DCS Mslice User Manual

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Powder Sample

1. Select the data files, and press **Load Data** button.

Drive: G:\ C: C: C	Sample E Rebin Size	Powder 1	v v
20030807_011.dcs.gz 20030807_012.dcs.gz	Intensity Label	lintensity (arb. u	misj
20030807_013.dcs.gz	inte Labei		
20030807_014.dcs.gz 20030807_015.dcs.gz	Legend Label	l	
20030807_016.dcs.gz		Load Data	Add Data
20030807_017.dcs.gz		Clear D	CS Data

2. Choose the viewing axes, and press Calculate Projection button.

View	ing Axes:		
		Label	
u1	IQI		
u2	Energy	E	Calculate

3. Press **Plot Slice** button to view the color contour plot of the intensity over the chosen viewing axes, or **Surf Slice** to view the 3D surface plot.

Display:						
	horizontal range Q	0	to:	2.5	step	0.015
	vertical range E	-1	to:	2.5	step	
	intensity range	0	to:	0.2	color map	
	smoothing level	1	shading	Gourau 💌	PlotSlice	Surf Slice

The plot will look like the following, which is a superfluid LHe4 roton spectrum.



4. Choose the cutting axis, and press **Plot Cut** to plot the cut.



The plot will look like the following.



Single Crystal Sample

1. Select the data files, and press Load Data button.

Drive: G:\	Sample E Robin Sizo	Single Crystal	-
20021218_06.dcs.gz			•
20021218_07.dcs.gz	Intensity Label	Intensity (abs. u	units)
20021218_08.dcs.gz 20021219_01_dcs.gz	Title Label		
20021219_02.dcs.gz	Legend Label		
20021219_03.dcs.gz		Load-Data	Add Data
20021219_04.dcs.gz			Auu Dala
20021219_06.dcs.gz		Clear D	CS Data

2. Select the background (empty can) files, then in **Background** menu, press **Load Background File(s)**.

🚺Mslice for	🚺Mslice for DC5 ¥2.0									
File Parameter	Background Ma	k Option	Window	Help						
	Load Backgrou	d File(s)								
Drive: GA	Set Overall Ba	Rground Ra	te							
	Clear Backgrou	nd		Sample	Single Crystal	•				
🖸 🖻 G:\2	Load Vanadium	File(s)		F Bebin Size	1	_				
20021219_05	Clear Vanadiur	n								
20021219_06.	dcs.gz			ntensity Label	Intensity (abs. u	inits)				
20021219_07	des.gz			Title Label						
20021219_08	acs.gz des.az			egend Label	Í.					
20021220 02	dcs.gz			egena zaber	ľ.					
20021220_03	dcs.gz				Load Data	Add Data				
20021220_04	dcs.gz		-		Clear D(ng Data				
20021220_05.	dcs.gz					55 0 414				

3. Choose the Vanadium file, and in **Background** menu, press **Load Vanadium File(s)**.

	Mslice for	DC5 ¥2.0						_ 🗆 ×
File	Parameter	Background	Mask	Option	Window	Help		
		Load Back Set Overa	iground all Backg	File(s) pround Ra	ite			
	nve: ju:r al calless	Clear Back	kground			Sample	Single Crystal	•
20		Load Var	adium Fi	le(s)		E Rebin Size	1	•
20	021219_07.	dcs.gz	salum.			itensity Label	Intensity (abs. u	inits)
20	021219_08. 021220_01	des.gz des.gz				Title Label		
20	021220_02.	.dcs.gz			L	egend Label.		
20	021220_03. 021220_04.	des.gz .des.gz					Load Data	Add Data
20	021220_05.	dcs.gz			-		Clear D(CS Data
20	021220_06,	dcs.gz			۲		Ciedi Di	JS Dala

4. Enter the lattice parameters, crystal orientation, and the viewing axes, then press **Calculate Projection** button. Psi is the angle from ki to u, with counterclockwise being the positive direction.

