WCEN USER'S MANUAL

Version 1.1

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1. Introduction

WCEN is a fiber diffraction data processing program. The main features of the program include displaying fiber diffraction images, determining fiber diffraction parameters, refining the parameters, correcting systematic effects and mapping diffraction data into reciprocal space.

We assume that the users are familiar with X window environment and understand basic window operations.

1.1 Formatting Conventions

In this manual, there are several formatting conventions used to denote the different on screen interface commands.

- **Bold** indicates a command to click, such as buttons, options and drop down menus.
- SMALL CAPS indicate a new window opening on top of the main image window.
- *Italics* indicate a pane or input box within a window or a sub-window.
- `Courier` font is used for typed commands and on-screen text.

1.2 File Browser Windows

All files loaded and some saved in WCEN use a file browser window (see Fig. 1). There are four input fields and navigation tools – the *Directories* pane, *Filter* box, *Files* pane, and *File* box. You may click the **Cancel** button at anytime to close the browser window without loading or saving a file.

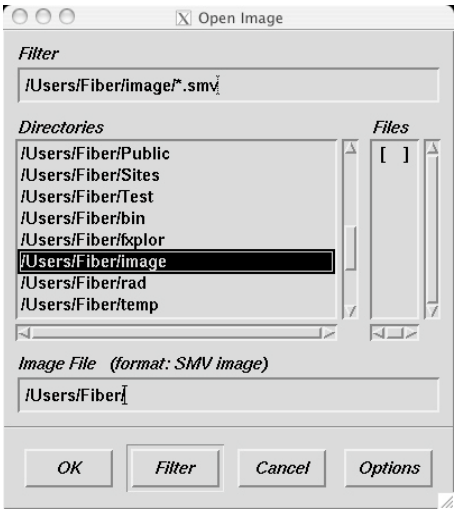

Fig. 1. A File Browser window

1.2.1 Loading a file in the browser window

1) Select the folder with the desired file in the *Directories* pane.
2) In the *Filter* box, use a wildcard command (*) to select the file extension you want to display in the *Files* pane. Click **Filter** to apply the criteria.
3) In the *Files* pane, select a file to load with the mouse.
4) The selected file will appear in the *Files* box, click the **OK** button.

1.2.2 Saving a file in the browser window

1) Select the destination folder with the *Directories* pane.
2) Type the file name in the *File* box with the desired extension.
3) Click the **OK** button.

1.2.3 Directories Pane

Use the *Directories* pane to navigate folders. In the *Directories* pane, select a folder by highlighting it with the mouse. The selected directory will then appear in the *Filter* box. Double clicking on a directory will act like the **Filter** button, and show the files from the *Filter box* in the *Files Pane*. Double clicking the directory ending `/..` takes the user up one level in the file hierarchy.

1.2.4 Filter Box

The *Filter* box can select specific file extension types to appear in the *Files* pane by using wildcards (*). Wildcards ignore text before or after them, some examples of use:

Filter box input	Files displayed in Files pane
/Users/Fiber/images/*.smv	all .smv files in /Users/Fiber/images
/Users/Fiber/NMV*	files in /Users/Fiber/ beginning with NMV
/Users/Fiber/images/*	all files in /Users/Fiber/images
/Users/Fiber/images/*284*	files in /Users/Fiber/images with 284 in their name

Click **Filter** to implement the wildcard constraints from the *Filter* box.

1.2.5 Files Pane

The *Files* pane will display filtered files from the *Filter* box or *Directories* pane. Click and highlight a file in this pane to write that file name into the *File* box for imminent selection.

1.2.6 File Box

The file name shown in the *Files* box will be loaded or saved. Click **OK** to load or save respectively. A progress bar will appear while loading image files.

1.3 File Naming Conventions

Users who wish to take advantage of WCEN's default filters should use these extensions for parameter and colormap files respectively.

.par default naming conventions for parameter files
.cmp default naming conventions for colormap files

2. Main Program Window

When first started, the main window of the program will come up. It has three parts, a title bar, a main menu bar and the image window.

2.1 Title Bar

The title bar is the very top bar of the program window. The title bar contains the name of the current version of WCEN, the name of the file last loaded and the width and height of the image in the image window. The title bar will also have close, minimize and maximize buttons that will vary depending on the operating system used.

2.2 Main Menu Bar

The main menu bar is immediately below the title bar and consists of seven drop down menus: **File**, **Image**, **Colormap**, **Draw**, **Process**, **Windows**, and **Help**. The menus will be discussed in order later in the manual.

2.3 Main Image Window

The main image window (Fig. 2) is used to display the fiber diffraction image. PseudoColor is used for efficient manipulation of colormap and image refreshing. There is virtually no restriction on the size of the image. Vertical and horizontal scroll bars can be used to scroll images through the window when the image is very large. Furthermore, the main window is revisable. There is a cross-box type cursor in the image window. The pixel position and intensity of the cursor position are shown in the window's title bar. Clicking the mouse button, or dragging the mouse while holding the mouse button down, changes the cursor's position.

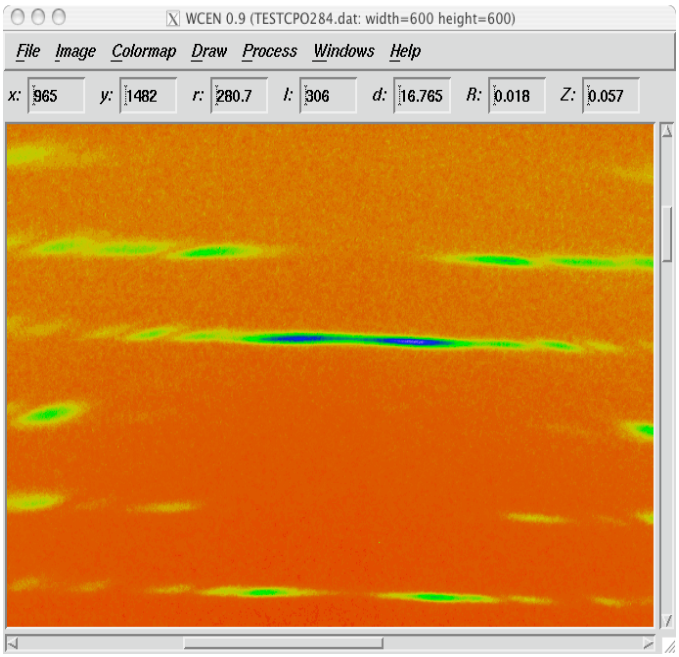

Fig. 2 MAIN IMAGE window

It should be noted that the key shortcut (an underscored letter) might not work on some systems. On Red Hat Linux, pressing ALT + a shortcut letter would activate the corresponding top-menu, and subsequent pressing of a shortcut letter in the sub-menu would invoke the corresponding command; on Mac OS X systems, the top-menu shortcut doesn't work because X Windows absorbs the ALT input, but the sub-menu shortcut still behaves the same.

3. File Menu

The **File** menu allows users to **Open**, **Save** and **Close** image files, **Load Parameters** and **Save Parameters** and **Exit** WCEN.

3.1 Open command

Go to the **File** menu and choose **Open** to bring up the file browser window OPEN IMAGE.
The image formats currently supported in WCEN are listed below:

Format	Description
BSL (CCP13)	This image format has a header file (xxx000.xxx) for image size and other information, and a binary file (xxx001.xxx) for image data.
MAR image plate	This image format includes 4000 bytes of header information followed by a 16 bit image data.
Perkin Elmer	Head information and image data are stored in two separated files. The image data are stored as 12-bit pixels. Any pixel with a value greater than 2400 is considered saturated.
Raw image	Image height and width, header size, bytes per pixel, and data type (unsigned, signed or float) must be specified before reading the image.
RAXIS (MSC)	Molecular Structure Corporation's X-ray diffraction Image format for R-axis IV. Image size and other information are included in the file.
SMV image	File format for ADSC CCD detectors. Image information is included in the header.
SPR image	Text image produced by Fit2d
TIFF	8,16-bit grayscale or 24-bit color TIFF image (without compression). Image information is included in the header.

