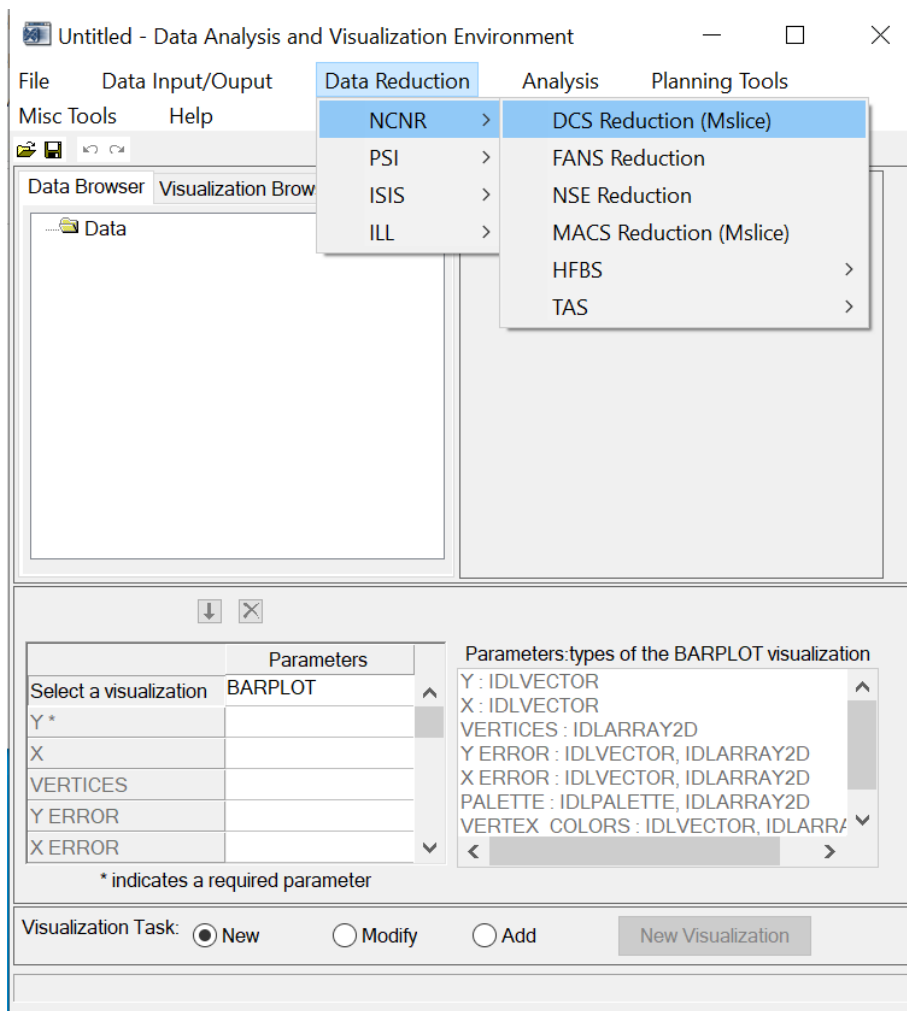


# DCS data reduction and analysis: a quick manual

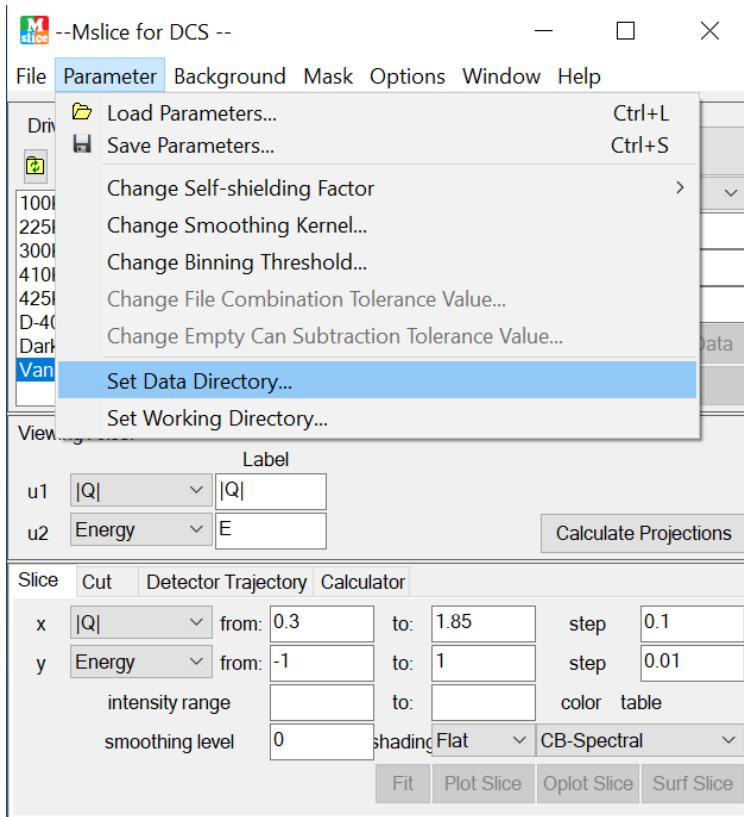
In the summer school, we are doing QENS experiments on powder samples using DCS. Here is a quick manual showing how we do data reduction and analysis. (Note that for DCS data on single crystal samples, the data reduction procedure would be significantly different.)

We use the program Mslice in the DAVE package for data reduction. (For detailed instructions on how to use Mslice, please refer to:

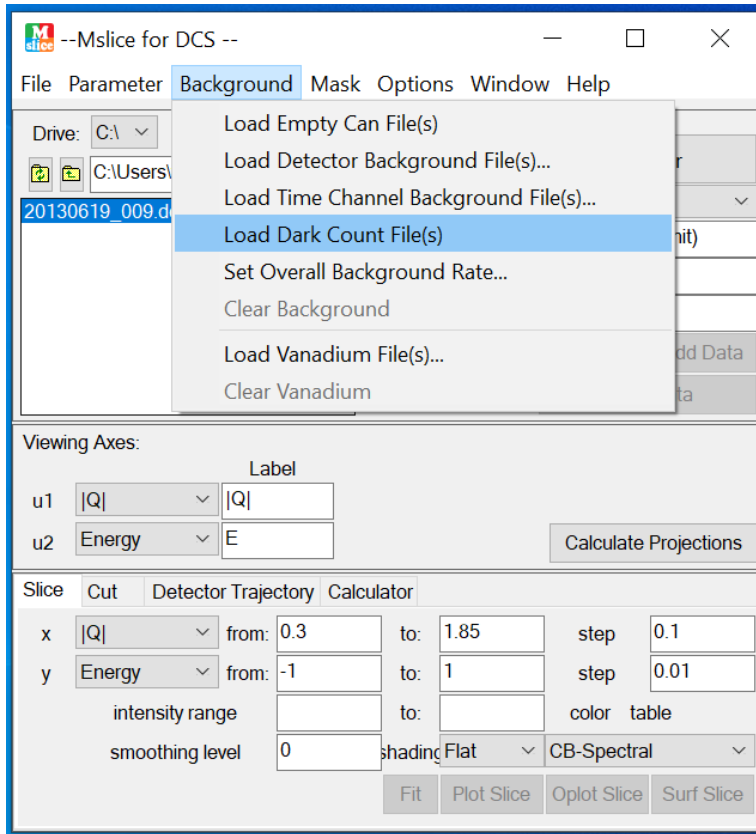
[http://www.ncnr.nist.gov/dave/documentation/dcs\\_mslice.pdf](http://www.ncnr.nist.gov/dave/documentation/dcs_mslice.pdf))