Unit Ce	II Lattice F	Paramete	ers:			Cryst	al Orien	tation:			
a (Å)	18.686	b (Å)	8.032	c (Å)	6.146	ux	0	uy	0	uz	1
α(°)	90	β (°)	90	γ(°)	90	vx	0	vy	-1	VZ	0
						Psi	95	angle	e of ki^u		
Orthogo	onal View	ing Axes	:								
	a*	b*	C*	Energy	Label						
u1	0	1	0	0	k						
u2	0	0	1	0	I						
u3	0	0	0	1	E			0	alculate	Rroje	ections

5. Choose the slice plane. Press **Plot Slice** button to view the color contour plot of the intensity over the slice plane, or **Surf Slice** to view the 3D surface plot.

Slice Plane:		1			
perp to [0,k,0] 💽 thick	-10	to:	10	🔽 Fold x-a	axis
horizontal range l	0.2	to:	1	step	0.015
vertical range E	-0.3	to:	3	step	0.015
intensity range	0	to:	0.1	color map	
smoothing level	1	shading	Gourau 💌	PlopSlice	Surf Slice

The plot will look like the following.



6. Choose the cutting axis and thickness over the other two axes, and press **Plot Cut** to plot the cut.

Cut							
along	E (meV)	from:	-0.2	to:	3	step	0.02
	thickness ra	nge k	-10	to:	10		
	thickness ra	nge l	0.43	to:	0.57	symbol	green 💌
У	Intensity	range	0	to:	0.2	circle 💌	solid 💌
						PlotQut	Oplot Cut
save as	none	-				Browse	Fit

The plot will look like the following.



Single Crystal Diffuse Scattering

1. Select the data files, and press **Load Data** button.

	Sample	Diffuse Scatteri	ing 💌
20020015_016_doo_dz	Energy Range	Elastic Peak	•
20030915_017.dcs.gz	Intensity Label	Intensity (arb. u	nits)
20030915_018.dcs.gz	Title Label		
20030915_019.dcs.gz	legendlabel		
20030915_021.dcs.gz	Logona Labor		
20030915_022.dcs.gz		Load Data	Add Data
20030915_023.dcs.gz		Clear D(CS Data

2. In the option menu, select the average binning method, show Al powder line, and log scale intensity. Enter the lattice parameters, crystal orientation, and the viewing axes, then press **Calculate Projection** button. Psi is the angle from ki to u of the first file, with counterclockwise being the positive direction.

Image: Second State of the second		
File Parameter Background Mask	Option Window Help	
Drive: G:\ ▼	View Intensity As Binning Method Monitor Count Viewing Axis Show Powder Line E-Dependent Detector Efficiency C ✓ Log Scale Intensity Legend Label	
20030915_021.dcs.gz 20030915_022.dcs.gz		Load Data Add Data
20030915_023.dcs.gz 20030915_024.dcs.gz		Clear DCS Data
Unit Cell Lattice Parameters: a (Å) 8.995 b (Å) 8.995 α (°) 90 β (°) 90	Crystal Or c (Å) 6.649 ux 0 γ (°) 90 vx 1 Pei 150	ientation: uy 0 uz 1 vy 0 vz 0
Orthogonal Viewing Axes: a* b* c* u1 1 0 0 u2 0 0 1	Label	Calculate Projections

3. Press **Plot Slice** button to view the color contour plot of the intensity over the viewing axes, or **Surf Slice** to view the 3D surface plot.



The plots will look like the following.



The white lines denote the positions of the Al powder line.

Load SPE File

To read a SPE file, use the **Load SPE File** button in the **File** menu. The following dialog window will appear. PHX file refers to the detector configuration file that is associated with the SPE file.

🛐 Input:		×
spe file:		Browse
phx file:		Browse
	Clear OK	

User will be asked to enter the incident neutron energy during the projection calculation.

Load DAVE File

To read a DAVE format file, use the **Load DAVE File** button in the **File** menu. The DAVE file should contain all necessary information, preferably a DAVE file reduced from the DCS files.

Convert DCS Files to SPE Format

Convert DCS Files To SPE Format button in the **File** menu starts a stand-alone application to convert DCS files into SPE format which can be processed by MATLAB <u>Mslice</u> program.

