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Manual of Red2D

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This is a small package for Igor Pro to reduce 2D elastic scattering data to 1D I-q or I-2θ profiles. This package is suitable for light users who focus on simple data reduction, including time, transmittance correction etc.. For more comprehensive data reduction, I recommend you use, *Nika*, developed by Dr. Jan Ilavsky. The accuracy of reduced 1D profiles from Red2D was confirmed by reducing the same 2D images with *Nika*.

It will be nice if you acknowledge me in your publications.

Example: The SAXS/WAXS/SANS data reduction is performed by using a reduction package Red2D (https://github.com/hurxl/Red2D) on a data analysis software Igor Pro.

Requirements:

- Igor Pro 8.0 or latter by WaveMetrics
- This package has been tested on MacOS Catalina and Windows 10.
- Red2D package 2.0.0 and newer cannot handle 1D data reduced with older Red2D packages because I have changed the naming rule of 1D waves to improve the compatibility with other software and packages, such as NSIT model fits package and SasView.

How to install

1. Download the package from GitHub and unzip the file.
   https://github.com/hurxl/Red2D/blob/master/README.md
2. Move the unzipped folder into your local WaveMetrics folder.
   e.g. ~/Documents/WaveMetrics/Igor Pro 8 User Files/Igor Procedures
3. Launch Igor Pro application and you will see a “Red2D” tab.

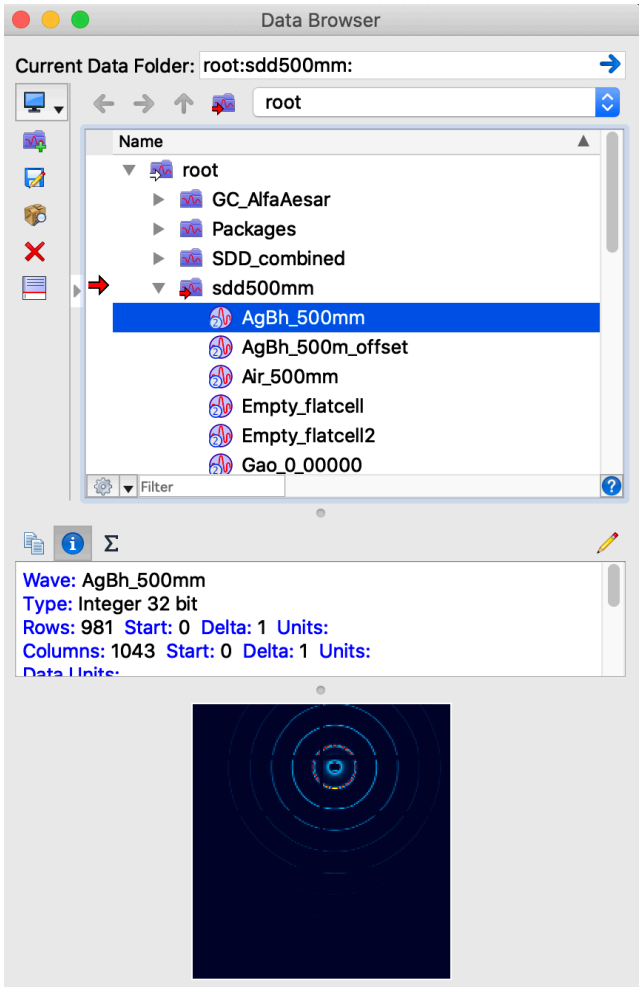
Common tips

1) Use data browser (Command + B) to organize your data.
2) Make different datafolders for different configurations (SDD, beam center, etc.).
3) Set datafolder to where the target data exist. The data in child folder will not be used.
   a) e.g. display images, mask image, circular average

      → set datafolder to where the images exist.

   b) Display 1D, normalization 1D

      → set datafolder to where1D data exist.
4) You can close any window, e.g. graph, table, panel, when you want.