See the Introduction for help navigating the file browser window.

Changing Image Format: In the OPEN IMAGE window, click the **Options** button to bring up the IMAGE FORMAT window (Fig. 3). Click the **select format** drop down button and select one of the image formats listed above. Click the **OK** button to change format or the **Cancel** button to ignore any changes. The selected format will be displayed above the **Image File** text box.

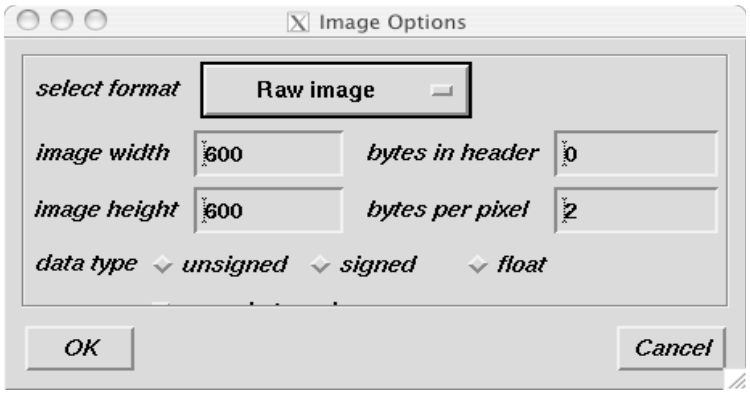

Fig. 3. IMAGE OPTIONS window

To load an image with an unlisted format (or no header), Raw image may be used. In this case, you need specify all of the following for your image: **image width** and **image height** (both in pixels), **bytes in header**, **bytes per pixel**, and type of **image data** (unsigned, signed, or float point number). For example, images in MAR image plate format can be loaded as Raw image format with a **bytes in header** of 4000 and **bytes per pixel** of 2.

There is an additional **swap byte** option available for Raw image and BSL image. When it is checked, WCEN will swap the byte order of the image data. Byte order is a concern when you transfer data across computers, for they might store numbers in a different way. For example, Intel X86 based systems (e.g. Linux and Windows PC) store the lower-order byte of a number at the lower memory address (Little Endian), while Mac and most UNIX systems store the higher-order byte of a number at a lower address (Big Endian). The following table lists the endianess of popular computer systems:

Processor Type	**Operating System**	**Byte Order**
Alpha AXP	Tru64 Unix	Little Endian
	Alpha VMS	Little Endian
	Linux	Little Endian
HP PaRISC	HP-UX	Big Endian
IBM RS/6000	AIX	Big Endian
Intel X86	Linux	Little Endian
	Solaris X86	Little Endian
	Windows	Little Endian
	Intel Macintosh OS X	Little Endian
Motorola PowerPC	Macintosh OS (Classic)	Big Endian
	Macintosh OS X	Big Endian
SGI R4000 and up	IRIX	Big Endian
Sun Sparc	SunOS	Big Endian
	Solaris	Big Endian

3.2 Save as

Go to the **File** menu and select **Save as**; choose one of the image formats to save the image to a file. The following are the sub-menu commands under the **Save image** command:

smv	save image in .smv format
bsl	save image in .bsl format
8-bit grayscale tiff	save image in .tiff format (8-bit grayscale, no compression)
16-bit grayscale tiff	save image in .tiff format (16-bit grayscale, no compression)
24-bit color tiff	save image in .tiff format (24-bit color, no compression)
8-bit raw	save image in an array of pixels (1 byte per pixel), no header
16-bit raw	save image in an array of pixels (2 bytes per pixel), no header
rad	save polar coordinates in txt file for angular deconvolution
postscript	save image in postscript format (.ps)

3.3 Close

To close the image currently open in the main image window, go to the **File** menu and click **Close**. This command will not exit WCEN.

3.4 Load Parameters

Open the **File** menu and choose **Load Parameters** to read a file of fiber diffraction parameters and reflections. The Load Parameter browser window will open (see section **1.2.1**). The default file type is `.par` for parameter files. If the size of the image in the parameter file is different from that loaded in the main image window, a warning message will appear on the screen to notify the user. A similar command is found in the Parameter menu of the REFLECTION-PARAMETER window (see section **8.2.2.8**).

3.5 Save Parameters

Open the **File** menu and choose **Save Parameters** to write the latest fiber diffraction parameters and reflection list to a file. The SAVE PARAMETER browser window will open (see section **1.2.2**). The default file type is `.par` for parameter files. Users should use this command to backup parameters periodically. A similar command is found in the Parameter menu of the REFLECTION-PARAMETER window (see section **8.2.2.9**).

3.6 Exit

To close the main window and exit WCEN, open the **File** menu and choose **Exit**. Before closing the program, be sure to save any changes to image data or parameters.

4. Image Menu

The **Image** menu allows users to **Flip** or **Rotate** images, **Repair** small areas of an image with a smoothing function, **Merge** a second image with the current one, and **Rescale** the intensities (mainly designed to work with the fiber diffraction simulation program **Disorder**, http://fibernet.vanderbilt.edu/Software/disorder).

4.1 Flip

In the **Image** menu select **Flip**; from the sub-menu that appears choose **vertically** or **horizontally** to flip the image in the selected manner.

4.2 Rotate

In the **Image** menu select **Rotate**; from the sub-menu that appears choose **90 degree**, **180 degree**, or **270 degree** to rotate the image clockwise by the amount selected.

4.3 Repair

WCEN can remove image defects caused by detector malfunction. The removal program takes a defined rectangle of pixels and revalues the intensities using a simple smoothing function based on the pixel intensity values immediately outside the defined area. Smoothing occurs across the narrowest direction of the rectangle defined. This function works best for a row or column of bad pixels.

4.3.1 Steps for Removing an Image Defect

1) In the **Image** menu, click **Repair** to open the IMAGE REPAIR window. Click **Show Pixels i**n the IMAGE REPAIR window to open the PIXEL INTENSITIES window.
2) In the Main Image window, drag the cursor to the top left region of the defective area.
3) Use the PIXEL INTENSITIES window to identify the edge of the defective pixel region – for lines of bad pixels note the one (or ones) that systematically differ as a column or row.
4) Enter the x/y coordinates of the top left corner of the region to be corrected in the boxes `x1` and `y1` of the IMAGE REPAIR window.
5) Repeat steps 2-4 for the bottom right corner and enter the x/y coordinates of the bottom right corner of the region to be corrected in the boxes `x2` and `y2` of the IMAGE REPAIR window.
6) Click **Repair** in the IMAGE REPAIR window.

4.3.2 Exiting the Repair function

In the IMAGE REPAIR window click **Close**.

4.4 Merge

From the **Image** menu click **Merge** to open the MERGE window (Fig. 4).

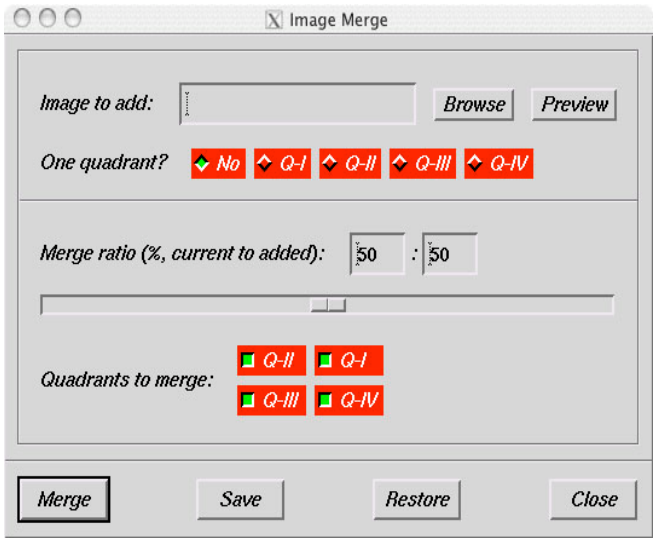

Fig. 4. MERGE window

4.4.1 Input Image

To select an image to merge, click the **Browse** button to locate the image file. Click the **Preview** button to view the image. If the image contains only one quadrant of a pattern, check the corresponding radio button.