Convert DCS data files to SPE for	mat		_ 🗆 🗙
File Mask Sample Help			
DCS file directory	Overall background rate	SPE file directory	
Drive: G:\	(cts/hr/det): 29.000000	Drive: C:\	
🚯 🔁 G:\data\200302	Associated error:	😰 🔁 C:\test	
20030206_001.dcs.qz	0.000000	20020919_15.spe	
20030206_002.dcs.gz	Energy binning size:	20020919_16.spe	
20030206_003.dcs.gz	5	20020919_17.spe	
20030206_004.dcs.gz		20020920_01.spe	
20030206_005.dcs.gz	Load BG Clear BG	20020920_02.spe	
20030206_006.dcs.gz		20020920_03.spe	
20030206_007.dcs.gz	Load V Clear V	20020920_04.spe	
20030207_001.dcs.gz		20021129_01.spe	
20030207_002.dcs.gz	Convert	combine.spe	
20030207_003.dcs.gz			
20030207_004.dcs.gz	Compine	save as: [combine.spe	

Choose one or more DCS *.dcs or *.dcs.gz files in the DCS file directory, press **Convert** button to convert them into *.spe files. The converted files will have the same names as the DCS files except for the file extension and they are saved in the SPE file directory.

To combine two or more DCS files, choose them in the DCS file directory, then press **Combine** button. The name of the combined SPE file can be specified in the **save as:** textbox. If no name is given, the default is 'combine.spe'.

Overall background rate and **Associated error** are used to apply an overall background rate to all the detectors. The background will be subtracted in Convert and Combine operations.

Energy binning size is used to rebin the time channel to reduce the size of data.

Load BG button is used to load background files, which will be subtracted in Convert and Combine operations. Once the background file is loaded, they will stay in the memory until **Clear Bg** button is pressed. The **Clear Bg** button will be sensitive only when a background file has been loaded.

Load V button is used to load vanadium files, which will be used to calculate the detector efficiencies. The detector efficiencies and divided from data in Convert and Combine operation. Once the vanadium file is loaded, the detector efficiencies will stay in the memory until **Clear V** button is pressed. The **Clear V** button will be sensitive only when a vanadium file has been loaded.

Both background files and vanadium files are selected in the DCS file directory.

Detectors can be masked in various ways in the **Mask** menu. Once set, the mask will stay in the memory until **Mask**->**Clear the mask** is pressed.

The data files can be saved as either single crystal or powder sample by choosing the corresponding sample type in the **Sample** menu. With the choice of powder sample, detectors with the same two theta angle will be combined.

Detector configuration file (*.phx) can be created during file conversion by choosing the **Yes** option in **Sample->Create Detector File**.

To exit the program, either go to **File**->**Exit** or simply close the window.

Exit

To exit the program, press the **File**->**Exit** button or simply close the window.

Load Parameters

To load a previously saved parameter file, click the **Parameter**->**Load Parameters** button. A file selection window will pop up. All the parameters shown in the main window plus some options will be restored. However, previous DCS data and projection are not loaded.

Save Parameters

To save the current settings in the main window, click the **Parameter**-> **Save Parameters** button. A file selection window will pop up. The default extension of saved file is *.*prm*. If no file name is entered or selected, no action is taken.

Change Self-Shielding Factor

The self-shielding factor is used in <u>background subtraction</u> according to the following equation:

```
\begin{split} I &= I_1\text{-ssfactor}*I_2 , \\ Err &= sqrt[Err_1^2 + (ssfactor*Err_2)^2] . \end{split}
```

Change Overall Intensity Factor

The overall intensity factor is multiplied to the intensity during <u>projection calculation</u>. This factor is reset to 1 every time a data file is loaded.

Change Smoothing Kernel

The smooth kernel for smoothing the 2D slice data can be changed in the **Parameter** menu. The default kernel is [[0.1,0.2,0.1],[0.2,0.8,0.2],[0.1,0.2,0.1]]. An error will be given if the entered matrix is not symmetric.

Set Data Directory

Set Data Directory in the **Parameter** menu will change the data directory to a new one.

Set Working Directory

Set Working Directory in the **Parameter** menu will change the working directory to a new one. The working directory is used as the default directory in saving files.

Load Background File(s)

To load a background file, use the upper left <u>file locator</u> to select the background file(s). Then press the **Background->Load Background File(s)** button. The background data will stay in the memory until the **Background->Clear Background** is pressed. The background will be subtracted in <u>projection</u> <u>calculation</u>. The intensity (I) and error (Err) are calculated as follow:

I =
$$I_1$$
-ssfactor* I_2 ,

 $Err = sqrt[Err_1^2 + (ssfactor^*Err_2)^2]$,

where ssfactor is the average self-shielding factor.