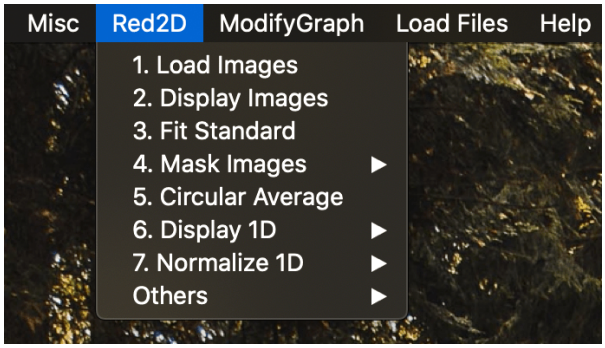


How to use

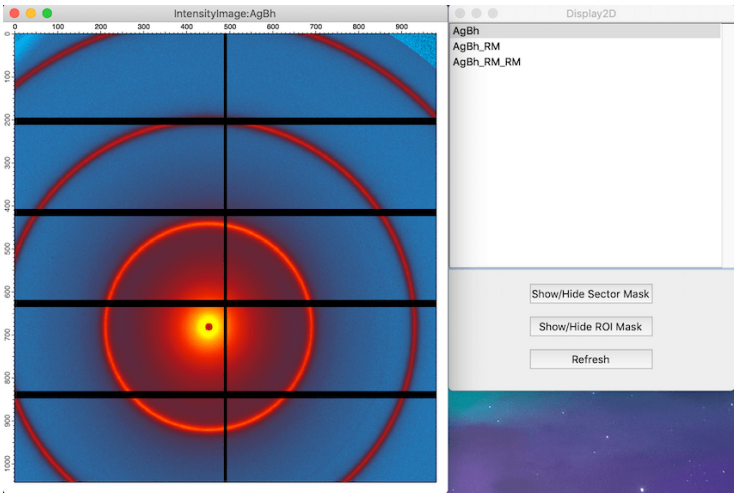
1. Click "Load Images" and select all the images you want to load.

Tips:

1) The files are loaded in the order as you selected.
2) The name of images will be used as the wave names. Therefore, you need to follow Igor Pro wave name rules:
   a) Starts from an alphabet. Do not start from a number.
   b) No space
   c) No symbol except underscore



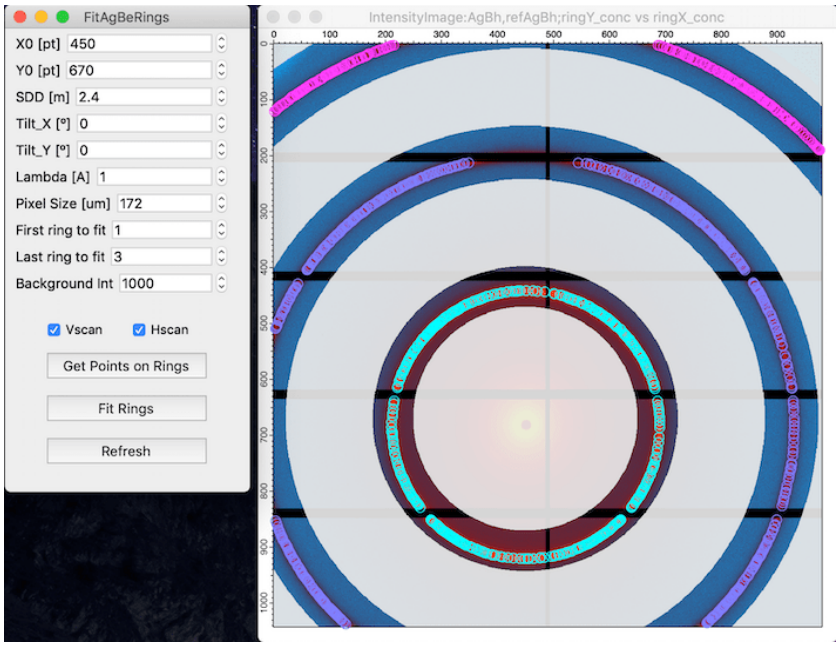
2. Use "Display Images" to show 2D images.