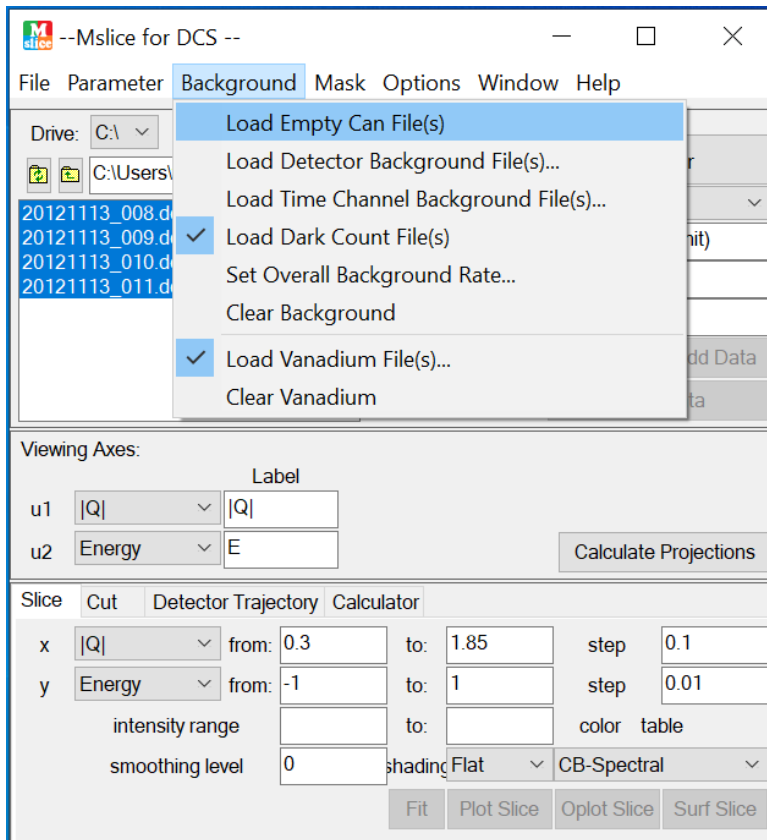
In Mslice, we can set the Data Directory and Working Directory, just for convenience.



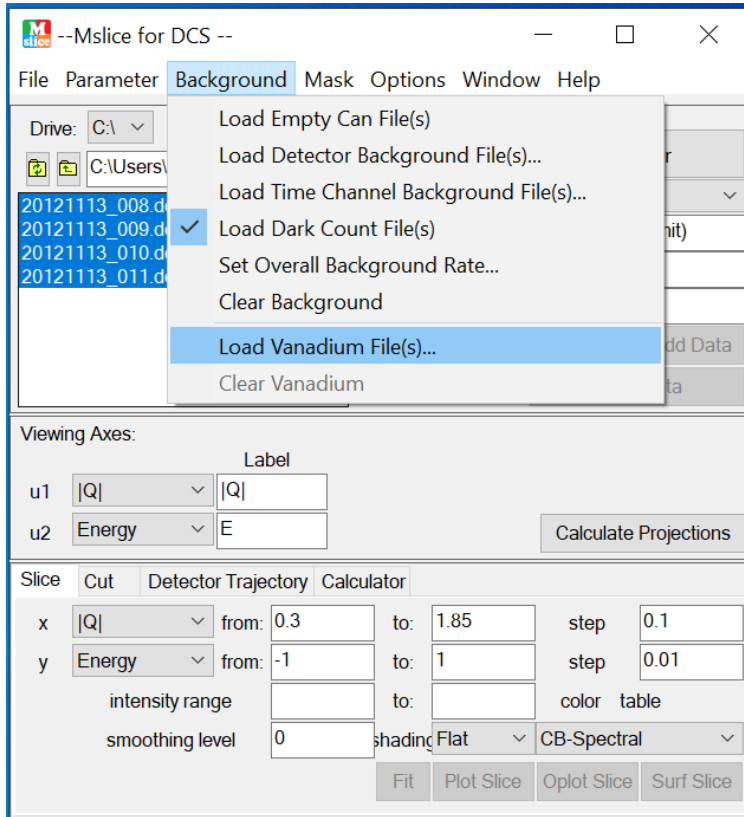
For the program to take care of background subtraction during data reduction, highlight the corresponding files and load them. Shown below is the “dark count” (beam closed) background subtraction.



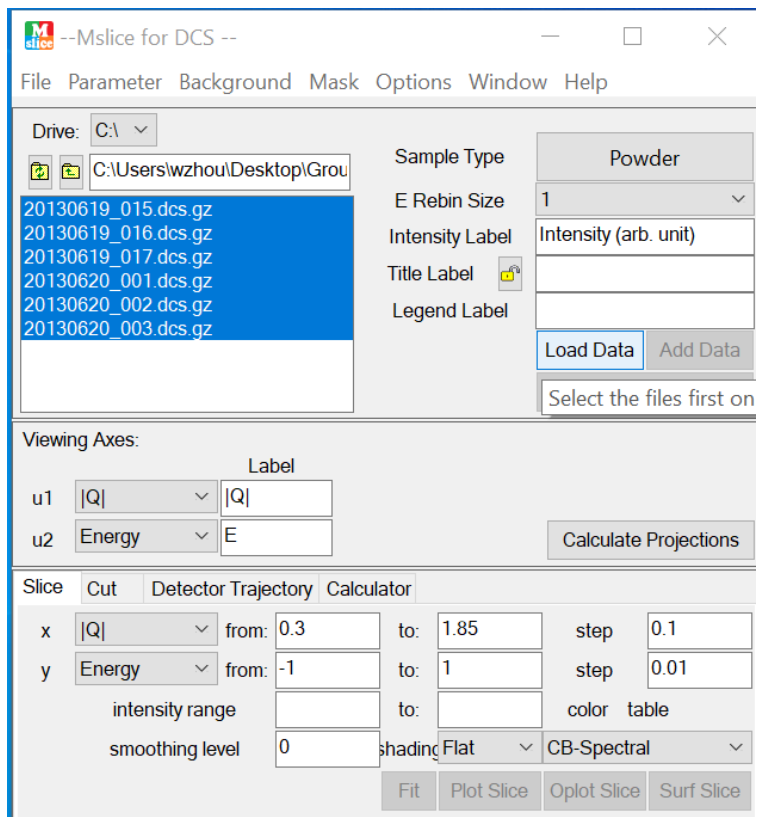
If we have data measured for the empty can, we can do empty can background subtraction, in which case we would not need the “dark count” background subtraction (the empty can data would already include dark count fast background).