Set Overall Background Rate

The **Set Overall Background Rate** button in the **Background** menu is used to input the overall background rate in counts/hour/detector. The value is then adjusted accordingly to be subtracted from DCS data in <u>projection calculation</u>. There is no error handling in this process. Use **Background**->**Clear Background** to clear it from the memory.

Clear Background

Background->Clear Background button is used to clear the background file and/or overall background rate from memory. To take effect, projection needs to be recalculated.

Load Vanadium File(s)

To calculate the detector efficiency factor of the spectrometer, first highlight the vanadium file using the upper left <u>file locator</u>, then press the **Load Vanadium File(s)** button in the **Background** menu. The detector efficiency factor is calculated as proportional to the integrated intensity of the elastic peak in each detector. This factor is divided from the raw data every time the <u>projection</u> is calculated. However, the raw data and the projection data are stored differently. Use **Background->Clear Vanadium** to clear the detector efficiency factor from memory.

Clear Vanadium

Background->Clear Vanadium button is used to clear the detector efficiency factor from memory. To take effect, projection needs to be recalculated.

Mask Upper and Lower Banks

To view the data from only the central bank detectors, press the **Mask Upper and Lower Banks** in the **Mask** menu. The mask takes effect when <u>projection</u> is calculated.

Once set, the mask stays in the memory. To clear the mask, press Mask->Clear Mask button.

Mask Central and Lower Banks

To view the data from only the upper bank detectors, press the Mask Central and Lower Banks in the Mask menu. The mask takes effect when projection is calculated.

Once set, the mask stays in the memory. To clear the mask, press Mask->Clear Mask button.

Mask Upper and Central Banks

To view the data from only the lower bank detectors, press the Mask Upper and Central Banks in the Mask menu. The mask takes effect when <u>projection</u> is calculated.

Once set, the mask stays in the memory. To clear the mask, press Mask->Clear Mask button.

Set Your Own Mask

To mask arbitrary detectors, press the **Set Mask** in the **Mask** menu. The detector number starts from 0. The mask takes effect when <u>projection</u> is calculated.

Once set, the mask stays in the memory. To clear the mask, press Mask->Clear Mask button.

Intensity Type

Use **Option->View Intensity As** button to choose the intensity type as one of the following three: **S(Q,omega)** ------ a factor of $(ki/kf)^4$ is applied to the normalized intensity, **Symmetrized S(Q,omega)** ------ a factor of $exp(-E/2k_BT)*(ki/kf)^4$ is applied to the normalized intensity, **d2(sigma)/d(Omega)d(Ef)** ------ a factor of $(ki/kf)^3$ is applied to the normalized intensity.

Binning Method

Two binning methods, **average** and **sum**, can be chosen from the **Option->Binning Method** menu button. The binning method is applied in rebinning time channel according to <u>E Rebin Size</u> for *powder* and *single crystal* or energy range in loading *diffuse scattering* data, and rebinning data in displaying slices and cuts.

Monitor Count

There are two options to calculate the monitor count: sum of beam monitor counts or the integrated intensity of the beam monitor counts after fitted by a Gaussian. The option is set in **Option->Monitor Count**. The monitor count is used to normalize data in loading DCS files.

Viewing Axis Type

For single crystal and diffuse scattering type, there are two options of viewing axis: orthogonal and arbitrary. They can be set in Option->Viewing Axis. If orthogonal option is chosen, the viewing axes given must be orthogonal to each other.

Show Powder Line

In diffuse scattering mode, either Al or Cu powder line can be overplotted to the intensity contour plots or detector trajectories (when the viewing axes are x and y axis). To do this, select the Al or Cu option in **Option->Show Powder Line** menu. The <u>projection</u> needs to be calculated to have the option in effect.

E-Dependent Detector Efficiency Correction

The energy dependent detector efficiency correction to the intensity can be applied to the data in <u>projection</u> calculation. To set this option on and off, press the **Option->E-Dependent Detector Efficiency Correction** button. When the program started, this option is off.

Warning: The intensity at high energy end could be overly corrected when this option is set.

