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Manual of Red2D

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Red2D 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 using *Nika*, developed by Dr. Jan Ilavsky. I have confirmed the accuracy of reduced 1D profiles from Red2D 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 was performed using a reduction package Red2D (https://github.com/hurxl/Red2D) on a data analysis software Igor Pro.

Requirements:

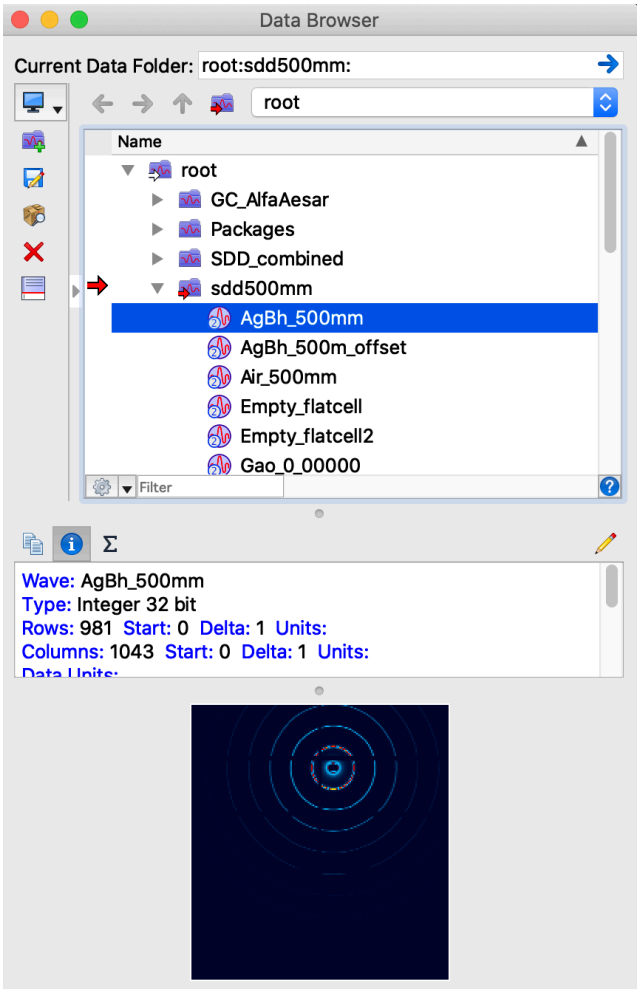
- Igor Pro 8.0 or later by Wave Metrics
- This package has been tested on macOS Big Sur and Windows 10.
- Red2D package 2.0.0 and newer cannot handle 1D data reduced with previous packages because I changed the naming rule of 1D waves to improve the compatibility with other software and packages, such 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) Create different datafolders for different configurations (SDD, beam center, etc.).
3) Use "Set Current Datafolder" to make the target datafolder active. A red arrow will appear on the left of the datafolder when the folder is activated. Only the waves stored in the active datafolder will be processed and displayed.
4) You can close any graphs, tables, panels whenever you want.
5) Do not use numbers for the wave name because Igor does not like it; do not use "_s", "_i", and "_q" because they have special meaning in this package.

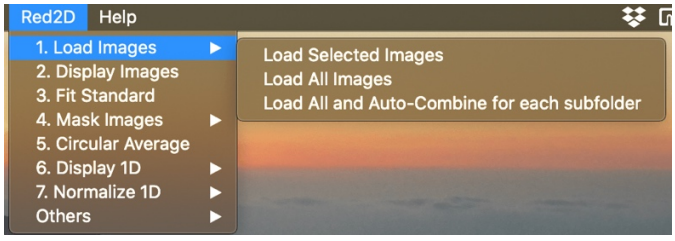


How to use

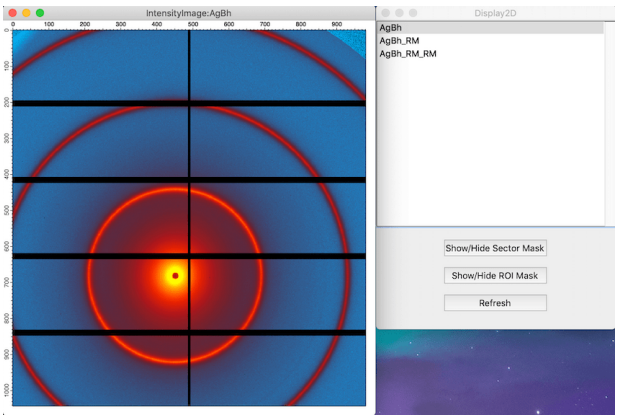
1. Click "Load Images" and select all the images you want to load.