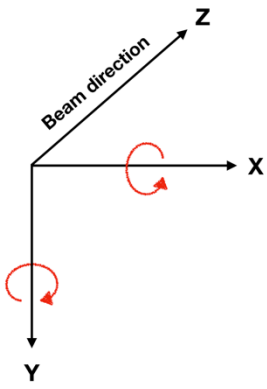


Tips:

1) Set datafolder to where the images exist.
2) Click "Refresh" button to get the list of images in current datafolder.
   - If sector mask or ROI mask is generated, you can show and hide the masks.

3. **Fit a standard (only silver behenate available for now) to get beam center and SDD**

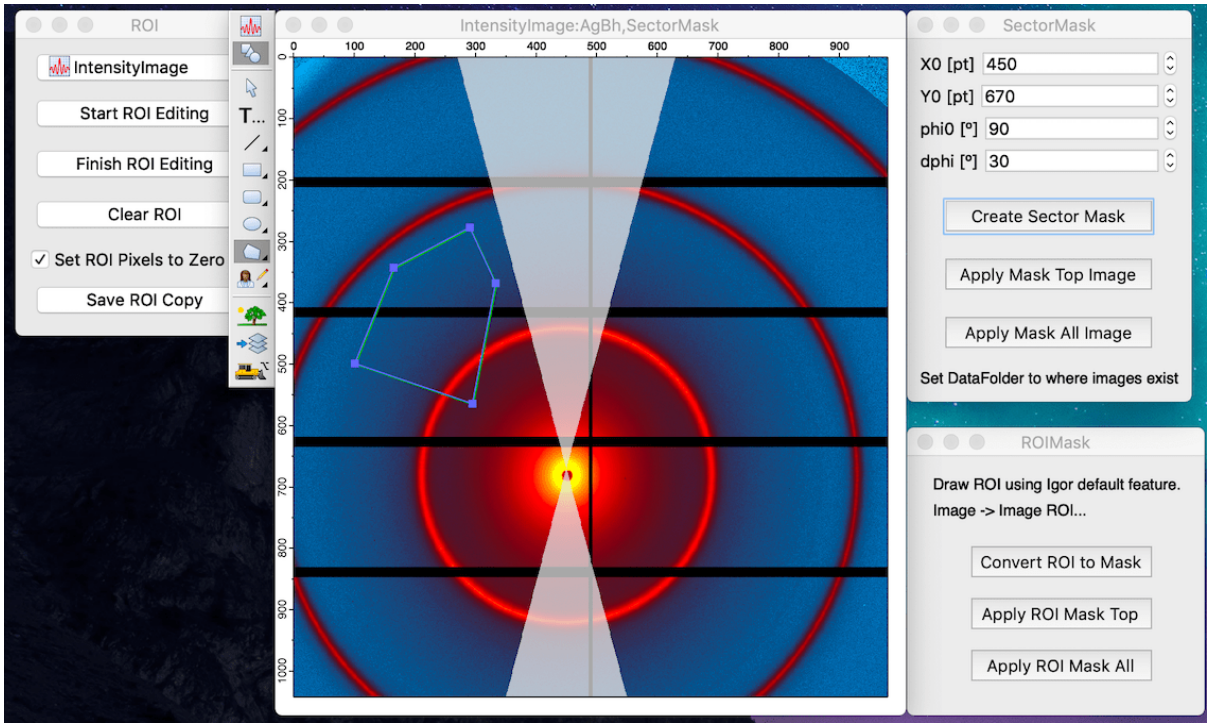




Tips:

1) Fill all the parameters. X0, Y0 are positions of the bema center. SDD is sample to detector distance. X0, Y0, SDD are fit parameters. You only need to give a guess for these parameters. However, all the other parameters, e.g. Lambda, Pixel size are independent variables and must be precise.
2) A white mask will appear based on the parameters you set.
   a) Only the non-masked pixels will be used to estimate beam center and SDD.
   b) Generally, fitting one ring is good enough.
3) Set background intensity to remove the noise and click "Get Points on Rings".
   a) Colorful points appear on the rings.
   b) If the points are not on the rings, change the background intensity then click "Get Points on Rings" again. You can also try to check/uncheck Vscan (vertical peak scan) and Hscan (horizontal peak scan).
4) Click "Fit Rings" to perform the fit.
   a) Fit result will appear in the command window of Igor Pro (Command + J). X0, Y0 and SDD will be stored as global variables in a datafolder "Red2Dpacakge".
5) Use tilt-X and tilt-Y to correct tilt angles of detector plane. We use right-hand coordinates and right-handed screws rule for tilt direction.