4.4.2 Merge Operations

Drag the scalebar to change the ratio of the two images for merging. By default, all 4 quadrants of both images are used, and the merged image is shown in the main window. Click **Merge** button to start the merging. The **Save** button saves the current image in display, while the **Restore** button restore the image in display to the last saved.

4.5 Rescale

From the **Image** menu click **Rescale** to open the RESCALE window (Fig. 5). This function is designed to optimize the contract of a simulated pattern from the program **Disorder**, by varying the scale factors for the calculated intensities, and the temperature factors.

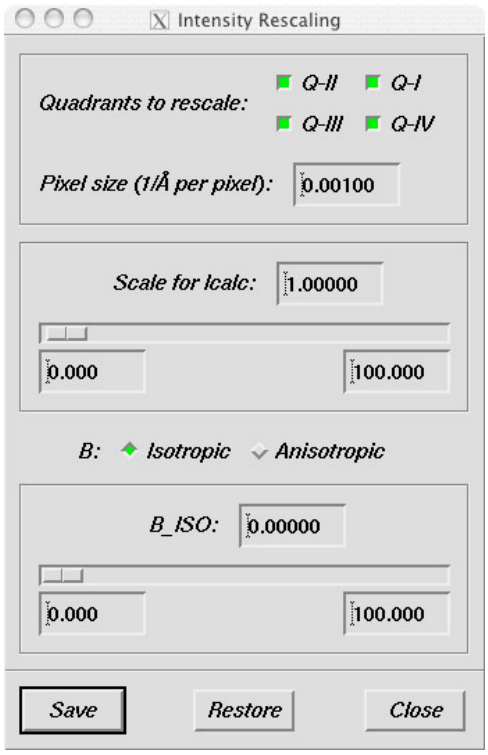

Fig. 5. RESCALE window

4.5.1 Rescale Parameters

By default all 4 quadrants are rescaled. To vary the temperature factors, the pattern has to be in reciprocal space, and the **Pixel size** has to be defined. The text boxes below a scalebar indicate the minimum and maximum values of the scalebar, and can be manually changed.

4.5.2 Rescale Operations

Dragging the scalebar to rescale the image. Click Anisotropic to bring out the anisotropic box to vary temperature factors in R and Z directions. The **Save** button saves the current image in display, while the **Restore** button restore the image in display to the last saved.

5. Colormap Menu

The **Colormap** menu allows users to **Customize** colormaps, **Save** colormaps, and **Load** them from a file.

5.1 Load

From the **Colormap** menu, select **Load** to open a file browser window. The default wildcard filter is `*.cmp` in the *Filter* box. Refer to section **1.2**, for assistance with the file browser.

5.2 Save

In the **Colormap** menu, click **Save** to open a file browser window. Type the file name in the *Write Colormap File* box after the directory name. The file browser filter default is `.cmp`, so users should use this file suffix if they wish the saved file to show up with the default configuration. The *histogram* range, colormap and the polynomial function are saved across colormap control sessions.

5.3 Customize

From the **Colormap** menu click **Customize** to open the COLORMAP CONTROL window (Fig. 6). This window has three control features: a drop down menu for **select colormap**, a *Histogram* pane, and a *Colormap* pane.

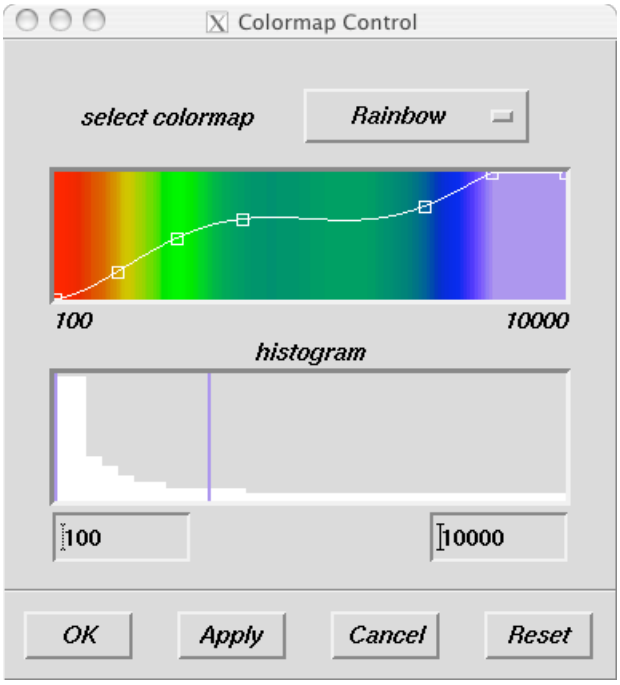

Fig. 6. COLORMAP CONTROL window

5.3.1 Colormap Selection

In **select colormap** drop down menu, click on one of the options (**Rainbow** is the default). WCEN has eleven colormap options and users should experiment with the available maps to achieve the best imaging of their data. Two of the colormap options, **Keiichi** and **Green-Purple**, are banded maps; all other maps are smooth. Changes made in **select colormap** are shown immediately in the main image window.

5.3.2 Histogram Pane

In the *histogram* pane, the white histogram represents the intensity distribution of the diffraction data. The horizontal axis is the intensity axis and the vertical axis is intensity frequency. Underneath the histogram pane are two input boxes; the left box is an input for the intensity range lower limit and the right box is the upper limit. Changes in these boxes

will be reflected by the vertical histogram lines in the *histogram* pane and by the intensity range of the *colormap* pane. Moving the histogram lines in the *histogram* pane will also change the intensity range of the *colormap* pane. To move a histogram line, click the mouse pointer on the line without releasing the button and move the line by dragging the mouse to a desired position before releasing the button. Right-click (or Option-click) to "release" a line so that you can move the other histogram line. Click the **Apply** button at the bottom of the COLORMAP CONTROL window to modify the intensity display range of the *colormap* pane. 8-bit image data have to be re-calculated to reflect the change of intensity display range. Calculating 8-bit image data may take much more time than changing the CCC depending on the size of the image.

5.3.3 Colormap Pane

The *colormap* pane displays the currently selected map. The horizontal axis of this pane is the intensity range of the colormap and the vertical axis is the range of different colors offered by the selected map. Below the pane at either end are two numbers that represent the intensity display range, which can be modified in the *histogram* pane (section **5.3.2**).

In the *colormap* pane, there is a white line going across the pane called the color control curve (CCC). Manipulating the CCC changes the colors at any given intensity. The default CCC is a straight line with three control points marked with open square boxes. Dragging any one of the square boxes on the curve alters the CCC. A control point can be added or removed by clicking the middle or right mouse button, respectively (option-click and "apple"-click for a Mac mouse):

CCC Action	3 button mouse	1 button mouse
move control box	Left button	Mouse button
add control box	Center button	Opt + Mouse button
remove control box	Right button	⌘ + Mouse button

Only ten control points can exist in the pane at a time, including the boxes at the ends. The control points at the ends of the curve cannot be removed, but can slide up and down the y-axis.

To restore the last saved settings, click the **Reset** button in the COLORMAP CONTROL window. Click the **OK** button to accept the new CCC and close the window. Click the **Cancel** button to restore the default CCC and close the window.

Tip: The control points are fixed points on the CCC, with the line curving as a polynomial function. Because of their nature, you cannot slide control points horizontally past other control points. The position of the CCC on the vertical axis assigns color to the intensity on the horizontal axis. Also, control points close to each other will tend to create large slopes and thus abrupt or radical changes to the colormap. Thus, use of many control points on a smooth colormap can create the effect of a banded colormap (**Keiichi** or **Green-Purple**).