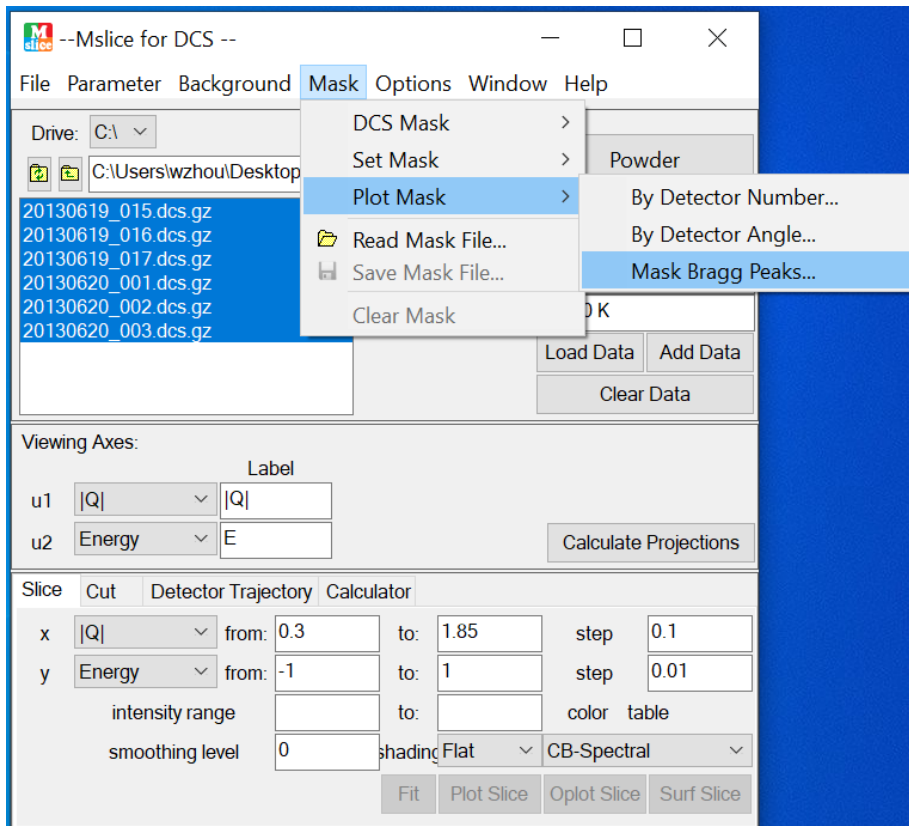


To correct detector efficiencies, we load the vanadium files.



For QENS analysis, to omit detectors that contain Bragg peak intensity, we load the sample data first, and then “Mask Bragg Peaks”.