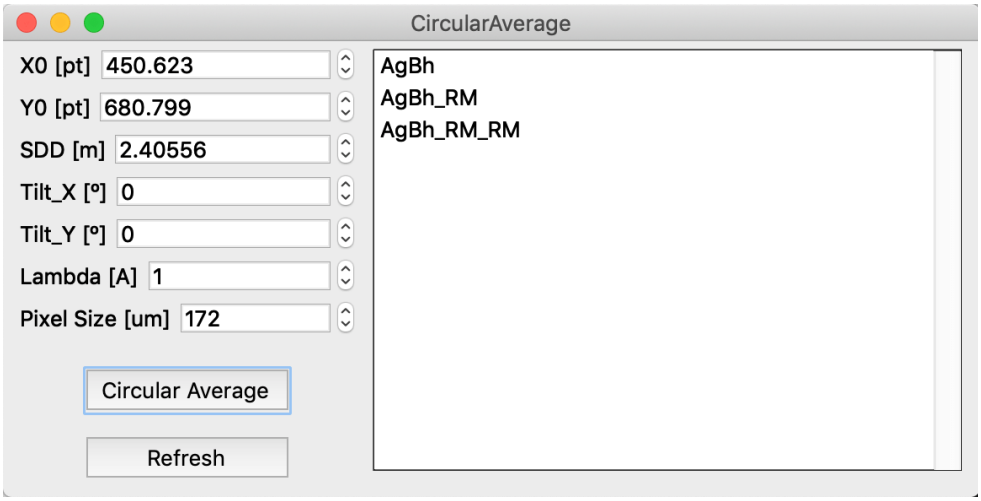
4. Create and apply sector or ROI mask to images [optional]



Tips:

1) X0, Y0 will be automatically filled if you have performed “Fit Standard”.
2) phi0 is the starting angle of the sectormask and dphi (i.e. Δphi) denotes the range.
3) “Create Sector Mask” generates a sector mask.
4) “Apply Mask” creates masked images. The masked image will be saved in a separate datafolder. The original image will not be changed.
5) To use ROI mask, you need draw a ROI first by select “Image” ≫”Image ROI…” in the Igor menu bar. Then click “Convert ROI to Mask”.
6) You can apply another mask to an already masked image.
7) The pixels with negative values, e.g. space between panels, dead pixels, will be automatically removed when performing circular average. You do not have make a mask for the spaces between panels.

5. Circular Average [Panel]



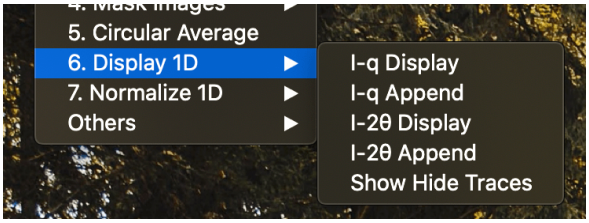
Tips:

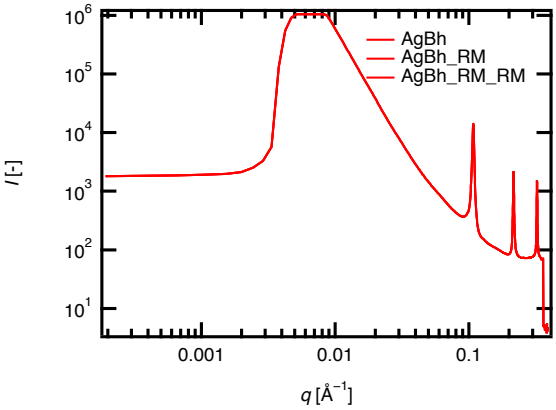
1) Click "Refresh" to get the image list in current datafolder and corresponding parameters (X0, Y0 etc.).
2) The parameters will be automatically filled if you have performed "Fit Standard".
3) Click "Circular Average" and a new datafolder "Iq1D…" will be generated, which contains the reduced 1D data.
4) Reduced 1D data follows the name rule of NIST data analysis package (NCNR_SANS_package:https://www.ncnr.nist.gov/programs/sans/data/red_anal.html). You can use the NIST package to perform basic model fits on your 1D data.
5) Other notes
   a) Negative pixels will be automatically removed. You do not need to make a mask for panel spaces, where the intensity is generally -1.
   b) Relative pixel area difference, which depends on scattering angle and SDD, is properly corrected based on B. R. Pauw, Everything SAXS: small-angle scattering pattern collection and correction. J Phys Condens Matter. 25, 383201 (2013).