Tips:

1) You can load all images in a folder, including its sub-directories, using "Load All Images in Selected Folder".
2) "Load All and Auto-Combine for each subfolder" is similar to "Load All Images" but it will add all images from the same subfolders to make one new image. This feature is useful when you take a series of images but want to add them together.
3) The name of images will be used as the wave names. Therefore, you need to follow Igor Pro wave name rules:
   a) Do not start from a number. Names should begin with an alphabet.
   b) Do not use space and symbols for wave names except the underscore.
   c) Do not use "_s" "_i" and "_q" as the suffix of the wave names because they have special meaning in this package.



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

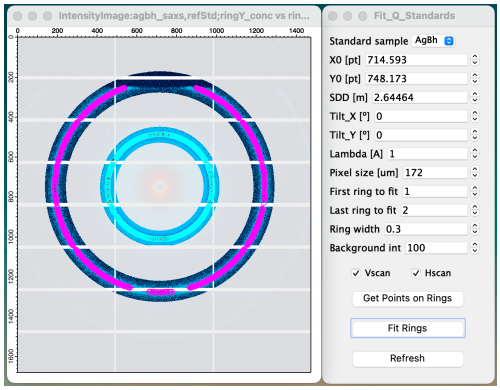


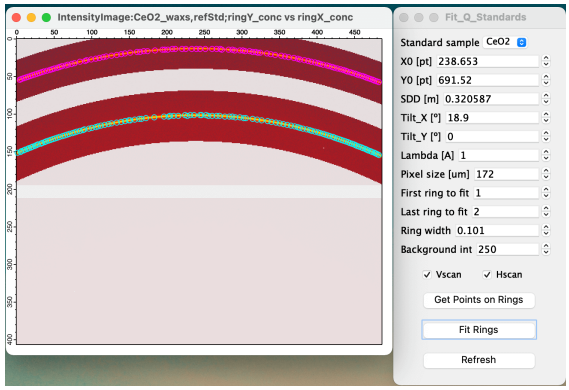
Tips:

1) Set datafolder to where the image data exist.
2) Click the "Refresh" button to get the list of images in the current datafolder.

- If a sector mask or ROI mask is generated, you can show and hide the masks.

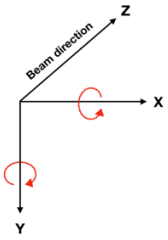
3. **Fit a standard (only silver behenate available for now) to get beam center and SDD**