6. Draw Menu

The Draw menu allows users to draw a **Circle**, a **Resolution Circle** or **Layerline**. This menu also allows users to **Move Objects**, **Refresh**, and **Close All** objects.

6.1 Circle

From the **Draw** menu click **Circle** to open the DRAW CIRCLE popup window (Fig. 7). This window has a color display area, a scalebar, a palette, an input field for radius (in pixels), two arrow buttons for increment/decrement of the radius, and an input field for step size (in pixels). The *color selected* area shows the current color for drawing, and it can be changed by dragging the scalebar or clicking the palette. After selecting color, enter the radius (in pixels) to draw a circle (from the pattern center) onto the main image window. The default value in the *radius* box is the radius from the last cursor position to the pattern center. Drawing circle is useful in determining the specimen to detector distance (see section **8.2.2.4**), and helpful in identifying symmetry related reflections. The **Clear** button will clear the last drawn circle.

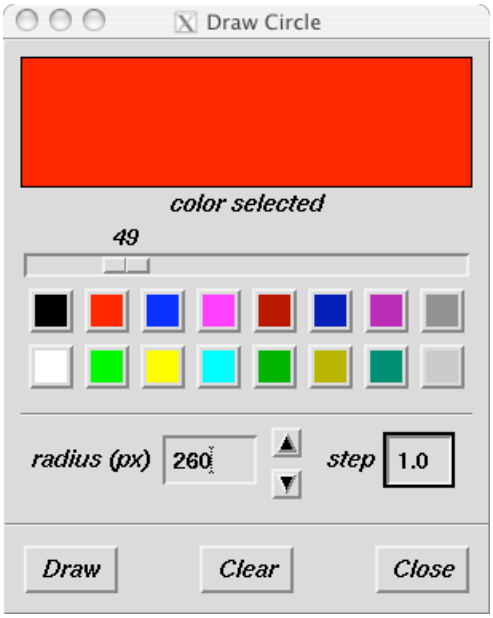

Fig. 7. DRAW CIRCLE window

6.2 Resolution Circle

From the **Draw** menu click **Resolution Circle** to open the DRAW RESOLUTION CIRCLE window. The window is similar to **Draw Circle**, except that the radius unit is Å and the default value is the resolution of the last cursor position. In order to draw a resolution circle, the parameters *distance*, *wavelength*, and *raster* must be defined (section **8.1.1**).

6.3 Layerline

From the **Draw** menu click **Layerline** to open DRAW LAYERLINE Window. The drawing interface is similar to that of **Circle**, except that the *repeat (Å)* box is for fiber repeat. In order to draw layerlines, the parameters *distance*, *repeat*, *wavelength*, and *raster* must be defined (section **8.1.1**). Layerlines are calculated using the most recent parameter values. This is a very useful option for checking the accuracy of the parameters, because a mismatch between the layerlines and the diffraction pattern indicates errors in the parameters. However, caution should be taken for a diffraction pattern with severe layerline splitting, such as tobacco mosaic virus. In this case, mismatch may not indicate errors in the parameters.

Tip: Drawing an additional set of layerlines at 90 degrees from the refined twist parameter will give a grid showing the refined center. This is useful for visualizing the image center.

6.4 Move Objects

From the **Draw** menu click **Move Objects** to open MOVE OBJECTS/CENTER window (Fig. 8) and it can be also accessed from the REFLECTION-PARAMETER window (Section **8.2.2.3**). This allows you to move the center of the diffraction pattern, redrawn the objects (circles, resolution circles and layerlines) and watch the fit. Move can be done with either the arrow buttons on the window, or the arrow keys on your keyboard once you check **enable move by arrow keys**. Please note that you need to put the focus back into main image window in order to move objects using the arrow keys.

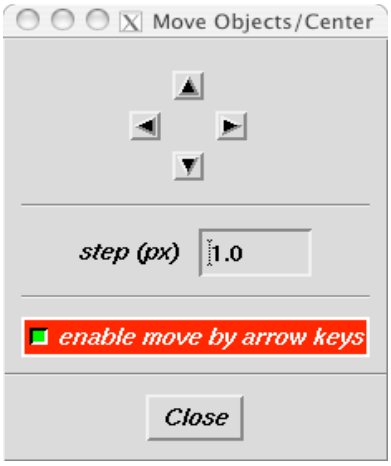

Fig. 8. MOVE OBJECTS window

6.5 Refresh

In the **Draw** menu choose **Refresh** to redraw the current objects on the main image.

6.6 Clear All

In the **Draw** menu choose **Clear All** to erase all the objects drawn on the main image.

7. Process Menu

The **Process** menu has three options, **Plot**, **Correction** and **Transform**. **Correction** compensates for film absorption, incident beam type, and detector fog/dark current. **Transform** is used for changing image data into reciprocal, polar reciprocal or RAD-Polar-reciprocal formats.

7.1 Plot

In the **Process** menu click **Plot** to open the DATA PLOT window (Fig. 9). It consists of three panes: the *Object* pane, the *Plot* pane and the Command pane.

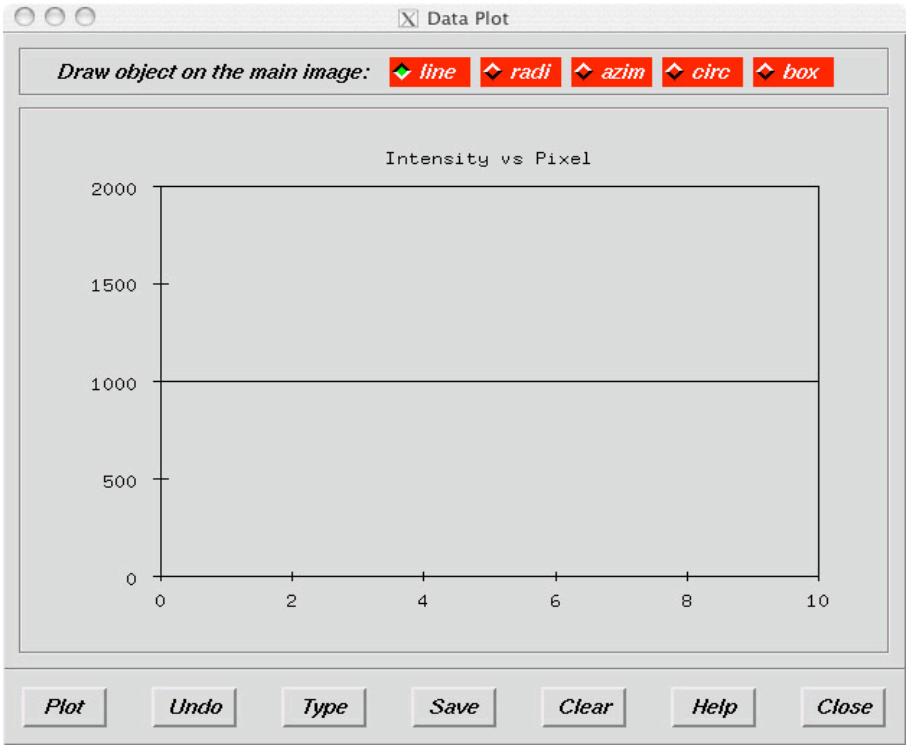

Fig. 9. PLOT window

7.1.1 Object Pane

Five types of objects can be selected in the main window. To select a **line**, left-click the starting point, drag the mouse pointer to the end point, and left-click. To select a **radi**, drag mouse pointer and left-click. To select an **azim**, i.e., an arc, left-click the starting point, then drag the mouse pointer to draw the arc, and left-click to stop. To select a **circ**(le), drag the mouse pointer to draw and left-click to stop at desired radius. To select a **box**, left-click the starting point (top-left corner of the box), drag the mouse pointer to the end point (the bottom-right corner of the box) and left-click. Data points are picked to be the nearest pixels if not exact. For a box, data are collected along its long dimension and averaged along the short dimension.