6. Click Display 1D and append 1D to show 1D data in a graph.

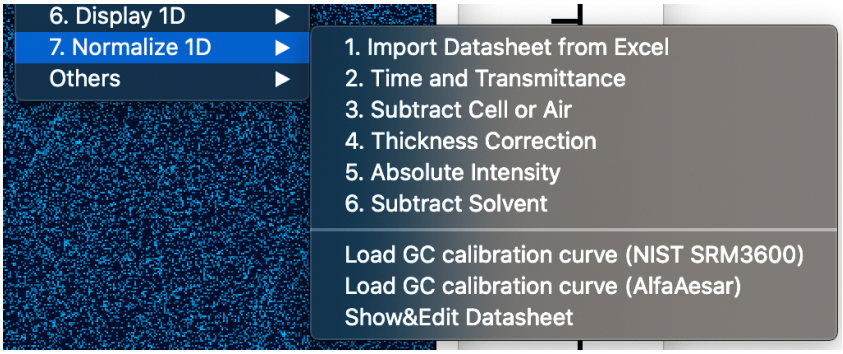
Tips:

1) Set the datafolder to where the 1D data exist then click display or append 1D.
2) I vs 2θ is supported.
3) "Show Hide Traces" is a handy tool to show and hide traces on graph.





7. Normalize 1D data



Datasheet_sdd500mm:Datasheet.ld

R0 Label

Row	Datasheet.I	Datasheet[][0].	Datasheet[][1].	Datasheet[][2].	Datasheet[][3].	Datasheet[][4].	Datasheet[][5].	Datasheet[][6].	Datasheet[][7].
	x y	ImageName	Time_s	Trans	Thick_cm	Comment0	Comment1	Comment2	Comment3
0		AgBh_500m_c	5.0000489999	0.2818788161	0.1	AgBh			
1		AgBh_500mm	5.0000489999	1.1363911901	0.1	AgBh_pf			
2		Air_500mm	300.002971	1	1	Air			
3		Empty_flatcell	300.00301999	0.5385910995	1	Empty_flatcell	streak at low q	not centerized	
4		Empty_flatcell:	300.00303700	0.5355126223	1	Empty_flatcell			
5		Gao_0_00000	120.00121799	0.3200109782	0.1	M2C120_air			

Tips:

1) First of all, set current datafolder to where the 1D data exist.
2) Create a datasheet using Excel and import that using "Import Datasheet from Excel".
   a) A template excel sheet is included in the zip file that you downloaded.

b) The first row in excel sheet is the header. Only the header named with “ImageName”, “Time_s”, “Trans”, “Thick_cm” and “Comment0-3” will be imported.

c) ImageName is the name of images that you loaded in the beginning.

d) I recommend storing the sample names in Comment0. Comment0-2 are in text format. So, you do not have to follow Igor Pro wave name rule and can name it as you like.

e) “Trans”, “Tims_s” and “Thcik_cm” must be filled. If you want to skip these normalizations for a sample, type “1” in these cells.

f) You can manually fill the datasheet if you want.

3) After datasheet is properly filled, you can start normalizing your 1D data by using “1. Time and Transmittance”, “2. Subtract Cell or Air.”, …

4) Notes for absolute intensity correction:

(i) Load calibration curve of glassy carbon

(ii) Calculate a ratio of [your data]/[Calibration curve]

(iii) Click “Absolute Intensity” and type the intensity ratio to perform the correction.

Appendix

Red2Dpackage folder

This datafolder will be automatically created in a directory where your images are stored. This datafolder stores global values, strings and waves used in background process. You can edit these values by yourself when necessary.