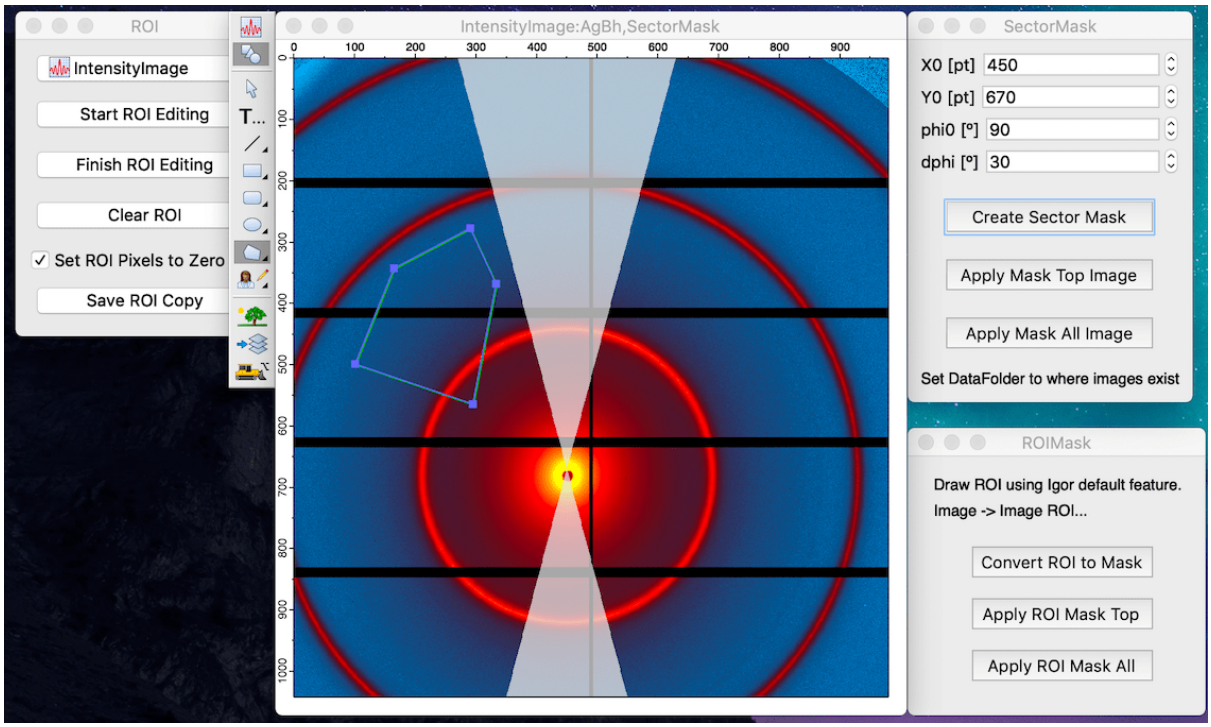


Tips:

1) Select the standard sample.
2) Give an initial guess for beam center (X0, Y0) and sample to detector distance (SDD). X0, Y0 and SDD are fit parameters.
3) Fill up the other information with accurate values.
4) A white mask with transparent rings will appear. The transparent rings indicate the rough position of the scattering peak rings. Change the parameters to make the transparent rings match the scattering rings of your standard sample.
5) Click "Get Points on Rings" to let Red2D find the scattering ring positions.
   a) If the points are not on the scattering peak 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) to improve finding accuracy.
6) Click "Fit Rings" to perform the fit.
   a) The fit result will be automatically stored and used in the following data reduction. The result also appears in the command window of Igor Pro (Command + J).
7) Use tilt-X and tilt-Y to correct tilt angles of the detector plane if your detector is tilted. We use right-hand coordinates, and right-handed screws rule for tilt direction (See the illustration below. The red arrows show the positive tilt angle.).



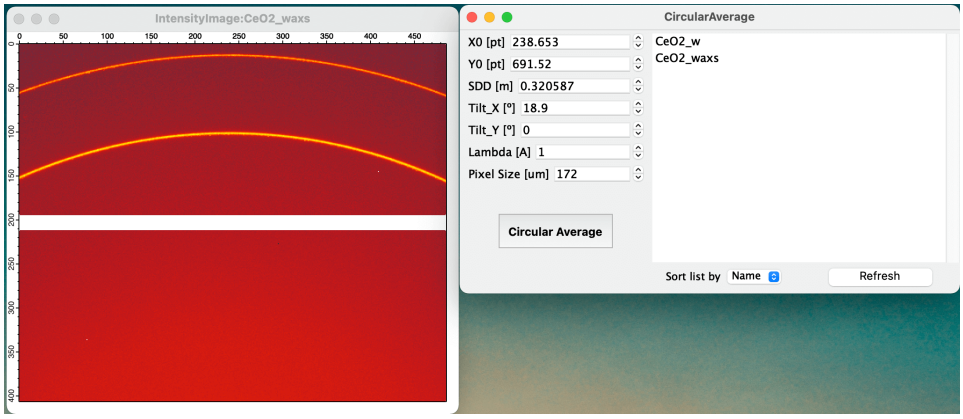
4. Create and apply sector or ROI mask to images [optional]



Tips:

1) X0, Y0 will be automatically filled if you have performed “Fit Standard.”
2) phi0 is the starting angle of the sector mask, 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 an ROI mask, you need to draw an 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 and dead pixels, will be automatically removed when performing a circular average. You do not have to make a mask for the spaces between panels.