Detector sum,

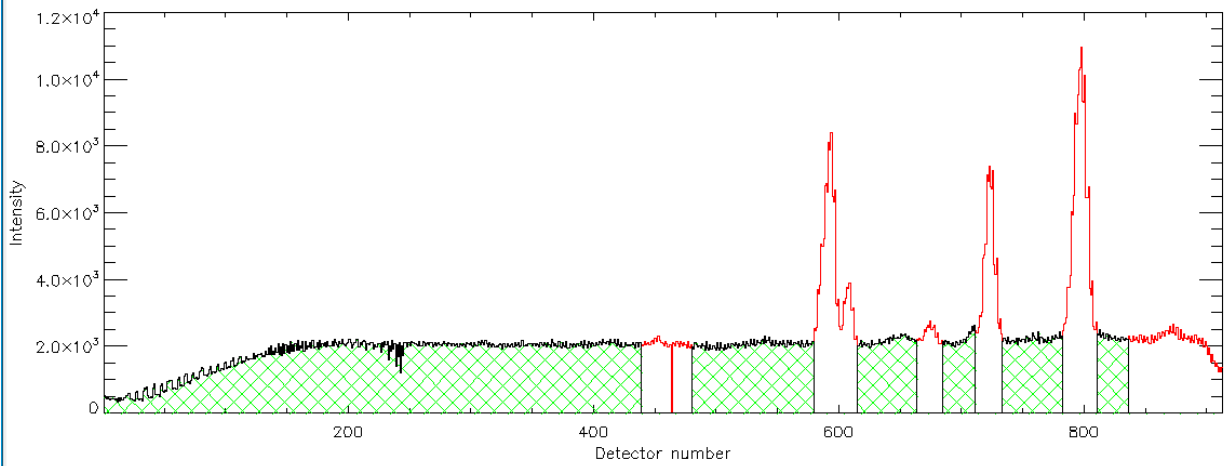


Detector 812

Intensity 2334

X ZOOM

MASK



1

913

Help

Show selected range of detectors

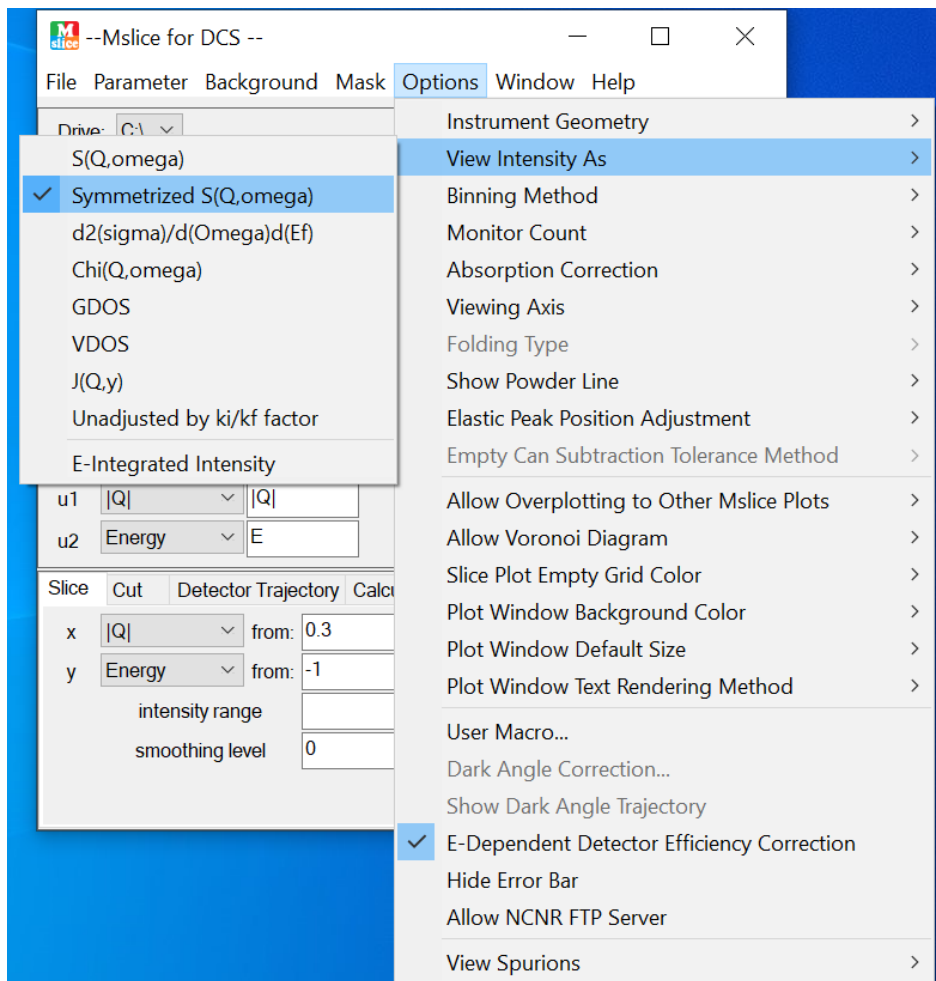
Show all detectors

Undo zoom

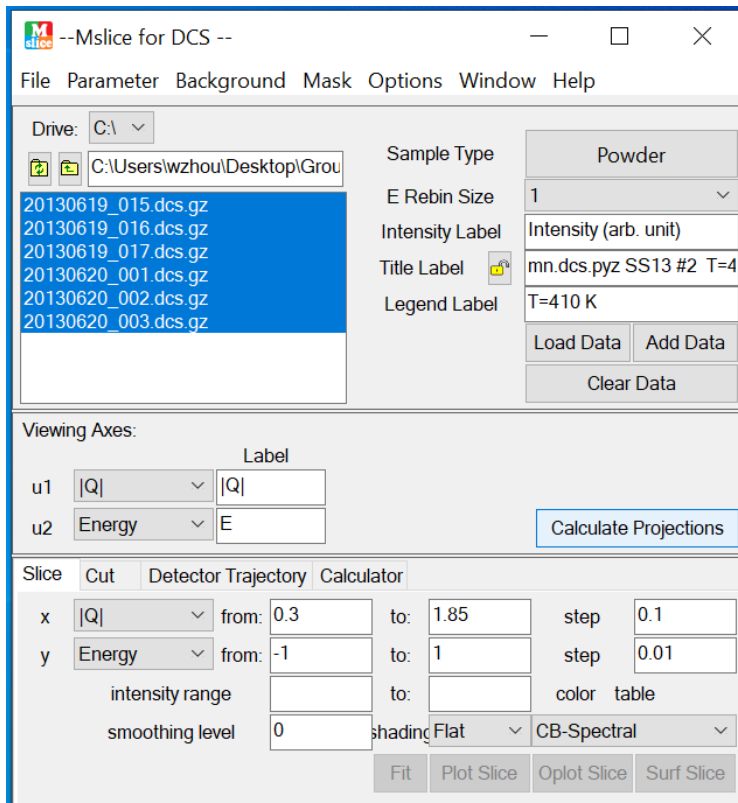
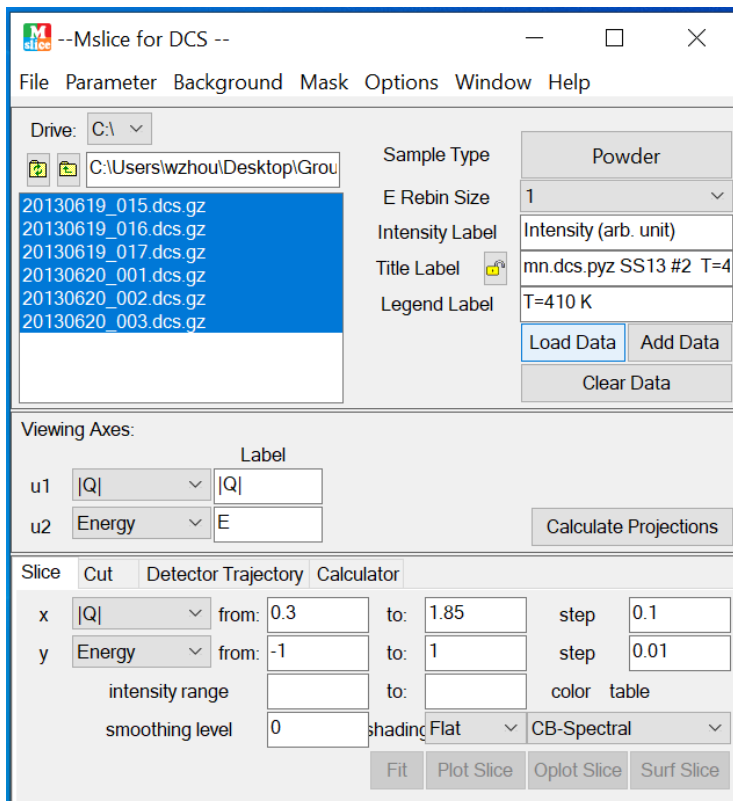
PROCEED



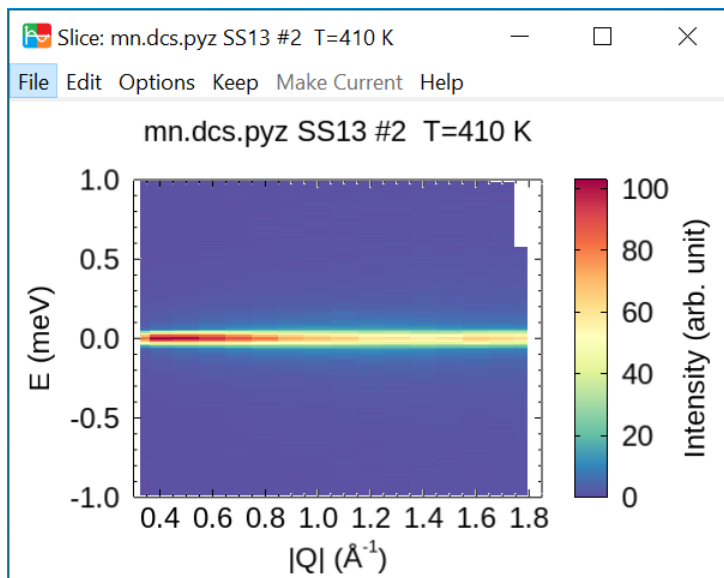
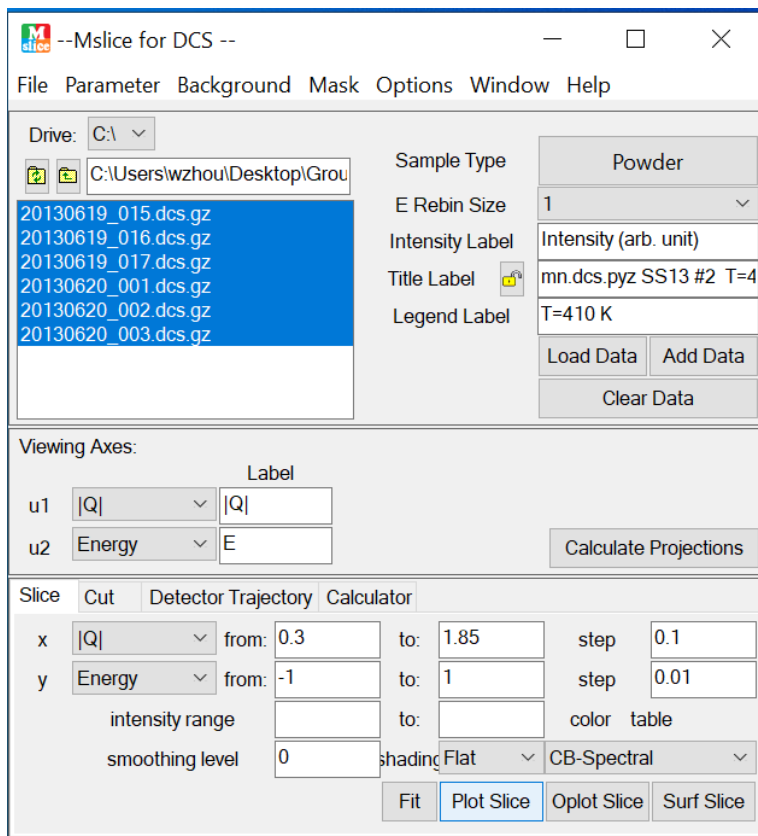
For QENS analysis, the symmetrized  $S(Q, \omega)$  is what we want, so we change the “View Intensity As” selection accordingly.