Log Scale Intensity

If **Option->Log Scale Intensity** menu button is set, subsequent plots will use log scale for the intensity. However, the log scale can be set back to linear in the plots.

Hiding Part of the Window

The projection, display, and detector trajectory frame of the window can be hidden by using the options in **Window** menu. This can be quite useful if the size of the window is larger than the screen. The following snapshot is an example.

Image: Second State S		
File Parameter Background Mask Option	Wir Yow Help	
	✓ Projection	
Drive: G:\	 Display Trajectory 	Powder 🖉
😰 🗈 G:\200309\	Current Plot Window	
20030916_006.dcs.gz	Intensity Label	Intensity (abs. units)
20030916_008.dcs.gz	Title Label	
20030916_010.dcs.gz	Legend Label	
20030917_001.dcs.gz 20030917_002.dcs.gz		Load Data Add Data
20030917_003.dcs.gz 20030917_004.dcs.gz	·	Clear DCS Data
Viewing Axes:		
Label	_	
	_	
u2 Energy Energy		Calculate Projections
Detector Trajectories:		
× [Q] 🔽 from:	to:	
y Energy 💌 from:	to:	
z None 💌 from:	to:	Plot Trajectories

View Current Plot Window

By pressing **Window**->**Current Plot Window** menu button, the current active (not kept) plot window will gain focus.

Load DCS File

To load DCS file(s) ending with .dcs or .dcs.gz, use the top left file locator to select one or more files. Press **Load Data** button to load the data. An error will be given if no file is highlighted. The data will be normalized by the monitor counts of beam monitor 1 if shutter is open.

For *powder* and *single crystal* sample type, the files will be combined. For *diffuse scattering* sample type, files are not combined, and energy range needs to be specified beforehand.

The loaded data will not be modified by the program until new data file is loaded or added, or the sample type is changed to or from *diffuse scattering*. Press **Clear DCS Data** button to remove the data from memory.

Drive: G:\ Image: G:\2003087 20030807_010.dcs.gz 20030807_011.dcs.gz 20030807_012.dcs.gz 20030807_013.dcs.gz 20030807_014.dcs.gz	Sample E Rebin Size Intensity Label Title Label	Powder 1 Intensity (arb. u	Powder 1 Intensity (arb. units)	
20030807_015.dcs.gz 20030807_016.dcs.gz 20030807_017.dcs.gz 20030807_018.dcs.gz		Load Pata Clear D	Add Data CS Data	

Add Data

The Add Data button will be activated when DCS data has been loaded.

Select the data files to be added by the upper left <u>file locator</u>. Then press the **Add Data** button. An error will be given if the file selected and the existing data are of different wavelength, master speed, speed ratio, resolution mode, or tsdmin.

For *powder* and *single crystal* data, the data are added to existing data; for *diffuse scattering* sample type, the data are appended to the existing data.

The algorithm for computing added intensity(I) and error(Err) with weights(W) taken into account is as follows:

$$\begin{split} I_3 &= (I_1 * W_1 + I_2 * W_2) / (W_1 + W_2) \ , \\ Err_3 &= sqrt[(Err_1 * W_1)^2 + (Err_2 * W_2)^2] / (W_1 + W_2) \ , \\ W_3 &= W_1 + W_2 \ . \end{split}$$

Clear DCS Data

Press **Clear DCS Data** to clear from memory the loaded DCS data and calculated projection data if existed.

Sample Type

There are three sample types: single crystal, powder, and diffuse scattering.

For **single crystal** sample, <u>lattice parameters</u>, <u>crystal orientation</u>, and three <u>viewing axes</u> need to be given to enable proper <u>projection calculation</u>. The data is plotted as 2D intensity color map on the plane defined by two of the viewing axes. The third axis is used to restrict the slice range. The data can also be cut along one of the three viewing axes with restrictions on the other two axes, and plotted as 1d plot.

For **powder** sample, two <u>viewing axes</u> need to be specified. In the <u>projection calculation</u>, detectors with the same two-theta angle are combined. The data is plotted as 2D intensity color map on the plane defined by the viewing axes. The data can also be cut along one of the two viewing axes with restrictions on the other axis, and plotted as 1d plot.