5. Circular Average [Panel]



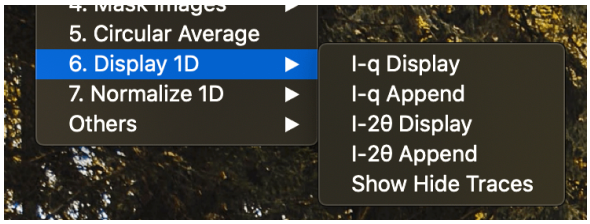
Tips:

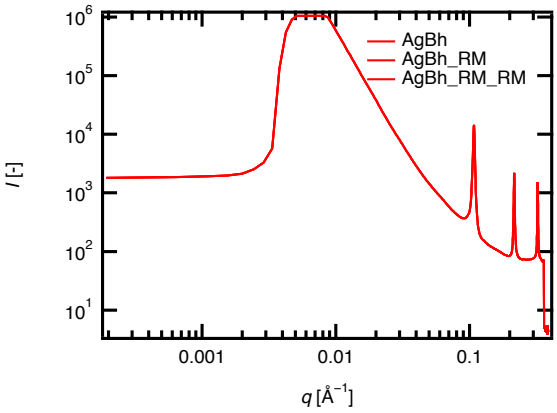
1) Click “Circular Average,” and a new datafolder, “Iq1D…” will be generated, containing the reduced 1D data.
2) Reduced 1D data follows the name rule of the NIST data analysis package (NCNR_SANS_package:https://www.ncnr.nist.gov/programs/sans/data/red_anal.html). You can use the NIST package to perform basic model fits on your 1D data.
3) Negative pixels will be automatically removed. You do not need to make a mask for panel spaces, where the intensity is generally -1.
4) 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).
5) If something wrong, click refresh.

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 a graph.





7. Datasheet

Datasheet_sdd500mm:Datasheet.ld

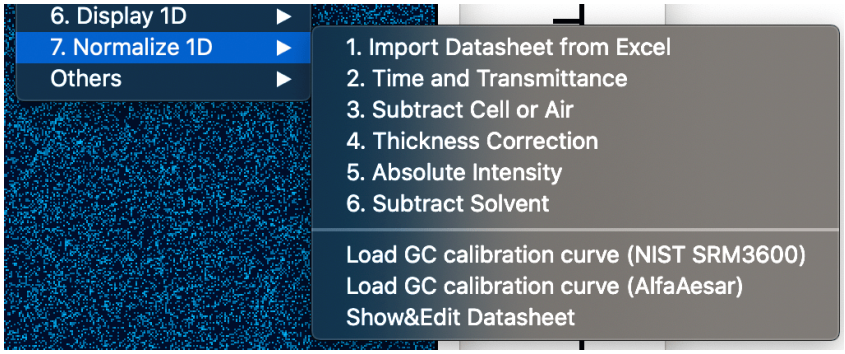
R0 Label

Row	Datasheet.I x \ y	Datasheet[][0]. ImageName	Datasheet[][1]. Time_s	Datasheet[][2]. Trans	Datasheet[][3]. Thick_cm	Datasheet[][4]. Comment0	Datasheet[][5]. Comment1	Datasheet[][6]. Comment2	Datasheet[][7]. 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) The datasheet is used to normalize 1D data or 2D images.
2) You can manually create and fill a datasheet in Igor Pro or import a prefilled datasheet from an excel sheet.
3) "Trans," "Time_s" and "Thick_cm" **must** be filled if you want to skip these normalizations for a sample, type "1" in these cells.
4) Regarding "Import Datasheet from Excel"
   a) A template excel sheet is included in the zip file that you downloaded.
   b) The first row in the 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 the images that you loaded in the beginning.

8. Normalize 1D data



1) After the datasheet is filled correctly, you can normalize your 1D data by using "1. Time and Transmittance", "2. Subtract Cell or Air.", …
2) I recommend you normalize your data following the number noted in the menu unless you truly understand what you are doing.
3) The detailed equation of normalization is described at the end of this manual.
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.