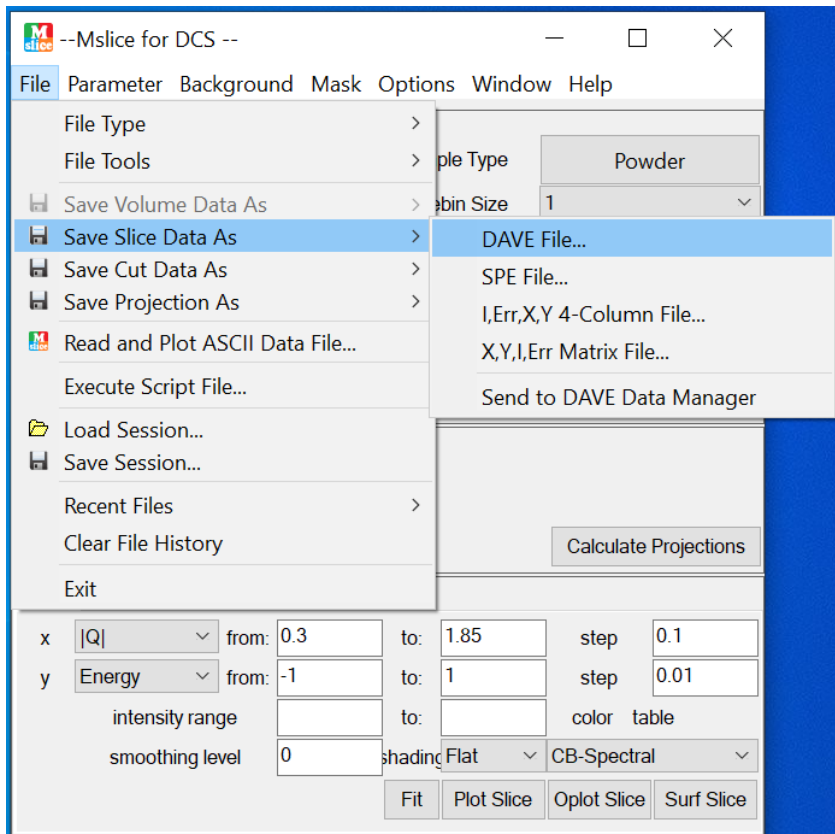
Now we can reload the data and click “Calculate Projections”.



Now we are ready to plot the data. We can use “Plot Slice” to plot the Intensity as function of both Q and E.



The Slice data can be saved as a DAVE file (to be analyzed using the PAN program) or in some other ASCII format.



The data can also be plotted as “Cut” (e.g., Intensity vs. Q or Intensity vs. E etc.)

Mslice --Mslice for DCS --

File Parameter Background Mask Options Window Help

Drive: C:\

C:\Users\lwzhou\Desktop\Grou

- 20130619\_015.dcs.gz
- 20130619\_016.dcs.gz
- 20130619\_017.dcs.gz
- 20130620\_001.dcs.gz
- 20130620\_002.dcs.gz
- 20130620\_003.dcs.gz

Sample Type: Powder

E Rebin Size: 1

Intensity Label: Intensity (arb. unit)

Title Label: mn.dcs.pyz SS13 #2 T=4

Legend Label: T=410 K

Buttons: Load Data, Add Data, Clear Data

Viewing Axes:

u1: |Q| Label: |Q|

u2: Energy Label: E

Calculate Projections

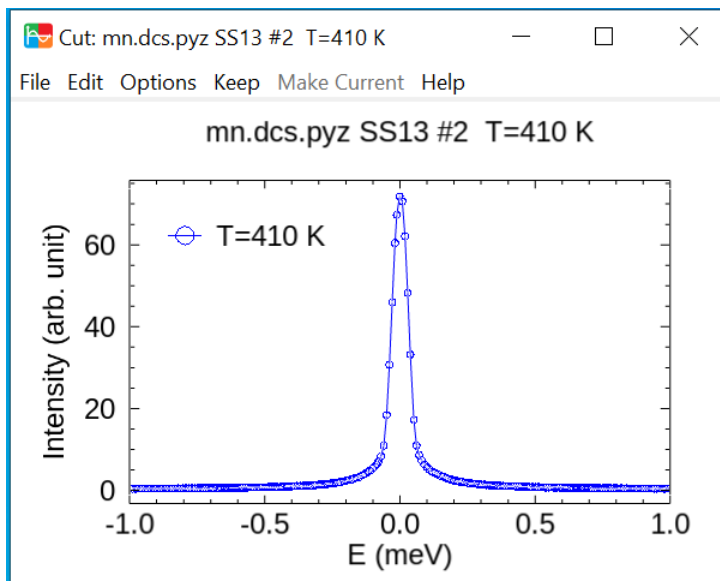
Slice: Cut, Detector Trajectory, Calculator

along: Energy from: -1 to: 1 step: 0.01

|Q| thick to: symbol: blue

y: Intensity range to: circle solid

Buttons: Fit, Plot Cut, Oplot Cut



We can compare different data sets by loading new data and using “Oplot” to plot the data.

--Mslice for DCS --

File Parameter Background Mask Options Window Help

Drive: C:\

C:\Users\lwzhou\Desktop\Grou

- 20130618\_025.dcs.gz
- 20130618\_026.dcs.gz
- 20130618\_027.dcs.gz
- 20130618\_028.dcs.gz
- 20130618\_029.dcs.gz

Sample Type: Powder

E Rebin Size: 1

Intensity Label: Intensity (arb. unit)

Title Label: mn.dcs.pyz SS13 #3 T=1

Legend Label: T=100 K

Load Data Add Data

Clear Data

Viewing Axes:

Label

u1: |Q| |Q|

u2: Energy E

Calculate Projections

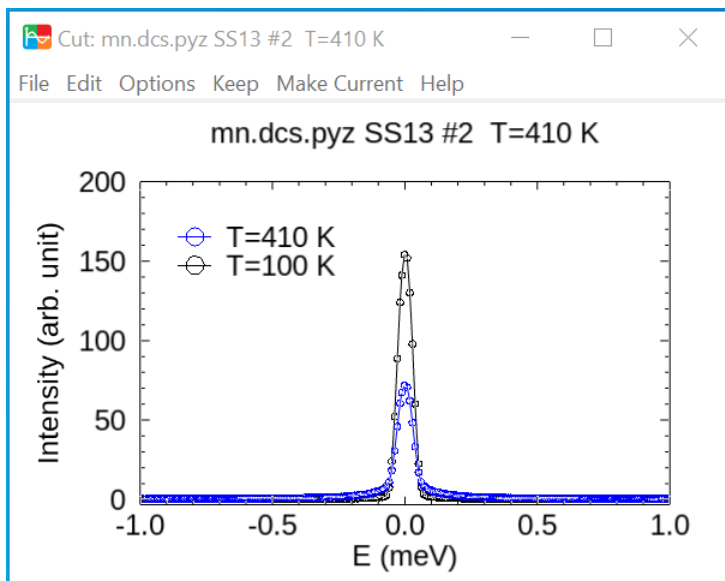
Slice Cut Detector Trajectory Calculator