Others

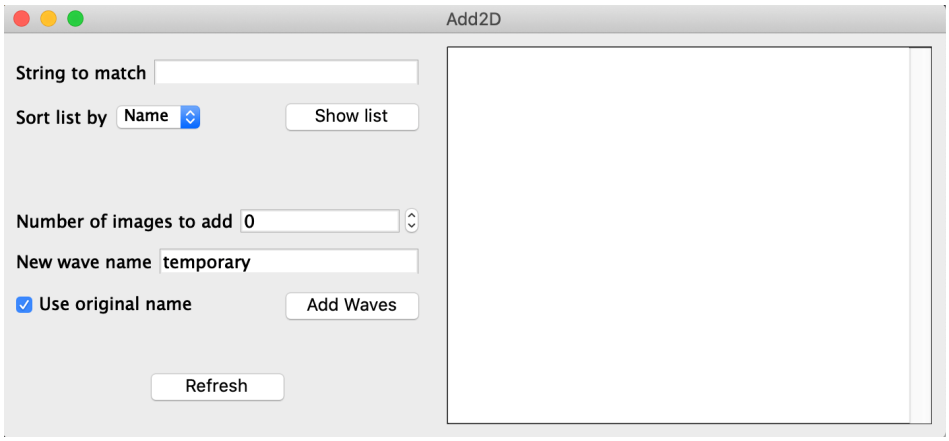
You can find several useful tools in “Others”.

- Load All 2D Images

Load all 2D images from selected folder and all the subfolders.

- Add 2D Images

You can add multiple images into 1 image by using “Add 2D images”.

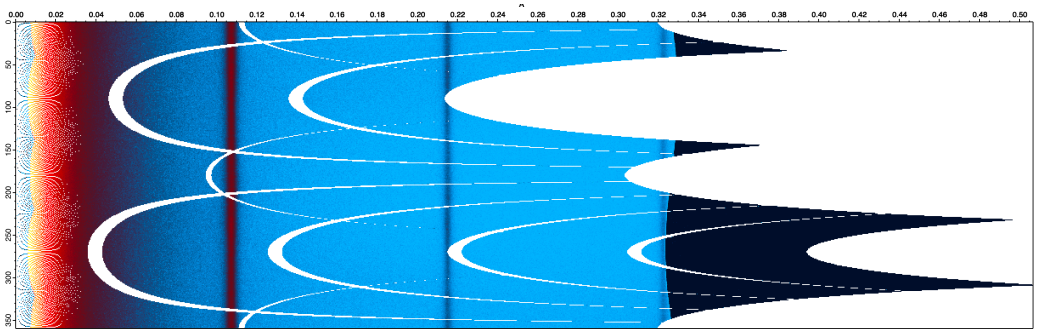


1) String to match: the common part of the image names. Use an asterisk (*) as a wildcard, e.g. use “*abc*” to get “testabctest”, use “*” to get all images.
2) Select a sort by list option, then click show list.

3) Numbers of images to add: the number of images to add together. e.g. If you have 10 images and "Numbers to Combine" = 2, then 5 added images will be generated.
4) New wave name: new name of added images. When multiple images generated, a sequential number will be added at the end of the names.
5) When "use original name" is selected, the 1st name in each group will be used as the new image name. The name in the "New wave name" will be overwritten.
6) Data will be saved in a datafolder "Added".

- Convert to azimuthal-q coordinates

You can convert normal X-Y Images to azimuthal degree vs q images as shown below. The vertical axis shows the azimuthal degree and the horizontal axis is q.



- Logarithmic 1D resampling

Resample or bin your 1D data on a logarithmic scale

- Shorten all 1D in current datafolder

You can delete unnecessary points from your reduced 1D waves. Note that this process is irreversible. You may want to save your original 1D data somewhere.