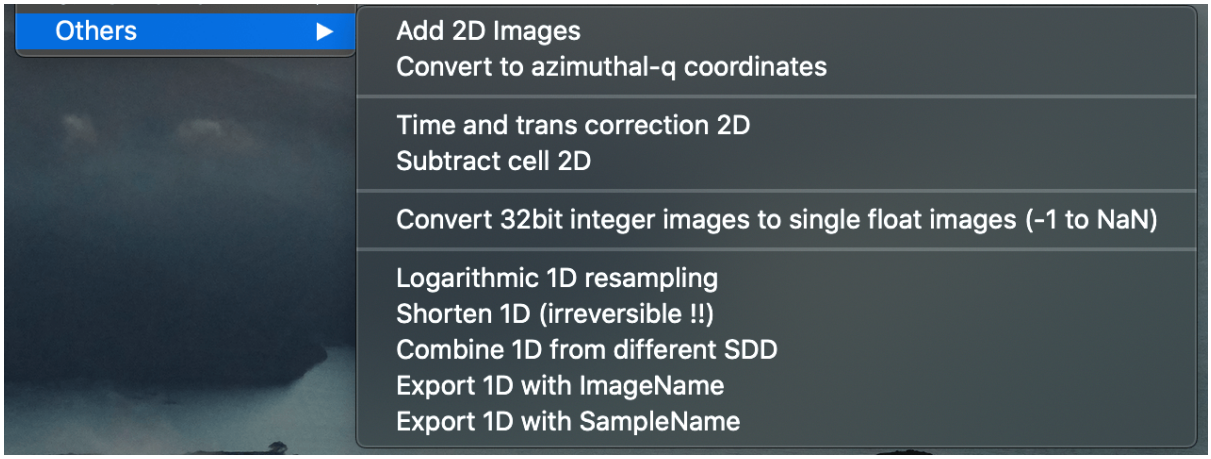
Appendix

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 processes. You can find stored parameters, such as beam center position, SDD, wavelength, pixel size, Image size, etc.

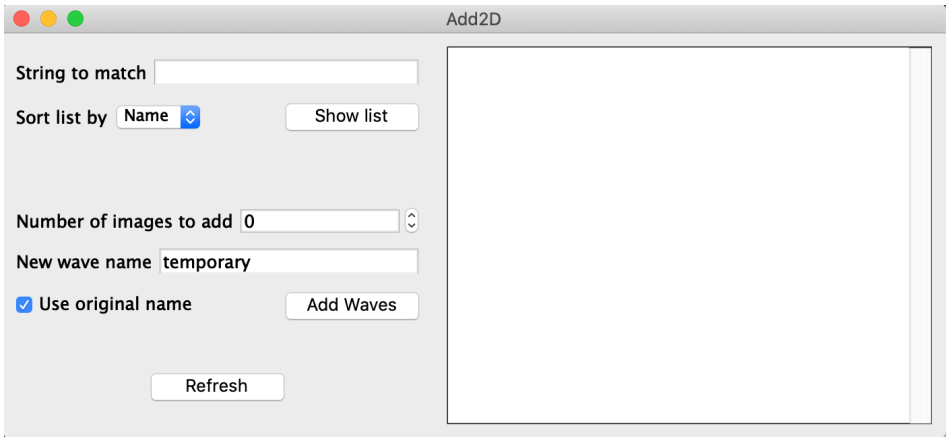
Others

You can find several helpful tools in "Others."



- Add 2D Images

You can add multiple images into one image by using "Add 2D images".

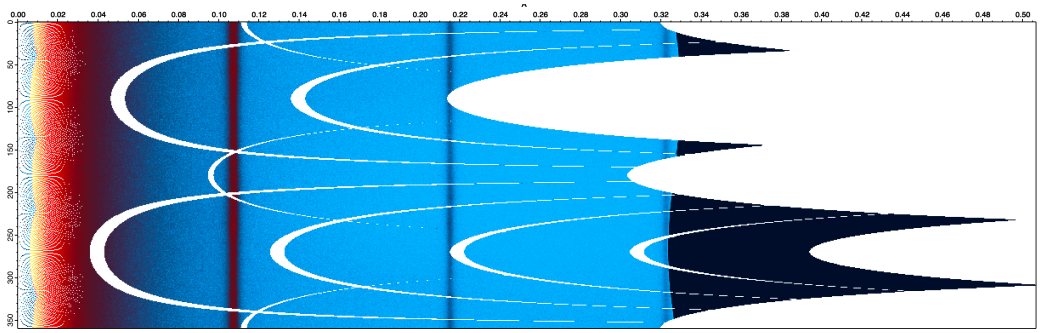


1) String to match: the common part of the image names. Use an asterisk (*) as a wildcard, e.g., use "*abc*" to get "testabctest", use "*" to get all images.
2) Select a sort by list option, then click show list.

3) Numbers of images to add: the number of images to add together. e.g., If you have ten images and "Numbers to Combine" = 2, then five added images will be generated.
4) "New wave name" is a new name for the output image. When multiple images are generated, a sequential number will be added at the end of the names.
5) When "use the 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 standard 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.