along: Energy from: -1 to: 1 step: 0.01

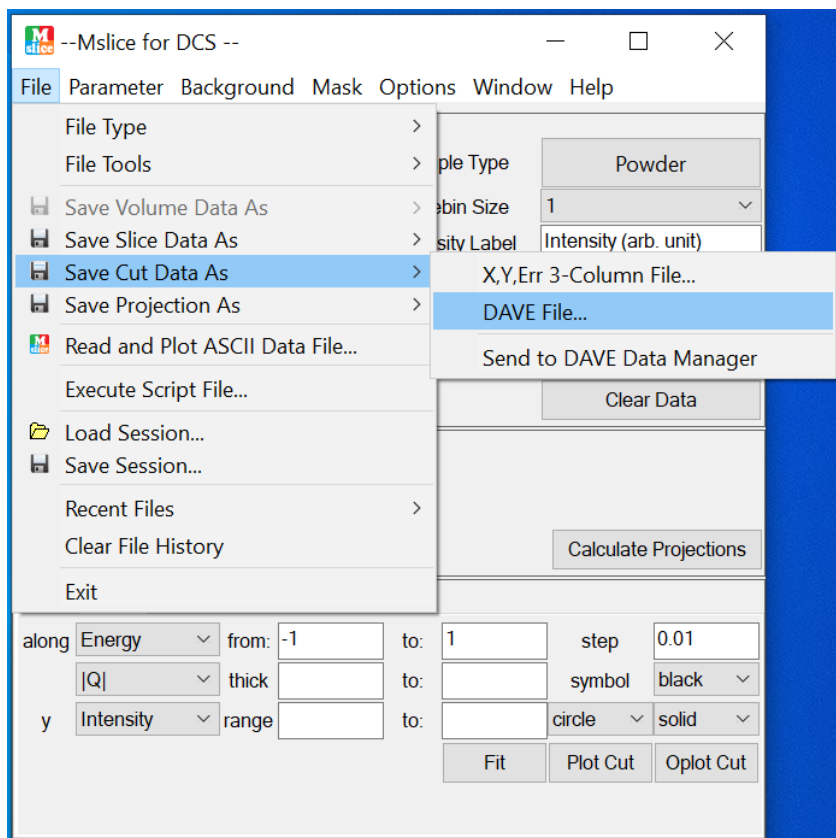
|Q| thick to: symbol: blue

y: Intensity range to: circle solid

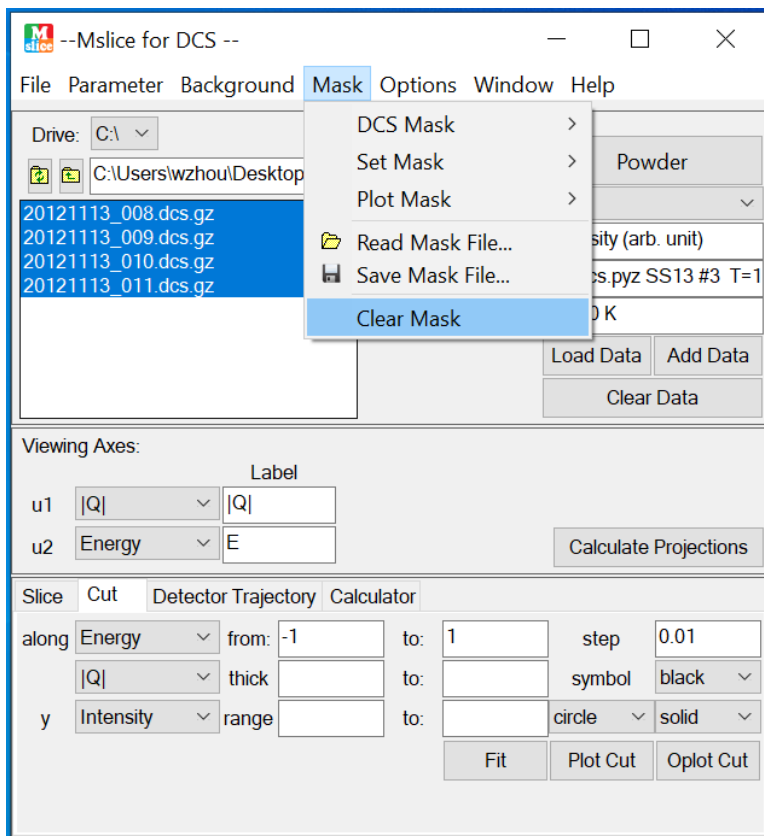
Fit Plot Cut Oplot Cut



The “Cut data” can be saved as well.

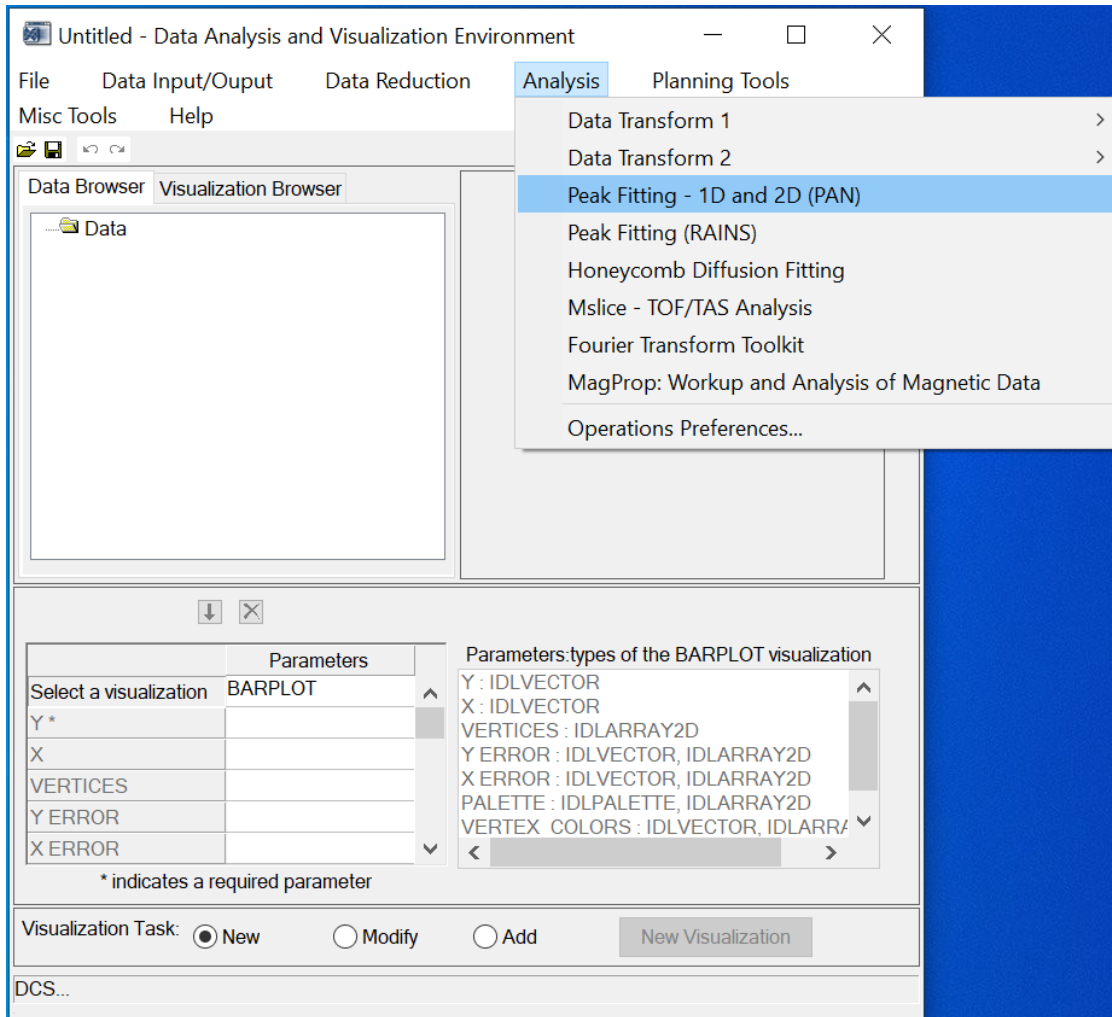


We also need to reduce the Vanadium data (to be used as instrument resolution). For Vanadium (no Bragg peaks), we don't want to use masks. Other than that, the procedure is the same.