7.1.2 Plot Pane

The data plot can be zoomed and saved, see **7.1.3**.

7.1.3 Command Pane

To plot data, select an object from the main image, and then click the **Plot** button; to zoom the plot, draw a box on area of interest; to undo a zoom, click the **Undo** button; click the **Type** button to switch the type of the plot between line, line with data points, and data points only; to save the plot data or picture into a file, click the **Save** button; to clear the plot and clear all plot objects in the main image, click the **Clear** button.

7.2 Correction

In the **Process** menu click **Correction** to open the DATA CORRECTION window (Fig. 10). The window consists of three panes: the *Absorption* pane, the *Polarization* pane and the *Detector Fog* pane. At the top of each pane, there is a toggle button. When the toggle button is off (in red), the corresponding pane is collapsed and the systematic effect will not be corrected for the data. When the toggle button is on (in green), the corresponding pane is expanded and the systematic effect will be corrected for the data.

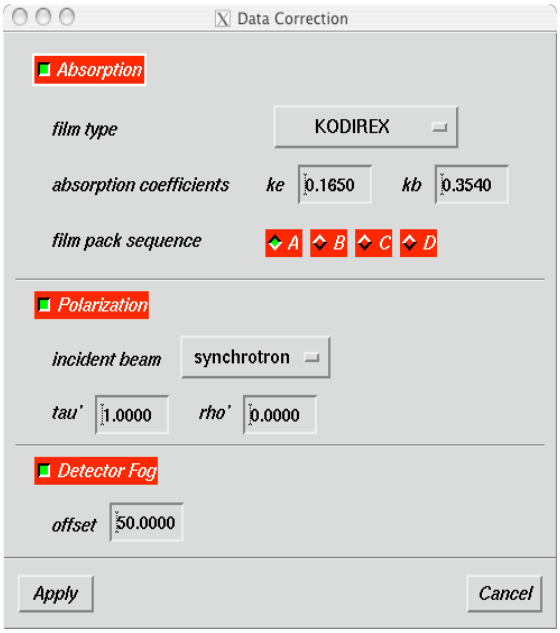

Fig. 10. DATA CORRECTION window

All the experimental parameters must be determined or defined before any correction can be made. The corrections must be made in detector space. After selecting the appropriate conditions, click **Apply** in the DATA CORRECTION window to correct for the selected factors. Click **Cancel** to exit **Correction** and close the DATA CORRECTION window.

7.2.1 Absorption Pane

WCEN includes preset mass absorption coefficients (**ke** and **kb**) for several film types. To select a provided film type, go to the *Absorption* pane and click the **film type** drop down menu to select **KODIREX** (Kodak), **ILFORD**, **CEA**, and **Kodak NoScreen**. Selecting a preset film type enters the correct emulsion (**ke**) and base (**kb**) values into the **absorption coefficients** boxes.

Non-listed film types can be corrected in the *Absorption* pane. In the *Absorption* pane, go to **film type** and from the drop down menu select **Other**. Now enter the correct emulsion (**ke**) and base (**kb**) values into the **absorption coefficients** boxes.

Select **film pack sequence** if you wish to correct for x-ray absorption of film pack wrappers and other film packs. The toggle buttons **A**, **B**, **C**, and **D** correspond to the

sequence of film packs out of four stacked together. Use **A** if only a single film pack was used.

Non-linearity due to the limited dynamics range of films is also corrected (Phillips, et al., *J. Appl. Cryst.* (1985). **18**, 3-7). The correction parameters are built into the program.

This only applies to data when photographic films were used. The absorption of an oblique incident beam by films must be corrected for by a factor of $C(0)/C(\tau)$. For a double side film $C(\tau)$ has the following form (Fraser, et al., *J. Appl. Cryst.* (1976). **9**, 81-94):

$$C(\tau) = 1 - \exp(-k_e \sec\tau) + \exp[-(k_e + k_b) \sec\tau] - \exp[- (2k_e + k_b) \sec\tau]$$

where τ is the angle between diffraction vector and the normal of the detector.

7.2.2 Polarization Pane

In the *Polarization* pane, three types of incident beam can be chosen from the drop-down menu: **Unpolarized**, **Polarized**, or **Synchrotron**. The current version of WCEN provides polarization correction for three types of radiation: unpolarized X-ray beam, crystal-monochromatized X-ray beam, and highly polarized synchrotron X-ray beam.

For unpolarized X-ray beam, the correction factor can be found from any X-ray crystallography textbook:

$$(1 + \cos^2 2\theta) / 2$$

where 2θ is the Bragg angle.

For crystal-monochromatized X-ray beam, the correction factor is given by (Azaroff, *Acta. Cryst.* (1955). **8**, 701-704):

$$\frac{\left(\cos^2 2\theta'\cos^2\rho + \sin^2\rho\right)\cos^2 2\theta + \cos^2 2\theta'\sin^2\rho + \cos^2\rho}{1+\cos^2 2\theta'}$$

where $2\theta'$ is the Bragg angle of the monochromator, and ρ is the "dihedral angle" between the incident beam (into the monochromator) and the diffracted beam (by the specimen).

For polarized synchrotron X-ray beam (with a monochromator), the correction factor is given by (Kahn et al., *J. Appl. Cryst.* (1982). **15**, 330-337):

$$(1 + \cos^2 2\theta) / 2 \; - \; (\tau' \cos 2\rho \sin^2 2\theta) / 2$$

where ρ is the same as in the case of crystal-monochromatized beam, and τ' is a factor depending on the monochromatic crystal and synchrotron radiation source. τ' is usually very close to 1, and you should be able to obtain its exact value from your synchrotron source staff.

Please note that for the crystal-monochromatized beam and the synchrotron beam, ρ varies with each reflection. What WCEN asks for, ρ', is the angle between the incident beam (y_0) and the upper vertical axis of the detector (z), which is constant. ρ' is positive if y_0 is to the left of z, negative otherwise. WCEN calculates ρ by adding the angle between the reflection and vertical axis to ρ'.

7.2.3 Detector Fog Pane

To correct for detector fog, toggle on the *Detector Fog* pane and enter a value into the *offset* box. WCEN can automatically enter a value using the **Detector Fog** command in the **Parameter** menu of the REFLECTION-PARAMETER window. See section **8.2.2.6** for details.

7.3 Transform

WCEN can map images in the main image window from detector space into reciprocal space. From the **Image** menu choose **Transform** to bring up the DATA TRANSFORMATION window (Fig. 11) Under **Transformation Type** WCEN provides three options: **Cartesian reciprocal**, **polar reciprocal**, and **polar reciprocal for angular deconvolution**. Select the desired transformation by switching the appropriate toggle button to green. By default, symmetry equivalent data from four quadrants will be merged/averaged in the transformation, to turn this option off, set the toggle button under **Merge Data** to **none**. **Resolution Range** (*lower* and *upper*, in Å) and reciprocal **Bin Size** (*x-rad* and *y-angle*) values can be specified or changed in the appropriate text box. **Resolution Range** defaults to a *lower* limit of 1000 Å and *upper* limit of 2.500 Å for all transformation types.

