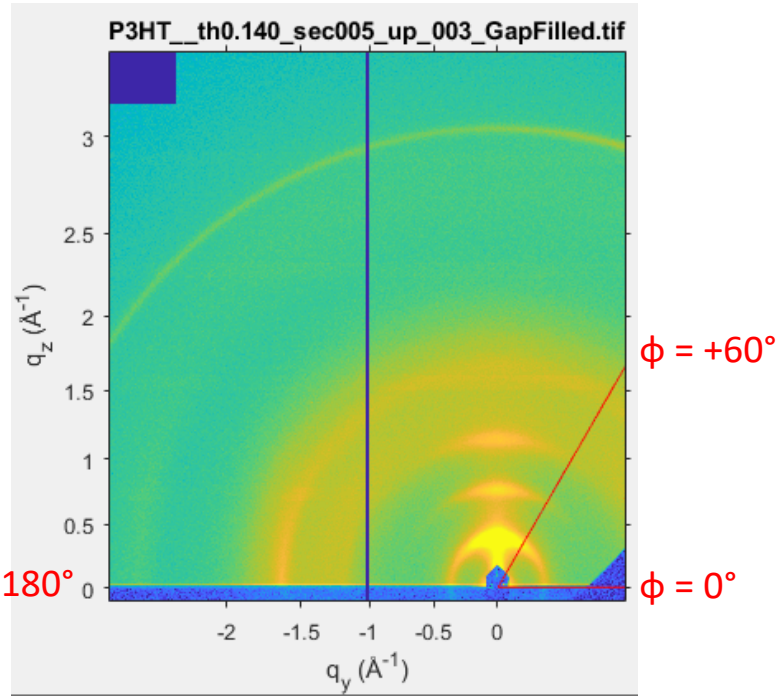






Note the difference between the azimuthal/polar angles phi (ϕ) and chi (χ).

ϕ: polar angle in the detector plane



χ: polar angle in the q_z-q_r plane