We use the PAN program for data analysis.



We first load the DAVE file of the sample.

The screenshot shows the PAN: Peak Analysis software interface. The 'Data' menu is open, with 'Load DAVE file' selected. The interface includes a menu bar (File, Data, Resolution, Plot\_Options, Hot\_Keys, Print, Help), a toolbar with buttons like 'Fit all groups', 'Interrupt fit', and 'View CORR matrix', and a control panel on the right with various settings and a table of parameters.

**Data Menu Options:**

- Load DAVE file
- Load ASCII Data File >
- Load test data
- Load 2nd test data
- Display current file information
- Rebin data
- Crop data
- Edit Pan Mask
- Restore Original data
- Save data and fits to text file
- Save data, fits, and selected curve to text file
- Save data and fits to EXCEL-readable ASCII
- Save fits only to EXCEL-readable ASCII
- Flush and close all open files

**Control Panel:**

- Fit all groups
- Interrupt fit
- Groups to fit: 1
- Fitting status: Resting
- View CORR matrix
- Refresh Fit Results
- Analyze Fit Parameters
- Plot EISF
- # of MC data sets: 100
- Monte-Carlo error estimate

**HTML Log Controls:**

- Create new HTML log file
- Open existing HTML log file
- Enter comment
- Add plot to log
- Close HTML log file
- Log file status: closed
- Log file name:

**Parameters Table:**

Differential Evolution Algorithm	
Enable DE Algorithm?	No
Method of Evaluating ChiSq	Mean square error (MSE)
Population factor (x nos params)	10
Max function evaluations	10000
Param Error: ChiSq Threshold (%)	5
Terminating ChiSq Tolerance	0.029999999329448
Function Evaluation Count	0
Generation Count	0
Current ChiSq	0

**Status Bar:** X: -53.9 Y: 8.90E+03

We then load the DAVE file of Vanadium (or the data file of the sample measured at very low T if it).

The screenshot shows the PAN: Peak Analysis - V.dave software interface. The main window displays a plot of Intensity (arb.) versus Energy (E) in meV. The plot shows a sharp peak at approximately 0.32500 meV, with a vertical dashed line indicating the peak position. The x-axis ranges from -1.0 to 1.0 meV, and the y-axis ranges from 0 to 40. The plot is titled "No Curves/Functions present".

The "Resolution" menu is open, showing the following options:

- Load DAVE data as resolution function
- Load ASCII Resolution File
- Load test resolution function
- Change resolution domain (crop)
- Rebin Resolution data
- Restore Resolution data
- Clear resolution function

The left sidebar contains various controls:

- Select
- Select
- Group
- Modify
- Clear current curves
- Clear all curves
- Remove selected curve
- Curve selection (1)
- Fit current group
- Fit all groups
- Interrupt fit
- Groups to fit (1-16)
- Fitting status (Resting)
- View CORR matrix
- Refresh Fit Results
- Analyze Fit Parameters
- Plot EISF
- # of MC data sets (100)
- Monte-Carlo error estimate

The right sidebar contains HTML Log Controls and Differential Evolution Algorithm settings:

HTML Log Controls:

- Create new HTML log file
- Open existing HTML log file
- Enter comment
- Add plot to log
- Close HTML log file
- Log file status: closed
- Log file name:

Differential Evolution Algorithm:

Parameter	Value
Enable DE Algorithm?	No
Method of Evaluating ChiSq	Mean square error (MSE)
Population factor (x nos params)	10
Max function evaluations	10000
Param Error: ChiSq Threshold (%)	5
Terminating ChiSq Tolerance	0.029999999329448
Function Evaluation Count	0
Generation Count	0
Current ChiSq	0

Coordinates: X: -1.12 Y: 84.3

Now we can fit the data. In this case, we use a linear background, a Delta function and a Lorentzian function.

PAN: Peak Analysis - T410K.dave

File Data Resolution Plot\_Options Hot\_Keys Print Help

Select 1D Function

- Background >
- Exponential >
- Momentum Dist >
- Quasielastic >
- Peak >
  - Delta (resolution)
  - Auto Gaussian
  - Auto Lorentzian
  - DHO
  - Gaussian
  - Lorentzian
  - Log-Normal
  - Bi Gaussian
  - Voigt
- Phase Transition >
- User Defined >
- Other >

Remove selected curve

1

< >

Curve selection

Fit current group

Fit all groups

Interrupt fit

Groups to fit

1-16

Fitting status

Resting

View CORR matrix

Refresh Fit Results

Analyze Fit Parameters

Plot EISF

# of MC data sets

100

Monte-Carlo error estimate

$|Q| (\text{\AA}^{-1}) = 1.39896$

E (meV)

No Curves/Functions present

HTML Log Controls

Create new HTML log file Open existing HTML log file

Enter comment Add plot to log

Close HTML log file

Log file status: Log file name

closed

ifferential Evolution Algorit

Enable DE Algorithm?	No
Method of Evaluating ChiSq	Mean square error (MSE)
Population factor (x nos params)	10
Max function evaluations	10000
Param Error: ChiSq Threshold (%)	5
Terminating ChiSq Tolerance	0.029999999329448
Function Evaluation Count	0
Generation Count	0
Current ChiSq	0

X: -0.982 Y: 69.3

Once the data fitting is done, we can “Analyze Fit Parameters” and “Plot EISF”

PAN: Peak Analysis - T410K.dave

File Data Resolution Plot\_Options Hot\_Keys Print Help

Select 1D Function

Select 2D Function

16  
Group selection

Modify fit parameters

Clear current curves

Clear all curves

Remove selected curve

1  
Curve selection

Fit current group

Fit all groups

Interrupt fit

Groups to fit  
1-16

Fitting status  
Resting

View CORR matrix

Refresh Fit Results

Analyze Fit Parameters

Plot EISF

# of MC data sets  
100

Monte-Carlo error estimate

$\backslash Q \backslash (E^{-1}) = 1.79599$

Intensity (arb. unit)

E (meV)

Residuals

E (meV)

Curve 1: LINEARBGD  
#0 : offset: 9.198e-01 +/- 2.688e-02  
#1 : slope: 2.112e-01 +/- 3.220e-02

Curve 2: DELTA  
#2 : area: 3.486e+00 +/- 3.403e-02  
#3 : center: -2.002e-03 +/- -1.904e-04