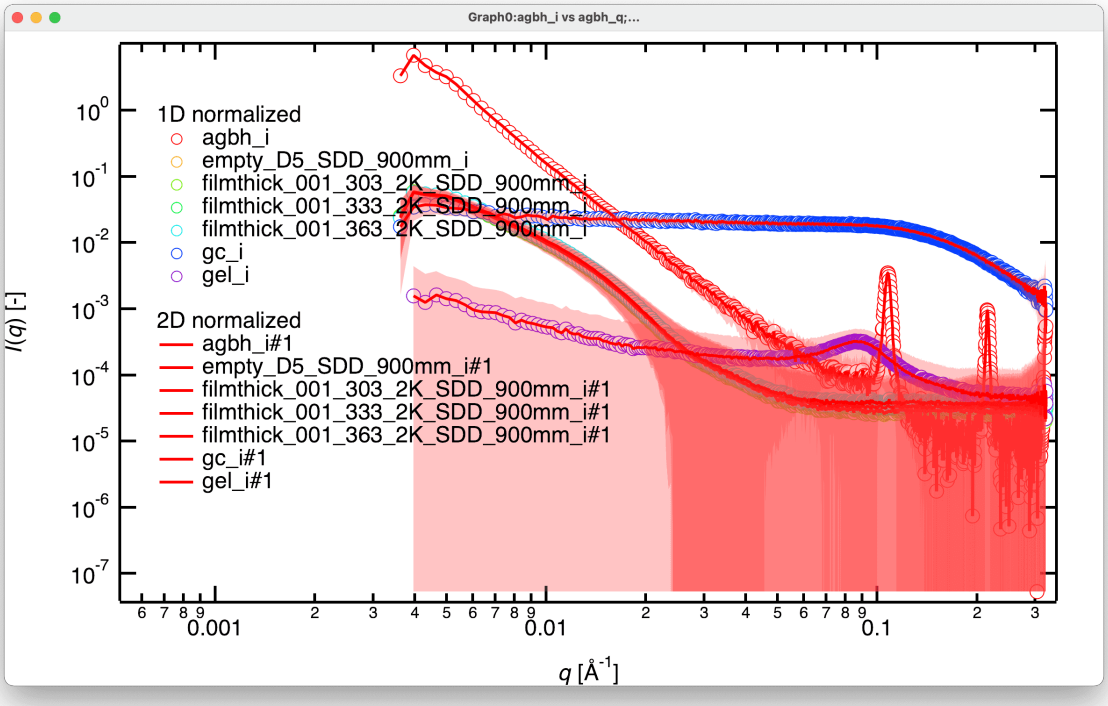


- Time and trans correction 2D

Perform the time and transmittance correction for 2D images. You have to load or create a datasheet using the functions located in the menu "1D normalization".

- Subtract cell 2D

Subtract cell or any background for 2D images. You have to load or create a datasheet using the functions located in the menu "1D normalization".



[Error report] The intensity was calculated correctly, but something wrong in the error calculation (2021-01-14).

- Convert 32bit integer images to single float (-1 to NaN)

This command converts 32-bit signed integer images to single float images in the selected datafolder. The masked pixel in 32-bit integer images, usually noted with -1, will be replaced to NaN during this process. This command is designed to maintain backward compatibility of Igor files created using old Red2D packages before v2.1.0. You do not have to run this command if you load the images using Red2D v2.1.0 or more recent.

- 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

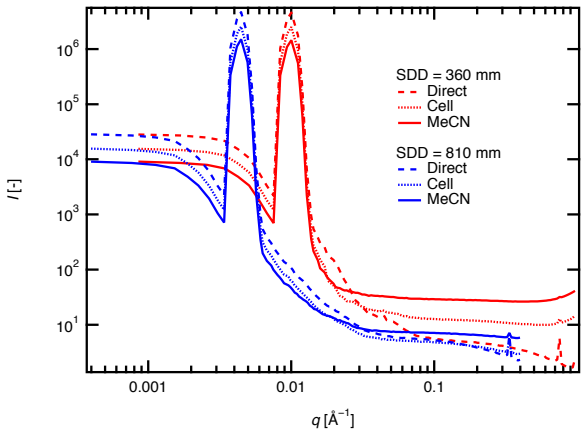
You can combine 1D data measured at different SDDs into a combined wave.