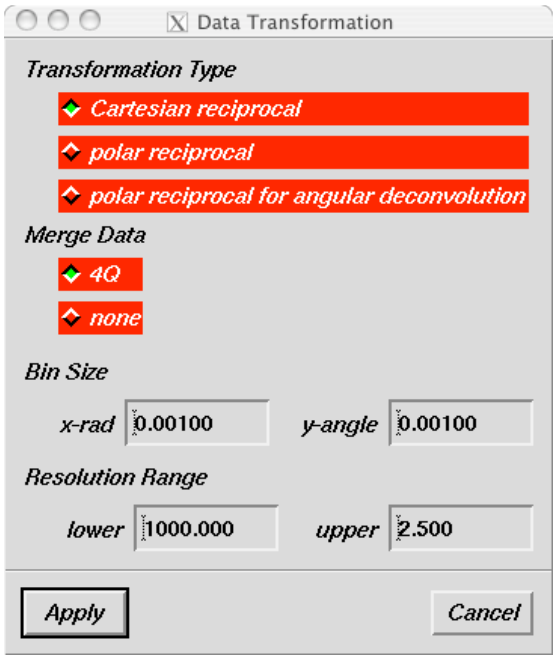

Fig. 11. DATA TRANSFORMATION window

7.3.1 Cartesian Reciprocal *Transform*

This option transforms image from detector space into Cartesian reciprocal space. The bin is a square in reciprocal space and is defined by the **Bin Size** text box *x-rad*. The bin size unit is $Å^{-1}$ and is determined by the value in the *x-rad* box. The value of y dimension of the bin in reciprocal Cartesian transformation has no effect on the size of the bin.

7.3.2 Polar Reciprocal *Transform*

This option transforms image from detector space into polar reciprocal space. The r dimension of the bin is in $Å^{-1}$ whereas the angle dimension of the bin is in degrees.

7.3.3 Polar Reciprocal Transform for angular deconvolution

This option transforms image from detector space into polar reciprocal space, in a format for use with angular deconvolution. The r dimension of the bin is in detector space pixel units whereas the angle dimension of the bin is in degrees. The polar coordinates can be saved in RAD format (see section **3.2**), which can be used directly by RADPV and other related programs. Four quadrants of data are merged after the transformation. After the merge, R-sym is reported in the Log window (see section **8.6**). The reciprocal image will be displayed in the main image window.

8. Windows

WCEN has many tools and functions that appear as popup windows and are contained in the **Windows** menu. Most important of these is the REFLECTION-PARAMETER window, which contains the majority of tools for refining parameters and selecting reflections. The REFLECTION-PARAMETER window has three main functional areas, the *Reflection* pane, *Parameter* pane and the *Zoom* sub-window. Section **8.1** will familiarize users with these functional areas, while section **8.2** will detail menu commands in the REFLECTION-PARAMETER window.

8.1 Functions in the REFLECTION-PARAMETER window

The REFLECTION-PARAMETER window can be opened with just the *Parameter* pane (the PARAMETER window), just the *Reflection* pane and *Zoom* sub-window (the REFLECTION window), or with both sides open together (the REFLECTION-PARAMETER window). Below is a screen shot of the REFLECTION-PARAMETER window, with the main functional areas labeled:

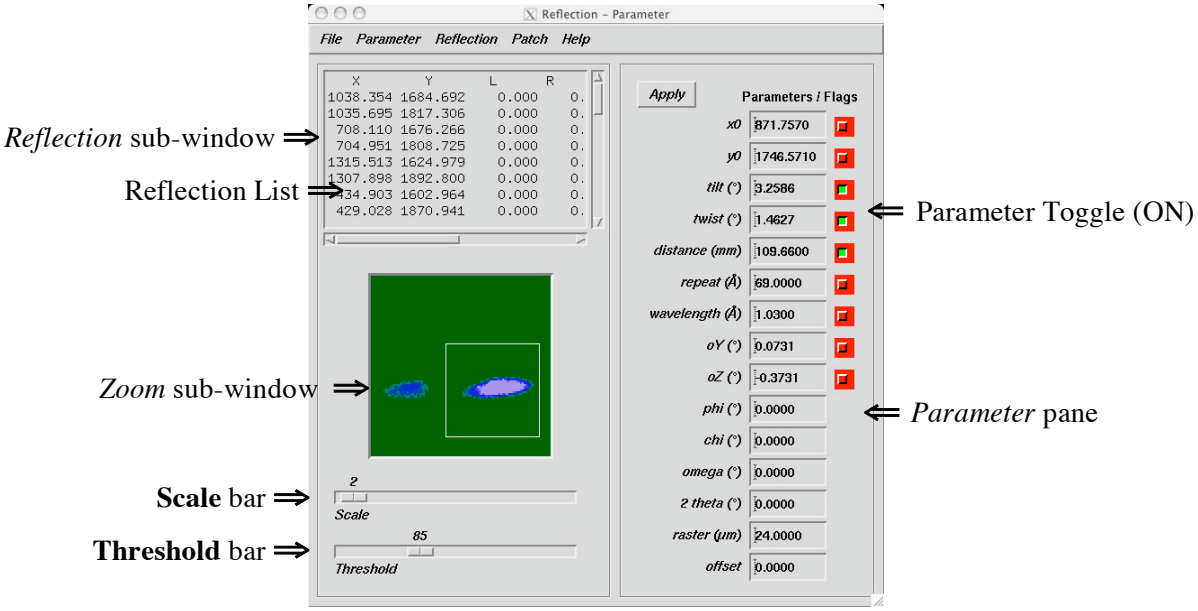

Fig. 12. REFLECTION-PARAMETER window

The *Reflection* pane and *zoom* sub-window are used for selecting reflections from the image loaded into the main window. The PARAMETER PANE is used for refining experimental parameters (see section **8.2.2.6**).

8.1.1 Parameter Pane

In the **Windows** menu select **Parameter** to open the *Parameter* pane in the PARAMETER window. If the REFLECTION window is already open, the *Parameter* pane will be added to the already open window. The following fiber diffraction parameters are listed in the pane:

- **x0, y0:** **pattern center (pixel location)**
- **tilt, twist:** **specimen missetting angles (in degrees)**

- **distance:** **specimen to detector distance (in mm)**
- **repeat:** **fiber repeat distance (in angstroms)**
- **wavelength:** **radiation wave length (in angstroms)**
- **oY, oZ:** **detector missetting angles (in degrees)**
- **phi, chi, omega:** **goniostat setting angles (in degrees)**
- **2 theta:** **2-theta angle (in degrees)**
- **raster:** **pixel size of detector bin or film (in micron)**
- **offset:** **film fog, dark current, or detector offset**
- **calibrant ring:** **the radius of the calibration additive if any (in angstroms)**

Parameter values are edited by changing the numbers in the text boxes. It is not necessary to press `[Return]` to register the changes. Changes to parameters due to refinement will be immediately reflected in these boxes.

Warning! **distance**, **repeat**, and **wavelength** are highly correlated. DO NOT refine any two or all of these parameters at the same time. DO NOT refine **wavelength** under normal circumstances.

8.1.1.1 Apply Button

In the *Parameter* pane, click the **Apply** button to read data from the input boxes into WCEN. The frequency with which WCEN automatically saves parameter data is system dependent, so **Apply** is used to immediately register input data. This is useful when manually changing parameters to fit layerlines (section **6.3**).

8.1.1.2 Parameter Flags

The parameters WCEN can refine using the **Refine selected** (see section **8.2.2.7**) feature have a toggle button to their right. The toggle is engaged when green, disabled when red, and can be switched with a mouse click. When using the **Refine selected** feature, only the parameters with the toggle button enabled (in green) will be refined. In default mode, all the toggle buttons are disabled.

8.1.2 Reflection Pane

In the **Windows** menu select **Reflection** to open the *Reflection* pane in the REFLECTION window. If the PARAMETER window is already open, the *Reflection* pane will be added to the already open window. The reflections listed in the *Reflection* sub-window contains the following data:

X, Y: center position of the reflection in detector space
L: layerline number assigned to the reflection
R: reciprocal space R value
ID: an ID number assigned to this reflection during indexing
Th: threshold value used in reflection centering
nP: number of pixels used in reflection centering

In the *Reflection* sub-window, a single reflection from the list is selected by clicking on it, while multiple reflections can be selected by clicking and dragging the mouse over them. Discontinuous reflections may be chosen by holding down the `Control` key while

clicking on the reflections. Selected reflections in the list will be highlighted if selected. All selected reflections will be marked in the main image window with a small square white box. Scroll bars will appear if the reflection data extends beyond the edges of the *Reflection* sub-window. The *Reflection* pane also contains the *Zoom* sub-window.