Curve 3: LORENTZIAN  
#4 : area: 3.485e+00 +/- 3.495e-02  
#5 : center: -1.777e-03 +/- -7.963e-04  
#6 : FWHM: 1.632e-01 +/- -4.172e-03

Chi-squared: 1.963

---

HTML Log Controls

Create new HTML log file Open existing HTML log file

Enter comment Add plot to log

Close HTML log file

Log file status: Log file name

closed

---

Differential Evolution Algorithm	
Enable DE Algorithm?	No
Method of Evaluating ChiSq	Mean square error (MSE)
Population factor (x nos params)	10
Max function evaluations	10000
Param Error: ChiSq Threshold (%)	5
Terminating ChiSq Tolerance	0.029999999329448
Function Evaluation Count	0
Generation Count	0
Current ChiSq	0

X: -0.279 Y: -17.0

Parameter plotting utility

Selected Parameter: Parameter #6: LORENTZIAN: FWHM

Plot Parameter

Fit in PAN

Export To Data Browser

Use parameter that is derived from the existing fitted parameters

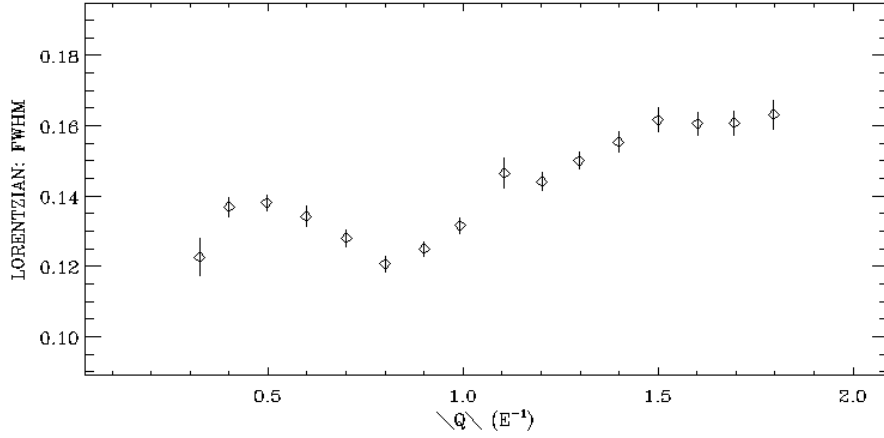
Derived Parameter Defn

Plot Derived Parameter

Fit it in PAN

Export to Data Browser

Parameter #6 in fit model



Save

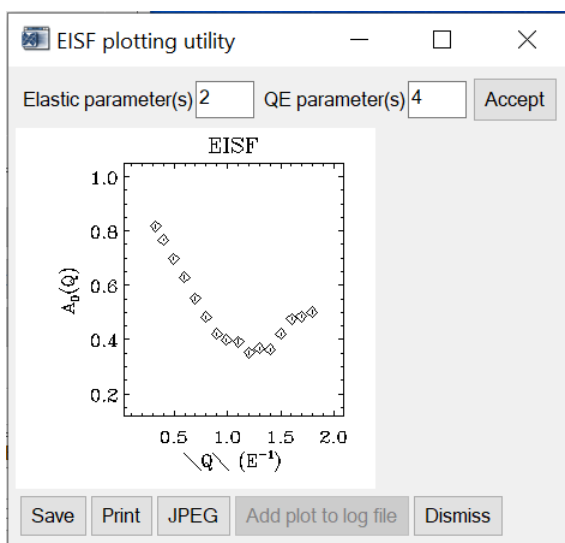
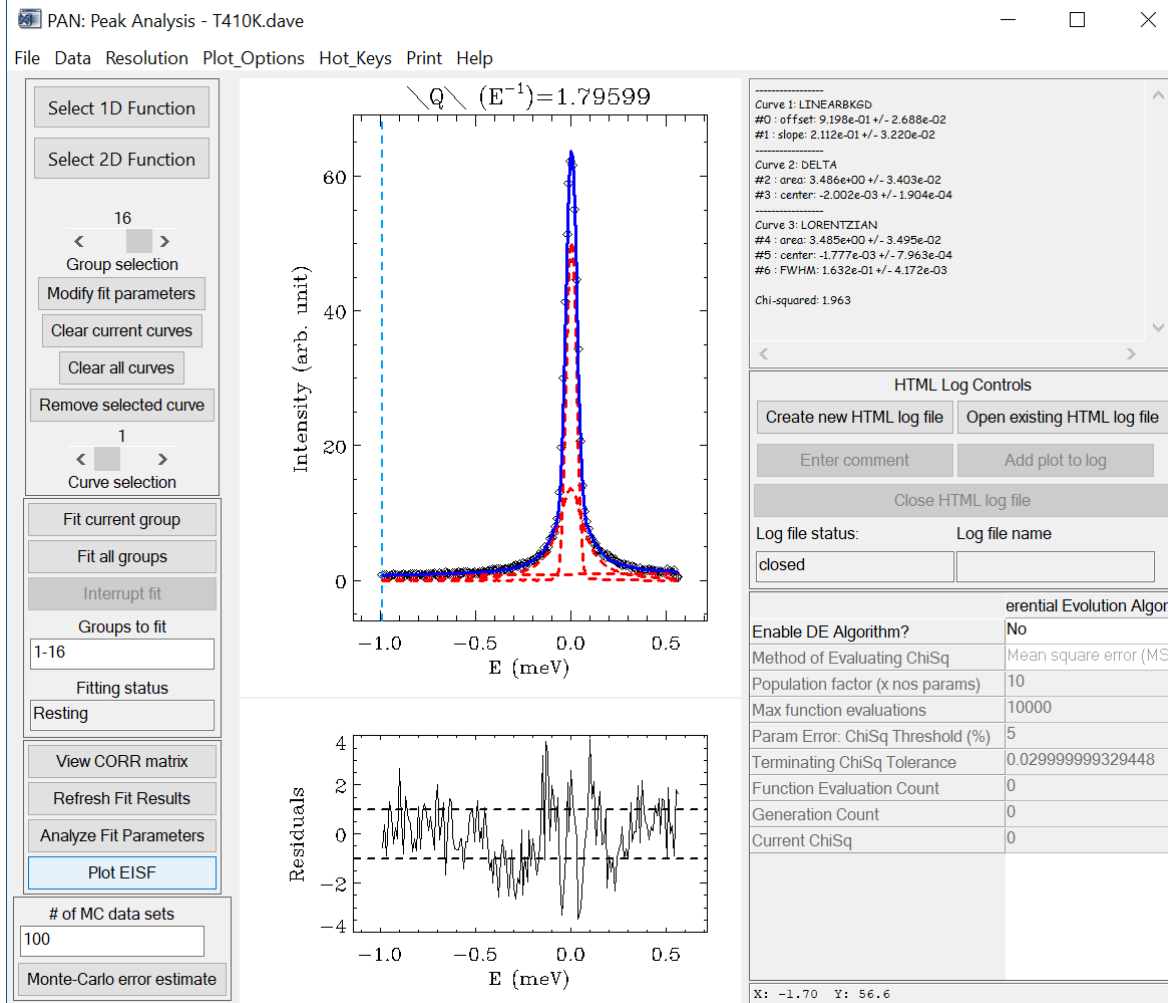
Save All

Print

JPEG

Add to log file

Dismiss



We can further save the EISF data as an ASCII file, and fit the data to investigate its Q dependence etc.