For **diffuse scattering** sample type, <u>lattice parameters</u>, <u>crystal orientation</u>, and two <u>viewing axes</u> need to be given to enable proper <u>projection calculation</u>. The data is plotted as 2D intensity color map on the plane defined by the viewing axes. The data can also be cut along one of the viewing axes with restrictions on the other axis, and plotted as 1D plot.

When the sample type is changed, the projection data is cleared and need to be recalculated before any plots can be made. The raw data is still stored in the memory if the change is between *powder* and *single crystal* type.

Lattice Parameters

For *single crystal* and *diffuse scattering* sample types, the direct lattice parameters of the unit cell are specified by **a**, **b**, **c**, α , β , and γ . α is the angle between **b** and **c**, β is the angle between **c** and **a**, and γ is the angle between **a** and **b**. An error will be given during projection calculation if any one of the six lattice parameters is missing.

Crystal Orientation

For *single crystal* and *diffuse scattering* sample types, the crystal orientation with respect to the spectrometer is defined by two reciprocal crystal axes ($\mathbf{u} \& \mathbf{v}$) in the principal scattering plane of the spectrometer and one angle (Psi) which uniquely identifies the rotation of the crystal in this plane.



(**ux**, **uy**, **uz**) and (**vx**, **vy**, **vz**) specifies the two *reciprocal* crystal axes. u x v should point to the vertically *upward* direction.

Psi is the angle between u and ki, and is positive if ki x u is pointing to the vertically upward direction. It should be the same as DCS A2 angle if A2=0 when ki//u. For *diffuse scattering*, Psi is the angle for the first file.

An error will be given in <u>projection calculation</u> if any value of u, v, or Psi is not set.

Viewing Axes

Powder

The viewing axes for *powder* are two axes out of (Energy, |Q|, 2Theta, and Det Group Number). They can be specified from the droplists. The labels of the viewing axes are used as corresponding axes titles in the 2d plots. The Most commonly used set of viewing axes for powder sample is u1=|Q| and u2=Energy.

Single Crystal

The viewing axes for *single crystal* are either wave vector directions or energy. They must be orthogonal if the orthogonal option is chosen for the <u>viewing axis type</u>. The energy axis is orthogonal to any wave vector direction. An example is

```
u1 = [1 \ 0 \ 0 \ 0] ;a^*
```

```
u2 = [0\ 1\ 0\ 0] ;b^*
```

```
u3 = [0\ 0\ 0\ 1];E
```

An error will be given in <u>projection calculation</u> if any value of the viewing axes is not given or the axes are not orthogonal when required.

Diffuse Scattering

The viewing axes for *diffuse scattering* are wave vector directions. They must be orthogonal if the orthogonal option is chosen for the <u>viewing axis type</u>. An example is

 $u1 = [1 \ 0 \ 0]$; a^*

 $u2 = [0 \ 1 \ 0] ;b*$

An error will be given in <u>projection calculation</u> if any value of the viewing axes is not given or the axes are not orthogonal when required.

Energy Rebin

To reduce the amount of data being processed and plotted, the raw data can be rebinned in the <u>projection</u> <u>calculation</u> for *single crystal* and *powder* sample types. Time channels are binned according to the size specified in the **E Rebin Size** textbox. No action is taken if the E rebin size is less than one or absent. The rebinning can be either average or sum according to the specified <u>binning method</u>.

Calculate Projection

Press **Calculate Projections** button to project the raw data into viewing axes. Detector masks and detector efficiency factors are applied if they are present. The background will also be subtracted if they have been previously loaded. Intensity data are also rebinned if <u>E rebin size</u> is greater than 1. The intensity will be calculated as one of three options chosen in **Option**->**View Intensity As** menu. Energy dependent detector efficiency will be calculated if the option is set. The projected data and the raw data are stored differently, i.e., the raw data are not changed by this calculation. If no DCS data has been loaded, the program will prompt for incident neutron energy Ei to calculate detector trajectories.

For *powder*, detectors with the same 2theta angle will be combined.

For *diffuse scattering*, data with the same sample rotation angles will be combined.

For *single crystal* and *diffuse scattering*, an error message will be given if any value of the lattice parameter, crystal orientation, and viewing axes is not given, or if the viewing axes are not orthogonal when required.