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

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

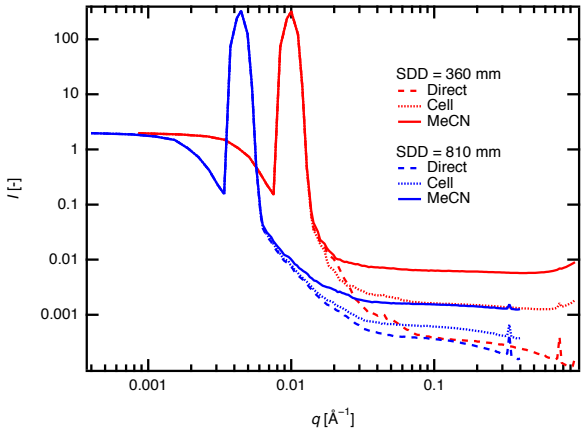
Screenshots of step by step data normalization

Raw



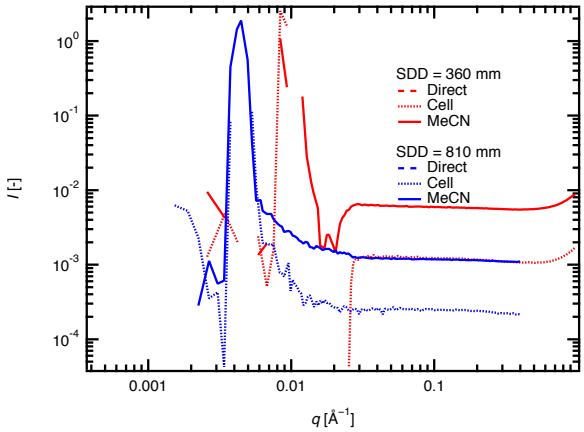
*In the above graph, the intensity is displayed per pixel. In the latest version, the intensity is shown per solid angle.

Time and transmittance corrected

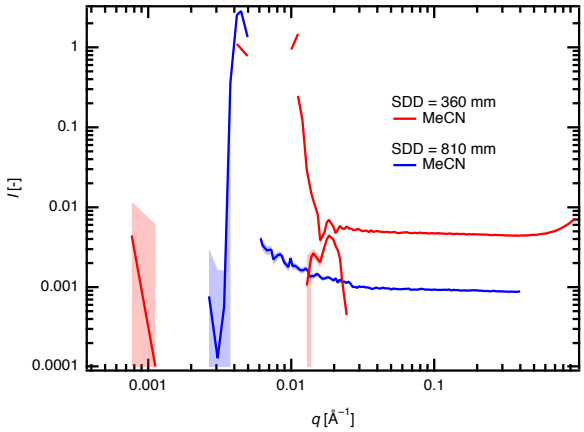


* The incident beam intensities of two distinct SDD overlap because the intensity is displayed per pixel. In the latest version, the intensity is shown per solid angle, and the incident beam intensities do not overlap for different SDDs.

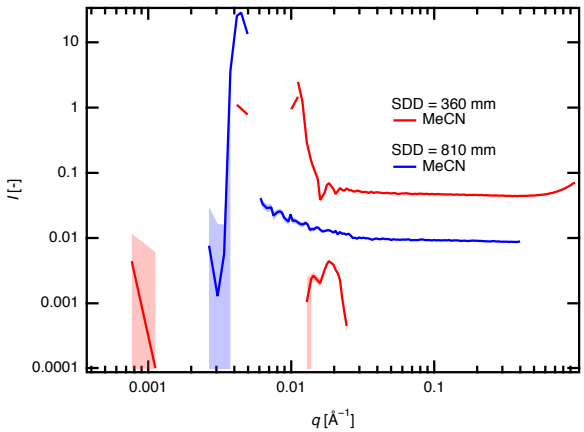
Air(Direct beam) subtracted



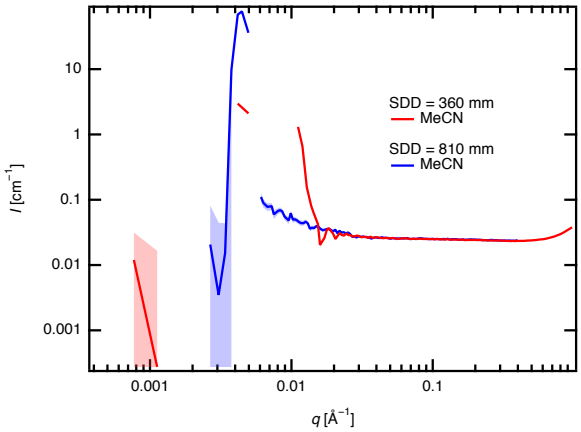
Cell subtracted



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.

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

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

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.