- Combine 1D from different SDD

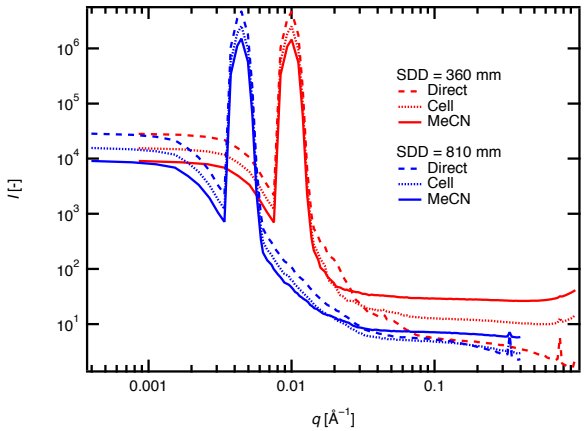
You can combine 1D data measured at different SDDs into a combined wave.

- Export 1D with ImageName
- Export 1D with SampleName

Export reduced 1D data in current datafolder as general text files.

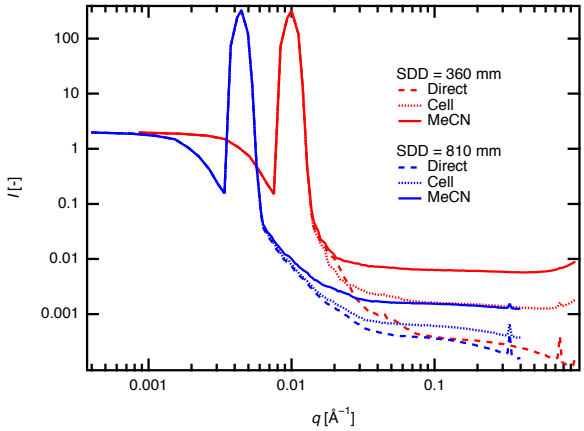
Screenshots of step by step data normalization

Raw



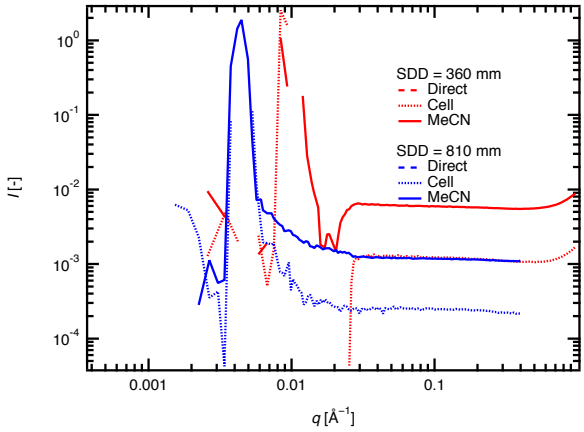
*In above graph, the intensity is displayed per pixel. In the latest version, the intensity is displayed per solid angle.

Time and transmittance corrected

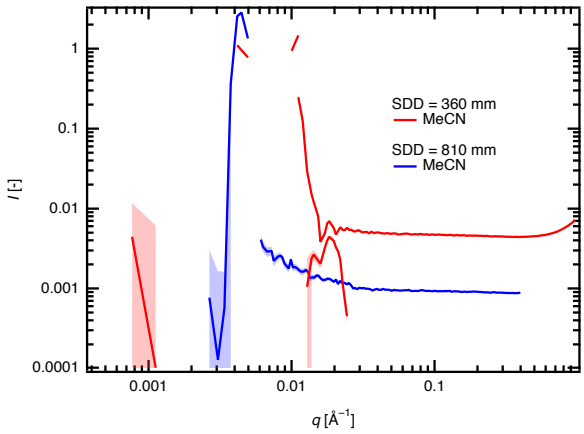


* The incident beam intensities of two different SDD overlap because the intensity is displayed per pixel. In the latest version, the intensity is displayed per solid angle and the incident bema intensities do not overlap for different SDDs.