8.1.3 Zoom Sub-window (Pixel Selection)

This pane is used to display a small section of the scaled image at the current cursor position in the main image window. To change the area of the image, click on the new area or drag the mouse pointer to the new area in the main image window. You can also make pixel by pixel adjustments to cursor position with the keyboard arrow keys. The *Zoom* sub-window image will change in real time with changes to the cursor's position in the main image window.

THE *Zoom* sub-window can be used to view the image in detail and is used to select pixels for other "actions". Pixels in the *Zoom* sub-window are selected by clicking and dragging the mouse cursor without releasing the mouse button to draw a white selection box. All the pixels within the box and above the threshold value are selected.

Under the *Zoom* sub-window are two control bars: the zoom scale control bar (**Scale**) and the pixel threshold control bar (**Threshold**). To adjust either control bar, click on it with the mouse (a dark box will outline the selected bar) and drag the bar or use the left and right keyboard arrow keys to change the value above the bar. **Scale** is used to change the scale factor of the *Zoom* sub-window, which is an integer from 1 to 64. **Threshold** is used to change the threshold value for pixel selection, which is an integer from 0 and 255. The pixels in the *Zoom* sub-window with a value below the selected threshold value are changed to the threshold color.

8.2 Menus in the Reflection-Parameter window

Experimental parameters including detector origin, specimen to detector distance, missetting angles, specimen tilt and specimen twist angles can be determined and refined in WCEN. Users select the specific parameters to be refined. Before the refinements are carried out, a list of symmetry equivalent reflections must be collected and indexed. For a diffraction pattern from a non-crystalline fiber specimen, a reflection is generally referred to an intensity peak with a well-defined boundary. The REFLECTION-PARAMETER window has all the menus and functions used for selecting reflections and refining diffraction pattern parameters.

8.2.1 File Menu

In the **File** menu users can **Close** the REFLECTION-PARAMETER window or toggle the individual panes opened or closed. Commands for the **File** menu are as follows:

Open/Close param pane:	Opens or closes the *Parameter* pane/window
Open/Close reflxn pane:	Opens or closes the *Reflection* pane/window
Close:	Closes the REFLECTION-PARAMETER window

8.2.2 Parameter Menu

The **Parameter** menu has all the commands directly related to calculation of parameter values in the *Parameter* pane. Users can determine the diffraction pattern **Center from reflection** or the **Center from cursor**, determine the specimen to detector **Distance from reflection** or **Distance from ring**, determine **Detector Fog**, **Save into file** or **Load from file** parameter values and **Refine selected** parameter values.

8.2.2.1 Center From Reflections

In the **Parameter** menu of the REFLECTION-PARAMETER window, click **Center from Reflections** to obtain the diffraction center coordinates (shown as **x0** and **y0** in the *Parameter* pane). It is calculated by a simple averaging of the positions of all currently highlighted reflections from the reflection list in the *Reflection* pane. Only even numbers of reflections will be accepted for averaging.

Warning! The center value calculated will be incorrect unless symmetry equivalent sets of reflections are chosen. Equatorial reflections may be chosen in sets of two and non-equatorial reflections in sets of four.

8.2.2.2 Center From Cursor

In the **Parameter** menu of the REFLECTION-PARAMETER window, click **Center from Cursor** to grab the diffraction center coordinates from the current cursor position in the main image window.

8.2.2.3 Center from objects

In the **Parameter** menu of the REFLECTION-PARAMETER window, open **Center from objects window** to adjust the center by moving objects to fit the pattern (see Section **6.4**).

8.2.2.4 Distance From Reflection

In the **Parameter** menu of the REFLECTION-PARAMETER window, click **Distance from Reflection** to calculate the specimen to detector distance. The radius of the calibration ring is calculated by a simple averaging of the distance to center of all currently highlighted reflections from the reflection list in the *Reflection* pane. For this command to function, the center must be determined accurately, the radius of the calibration ring must be input correctly in the *Parameter* pane, and the reflection in the reflection list must be from the calibration ring.

8.2.2.5 Distance from Ring

In the **Parameter** menu of the REFLECTION-PARAMETER window, click **Distance from Ring** to calculate the specimen to detector distance. The radius of the calibration ring on is taken from the radius of the last circle drawn on the pattern by the **Circle** command of the **Draw** menu in the main image window (see section **6.1**).

8.2.2.6 Detector Fog

In the **Parameter** menu of the REFLECTION-PARAMETER window, click **Detector fog** to define a value for **offset** in the *Parameter* pane. The value input into **offset** is the average pixel intensity of all pixels currently selected in the *Zoom* sub-window (see section **8.1.3**

on selecting pixels). If no selection box is used, all pixels in the *Zoom* sub-window are averaged to determine **offset**.

8.2.2.7 Refine Selected

From the **Parameter** menu of the REFLECTION-PARAMETER window, click **Refine selected** to refine selected parameters using all the reflections in the list. WCEN uses power minimization method for the refinements. The values of the selected parameters will be updated and changes are shown in the *Parameter* pane text boxes after the refinements. When using the **Refine selected** feature, only the parameters with the toggle button enabled (in green) will be refined (see section **8.1.1.2**). In default mode, all the toggle buttons are disabled (in red). Indexing of reflections should be done before parameter refinements (see sections **8.2.3.3** and **8.2.3.4**).

8.2.2.8 Load From File

From the **Parameter** menu of the REFLECTION-PARAMETER window choose **Load from file** to load fiber diffraction parameters and reflections list from a file. The LOAD PARAMETER browser window will open (see section **1.2**). A similar command can be found under the **File** menu in the main image window (section **3.4**). The default file type for the parameter file is `.par`.

8.2.2.9 Save Into File

From the **Parameter** menu of the REFLECTION-PARAMETER window choose **Save into file** to save fiber diffraction parameters and the current reflections list to a file. The SAVE PARAMETER browser window will open (see section **1.2**). A similar command can be found under the **File** menu in the main image window (section **3.5**). The default file type for parameter files is `.par`.

8.2.3 Reflection Menu

All the tools for adding to and deleting from the reflection list as well as indexing command are in the **Reflection** menu.

8.2.3.1 Box Select

From the **Reflection** menu of the REFLECTION-PARAMETER window click **Box select** to determine the weighted center of the selected pixels in the *Zoom* sub-window and add the coordinates to the reflection list of the *Reflection* sub-window (see section **8.1.2**). Pixels are selected using the normal selection method in the *Zoom* sub-window (see section **8.1.3**).

Tip: Select well-defined reflection peaks in the diffraction pattern. A well-defined peak is one with a clearly defined boundary and a symmetrical area. Make sure all symmetry equivalent reflections are well defined for the selected **threshold** value.

8.2.3.2 Mouse Select/Mouse Stop

From the **Reflection** menu of the REFLECTION-PARAMETER window click **Mouse select** to determine coordinates by the position of the cursor in the main image window. Once **Mouse select** is activated, each new cursor click in the main image window will add a new

reflection at the cursor coordinates to the reflection list. When done using **Mouse select**, return to the **Reflection** menu and click **Mouse Stop**.

8.2.3.3 Index

Selecting **Index** from the **Reflection** menu of the REFLECTION-PARAMETER window will bring up the INDEX popup window. Indexing of reflections assigns a layerline number and gives an ID number to reflections. The complete process for manually indexing reflections is given below.