Intensity Label

The intensity label is used as the axis title for intensity in plots. If not given, the default is *Intensity*. IDL formatting codes are supported.

Title Label

The title label is used as title in plots. IDL formatting codes are supported. It is set to the comment of a DCS data file after the file is loaded. The plot title can be easily modified in the plot window.

Legend Label

The legend label is used as the legend in plotting 1D cuts. It is set to the last word of the comment of a DCS data file after the file is loaded. The plot legend can be easily modified in the plot window.

Intensity Color Contour Plot and Slice

The intensity data projected into two viewing axes can be plotted as color contour plot by pressing the **Plot Slice** button.

For single crystal data, the axis perpendicular to the slice plane is chosen from the **perp to** droplist which contains the three viewing axes. The choice of the perpendicular axis automatically defines the slice plane axes as the remaining two viewing axes, and the horizontal and vertical label will change accordingly.

To fold the symmetrical data, choose the **Fold x-axis** option. The data can be folded into either positive or negative range depending on the sign of the horizontal range.

Data can be rebinned by specifying the horizontal and/or vertical step. If not specified, the default

binning size is 200 except for energy data. The binning algorithm is as follows: a grid of bins of size xstep x ystep is constructed with the lower left corner at (xmin-xstep/2, ymin-ystep/2) and not exceeding xmax+xstep/2 along x and ymax+ystep/2 along y. The x and y values for each bin are calculated by taking the average of the x and y values of all the data in that bin, and the intensity is the average or sum of all the data in that bin according to the specified <u>binning method</u>. The limits are inclusive to the left and exclusive to the right.

The grid can be smoothed by choosing a nonzero Smoothing level. The default smoothing kernel is

- 0.1 0.2 0.1
- 0.2 0.8 0.2
- $0.1 \ 0.2 \ 0.1$.

The kernel can be <u>changed</u> in the **Parameter** menu.

The color map of the contour plot can be chosen from the **color map** droplist. The names are the same as the predefined IDL color table names.

Two types of shading are available: Flat and Gouraud.

Flat: The color has a constant intensity for each face of the surface, based on the normal vector. Gouraud: The colors are interpolated between vertices, and then along scan lines from each of the edge intensities.

The 2D data can also be plotted as color surface plots by pressing the Surf Slice button.

Tip 1: Specify the horizontal and vertical range to reduce the amount of data and speed up the plotting.

Tip 2: If the energy step is not specified, the original energies corresponding to the time channels are used. This will prevent the energies from being changed by the binning process.

Cut

Cuts can be made along one of the viewing axes with integration over the other two directions for *single crystal* or the other one direction for *powder*. Use **along** droplist to select the x axis, and **y** droplist to select the y axis. The plotted data are the average or summed values over the integrated volume according to the specified <u>binning method</u>.

X and y range, integration volume (thickness) can be specified by the **from:** and **to:** textboxes. Data can also be rebinned by specifying the cut **step**. The x-range is divided into bins of length *step* starting at xmin-step/2 and not exceeding xmax+step/2. The x and y value for each bin is calculated by taking the simple average of the x and y values of all data in that bin, where the limits are inclusive to the left and exclusive to the right.

Plot **symbols** can be specified by the color, symbol style, and line style droplists. White color will be switched to black when the figure is printed or saved as a file. Press **Plot Cut** to plot the cut in the current plot window, or press **Oplot Cut** to overplot the cut in the current plot window. If **save as** type is other than *none*, the cut data will be saved as a .xye(x, y, yerr) file whose name can be either entered in a the filename textbox or chosen by pressing **Browse** button.

The cut data can also be sent to the Peak Analysis (PAN) program for fitting. To do this, simply press the **Fit** button. The cut data will be saved in this operation if the saving file name is specified.

Tip: If the cut is along energy and the step is not specified, the original energies corresponding to the time channels are used. This will prevent the energies from being changed by the binning process.

Plot Trajectories

The **Plot Trajectories** button is insensitive until projection is calculated. The projection can be calculated without loading any DCS data.

Detector trajectory is an x vs. y 1d plot. Both x and y are chosen from droplist. If None is chosen, the detector group number is used. Z can be used to restrict the range of data in extra dimension. If no ranges are set for x, y, and z, the default is to show all possible data. The following is an example in diffuse scattering mode.