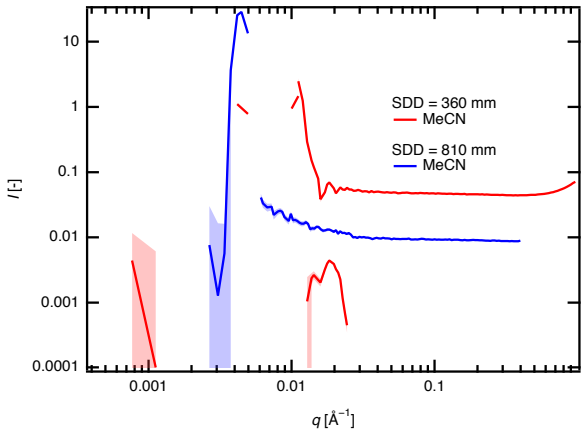
Air(Direct beam) subtracted



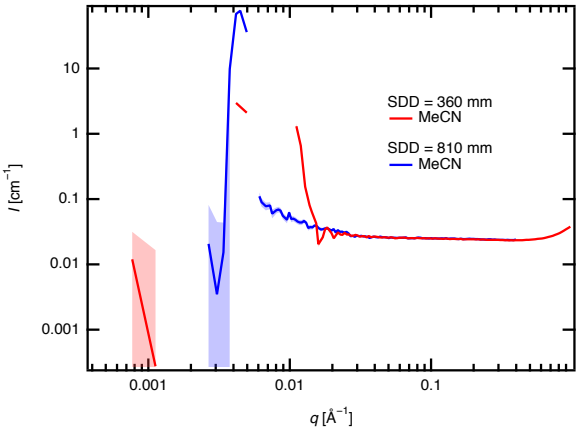
Cell subtracted



Sample thickness corrected



Absolute intensity corrected, using glassy carbon



Peak position of standards

$$q = \frac{2\pi}{d}, \qquad q = \frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right) \; or \; in \; \theta = 2\theta' \; q = \frac{4\pi}{\lambda}\sin(\theta')$$

Table. Silver behenate

PEAK NUMBER	D-SPACING [Å]	Q [Å^{-1}]
1	58.38	0.10762565
2	29.19	0.2152513
3	19.46	0.32287694
4	14.595	0.43050259
5	11.676	0.53812824
6	9.73	0.64575389
7	8.34	0.75337953
8	7.2975	0.86100518
9	6.48666667	0.96863083
10	5.838	1.07625648
11	5.30727273	1.18388212
12	4.865	1.29150777
DOUBLET		1.369
DOUBLET		1.387
13	4.49076923	1.39913342

Silver behenate d-spacing of (001) 58.38Å from Huang, T. C.; Toraya, H.; Blanton, T. N.; Wu, Y. X-Ray Powder Diffraction Analysis of Silver Behenate, a Possible Low-Angle Diffraction Standard. J Appl Crystallogr 1993, 26, 180–184

Table. Si

PEAK NUMBER	2Θ' (Λ 1.5405Å)	Q [Å^{-1}]
1	28.441	2.00376238
2	47.301	3.27217002
3	56.12	3.83694455
4	69.127	4.62753269
5	76.373	5.04274818
6	88.026	5.66754871
7	94.947	6.01130427
8	106.702	6.54429257
9	114.085	6.84419552
10	127.535	7.31674949
11	136.882	7.5861853

Basic knowledge

1) The error of intensity at each pixel is calculated based on Poisson probability distribution (e = I^0.5) and then averaged for multiple pixels with the same q value using error propagation equations (e = (e1^2 + e2^2 +…)^0.5/number of pixels = (I1 + I2 +…)^0.5/number of pixels). The error propagation is also used in normalizing 1D data.

2) The normalization of 1D data is performed based on the equations below.

$$\frac{d\Sigma}{d\Omega}(q)_{sample} = \left(\frac{I(q)_{sample\&cell}}{Time \cdot Trans} - \frac{I(q)_{cell}}{Time \cdot Trans}\right) \cdot \frac{1}{Sample\ thickness} \cdot \frac{1}{Instrumentatino\ factor}$$

$$\frac{d\Sigma}{d\Omega}(q)_{sample} = \phi \frac{d\Sigma}{d\Omega}(q)_{polymer} + (1-\phi)\frac{d\Sigma}{d\Omega}(q)_{solvent}$$

Instrumentation factor refers to beam size, incident beam flux, detector sensitivity, etc.. Instrumentation factor is irrelevant to sample and can be corrected by using a standard sample, e.g. glassy carbon.