Steps for Indexing Reflections

1) Select a reflection or set of symmetrically equivalent reflections from the *Reflection* sub-window.
2) From the **Reflection** menu of the REFLECTION-PARAMETER window select **Index** to bring up the INDEX window. In the INDEX window, the weighted center position of a reflection in detector space is shown in the top of the window as x, y coordinates.
3) Enter the layerline number in the **layerline** text box for the shown reflection position and an identifying number for the **ID** text box**.** It is not necessary to hit `[Return]` to register the changes in the INDEX text boxes. The **ID** number must be the same for all symmetrically equivalent reflections.
4) Use the **Next** or **Prev** buttons to move between selected reflections and enter or edit the indices. Alternately, click **Apply** if all the selected reflections have the same indices. **Apply** will assign the entered indices of the current reflection to all selected reflections.
5) Click **Close** when you are done indexing the selected reflections.

It is convenient to select only symmetry equivalent reflections when using the **Index** command since all symmetry equivalent reflections have the same indices. Enter the indices for the first reflection then click the **Apply** button to assign the indices to all the reflections in the list. Each reflection should have a unique **ID** number except symmetry equivalent reflections, which must have a unique set **ID** number.

8.2.3.4 Auto Index

From the **Reflection** menu of the REFLECTION-PARAMETER window click **Auto index** for WCEN to calculate the layerline number and assign an ID number to a set of symmetry equivalent reflections. The ID number assigned will be the lowest available integer. **Auto index** uses the repeat variable from the *Parameter* pane and **Z** (which can be shown in the *Coordinate* panel, see section **8.3**) to assign the layerline number. If these parameters are not accurate, the layerline designation may be wrong.

8.2.3.5 Delete

In the **Reflection** menu of the REFLECTION-PARAMETER window, clicking **Delete** will remove any highlighted reflections from the *Reflection* sub-window. The most recently deleted set of reflections are temporarily stored and can be restored to the reflection list using the **Undelete** command (see **8.2.3.6**).

8.2.3.6 Undelete

From the **Reflection** menu clicking **Undelete** restores to the *Reflection* sub-window the reflections removed by the most recent **Delete** command (see **8.2.3.5**).

8.2.4 Patch Menu

The **Patch** menu allows users to alter the intensity of individual image pixels. Users can **Set pixel value** or **Erase pixel value**, then **Make changes permanent** or **Reset pixel value** as needed. **Patch** is useful when trying to box select highly disordered reflections close to other reflections. In such a case, the rectangular box often cannot isolate a peak unless some pixel intensities are manually removed in the target peak's vicinity.

8.2.4.1 Set pixel value

From the **Patch** menu click **Set pixel value** to alter the intensity of the selected pixel or pixels. Use the *Zoom* sub-window to box select the pixels to be altered (section **8.1.3**). Next, click **Set pixel value** to open a popup window where you can specify a new pixel intensity in the *enter pixel value* text box. Click **Apply** in the window and the pixel values will be set to the specified value.

8.2.4.2 Erase pixel value

The **Erase pixel value** command will set the selected pixel or pixels to intensity -999. Pixel selection is identical to the **Set pixel value** command (section 8.2.4.1).

8.2.4.3 Make changes permanent

Make changes permanent will make the effects of all previous **Patch** menu operations permanent, that is, you will have to reopen the image to restore the original intensities.

8.2.4.4 Reset pixel value

Reset pixel value will restore the original intensities for the pixels you have altered provided that **Make changes permanent** has not been applied.

8.2.5 Help Menu

In the **Help** menu of the REFLECTION-PARAMETER window, click **Parameter Definition** to open the PARAMETER DEFINITION popup window. This window has a list with definitions of the parameters in the *Parameter* pane (see **8.1.1**). To close the PARAMETER DEFINITION popup window, click the **Close** button at the bottom of this window.

8.3 Coordinate

From the **Windows** menu, select **Coordinate** to open the *Coordinate* panel at the top of the main window (see Fig. 2). The *Coordinate* panel shows six values for the pixel closest to the current cursor position:

- **x:** x-coordinate of the cursor
- **y:** y-coordinate of the cursor
- **r:** cursor to center distance
- **I:** pixel intensity at cursor
- **d:** d-spacing

R: polar reciprocal radius
Z: z-coordinates of reciprocal vector

The values **d**, **R**, and **Z** are calculated from variables in the *Parameter* pane, so they are only as accurate as the refinement.

8.4 Pixel Intensities

From the **Windows** menu, choose **Pixel Intensities** to bring up the PIXEL INTENSITIES window. This window can also be opened from the Image Repair window (see section **4.3**). This window displays the intensity value of pixels in an 11x11 pixel area at the last cursor position before the window is brought up. The pixel location is given by x values along the top edge and y values along the left edge. Below the pixel table are these variables:

lmax: Maximum intensity value in the displayed area.
lmin: Minimum intensity value in the displayed area.
lave: Average intensity value of the displayed area.
lsig: Standard deviation of intensity values in the displayed area.
gmax: Maximum intensity value of the entire image.
gmin: Minimum intensity value of the entire image.

(l for local; g for global)

These values are not affected by manipulation of the histogram in the COLORMAP CONTROL window (section **5.3**). The pixel values can be updated to the current cursor position by clicking the **Update** button in the lower left of the PIXEL INTENSITIES window. Click the **Close** button at the bottom right to close the window when finished.

8.5 Full Pattern

From the **Windows** menu, select **Full Pattern** to open the FULL PATTERN window. The FULL PATTERN window will show a smaller version of the entire image with the x,y pixel dimensions of the scaled image on the window's title bar. The FULL PATTERN window will have the same orientation as the main image and can be manipulated, along with the main image, using **Flip** and **Rotate** (sections **4.2** and **4.3**). The FULL PATTERN can be resized by dragging the bottom right corner of the window with the mouse. To close the FULL PATTERN window, go to the **Windows** menu and click **Full Pattern** again, or click close on the title bar.

Tip: It is very helpful to pull up the full pattern when changing the colormap to see the complete effect of the changes.

8.6 Log

Go to the **Windows** menu and click **Log** to open the *Log* pane at the bottom of the main window. The *Log* pane will show calculations of WCEN during parameter refinement. To close the *Log* pane, go to the **Windows** menu and click **Log** again.

9. Help

WCEN was first released in 2006 (W. Bian, H. Wang, I. McCullough, G. Stubbs. WCEN: A Computer Program for Initial Processing of Fiber Diffraction Patterns. J. Applied Crystallography, 39:752-756, 2006), and now in version 1.1. The work is supported by *FiberNet*, formally known as Research Coordination Network: Fiber Diffraction from Biological Polymers and Assemblies, which is supported by the National Science Foundation's Division of Molecular and Cellular Bioscience, through grant MCB-0234001.

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For manuals, tutorials, and other resources, please visit

http://fibernet.vanderbilt.edu/software/wcen.

Appendix

Customizing WCEN

WCEN can be customized through an X resource file to be more effective. The file is usually located under directory /etc/X11/app-defaults or /usr/X11R6/lib/X11/app-defaults, or within the file .Xdefaults in your home directory.

Here are some customizable resources (Lines beginning with ! are comments):

```
!
! supported image format: IFM_BSL, IFM_MAR, IFM_PES, IFM_RAW, IFM_RAV,
!                          IFM_SMV, IFM_TIF
!
! default image format:
!
wcen.defaultImageFormat: IFM_SMV
!
!
! predefined colormap: CMP_Rainbow, CMP_Keiichi, CMP_RGB, CMP_BGR,
!                      CMP_BlackWhite,  CMP_WhiteBlack, CMP_BlueRed,
!                      CMP_BlueYellow, CMP_CyanRed, CMP_GreenPurple,
!                      CMP_GreenRed
!
! default colormap:
!
wcen.defaultColormap: CMP_Rainbow
!
!
! opticalDensityToPixel is used in non-linearity correction to
! convert optical density to pixel value, if a film is used.
!       * P-1000 Optronics: 136.0
!       * Perkin Elmer MicroDensitometer: 1216.0
wcen.opticalDensityToPixel: 136.0
!
!
```

The rest resources control the look and feel of WCEN and should be customized with caution.