Sample Rastering

Sample rastering is the process of collecting single frames at different sample locations (sample goni x,y, and z positions). This method can be used to find a crystal in a loop or to find the "best" region on a crystal. This method can also be used to align a crystal using diffraction.

The sergui implementation of this experimental technique is controlled through a stand alone gui that is opened from the main sergui/Automation/Sample Rastering pull down menu. The gui is divided into 2 sections: Collection Parameters and Results.

Collection Parameters

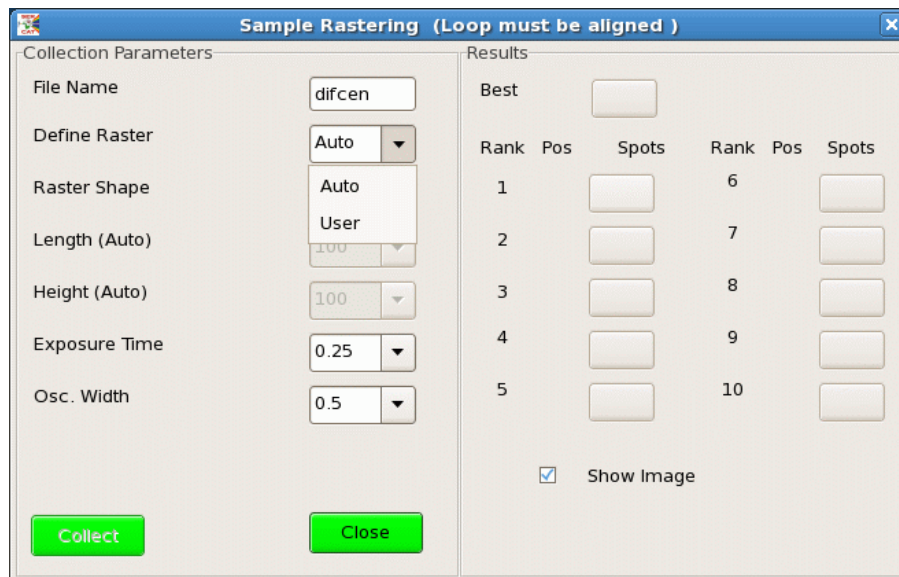All parameters except the file name, can be selected by use of the pull down options in this section

Figure 1. Image shows pull down menu usage for defining the type of raster.

File Name: input unique file name for file storage. All files will be saved to your archive
        directory.

Define Raster: The region of interest (roi) of the raster search can be defined
        automatically (Auto) or by the user (User).

Raster Shape: The shape of the roi for the automated method can be either a vertical
        Line, rectangular or 3D. The user method adds a parallelogram to
        the options.

Length (Auto): Enabled when an Auto Rectangle has been selected. This option will modify the horizontal range of the roi.

Height (Auto): Enabled when an Auto Line or Rectangle has been chosen. This option will modify the vertical range of the roi

Exposure Time: The exposure time in seconds used for each frame

Osc. Width: The oscillation width in degrees used for each frame

Defining an Automated ROI

The automated method will define a roi centered on the red cross hair in the sample image.
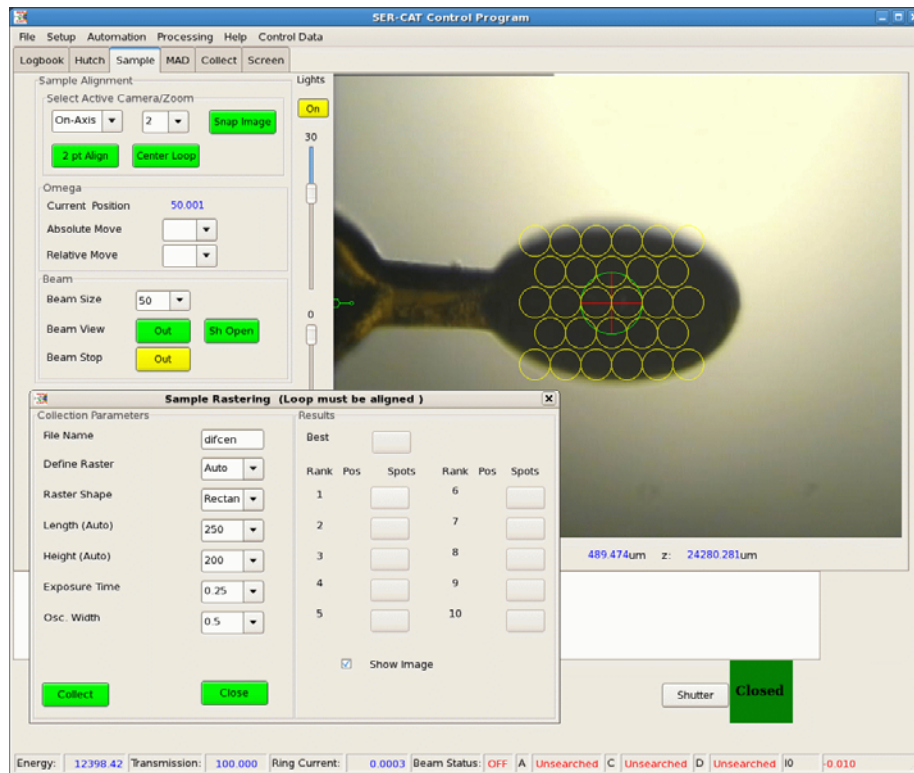

Figure 2. This image shows an automated rectangular roi with a horizontal range of 250 microns and a vertical range of 200 microns.
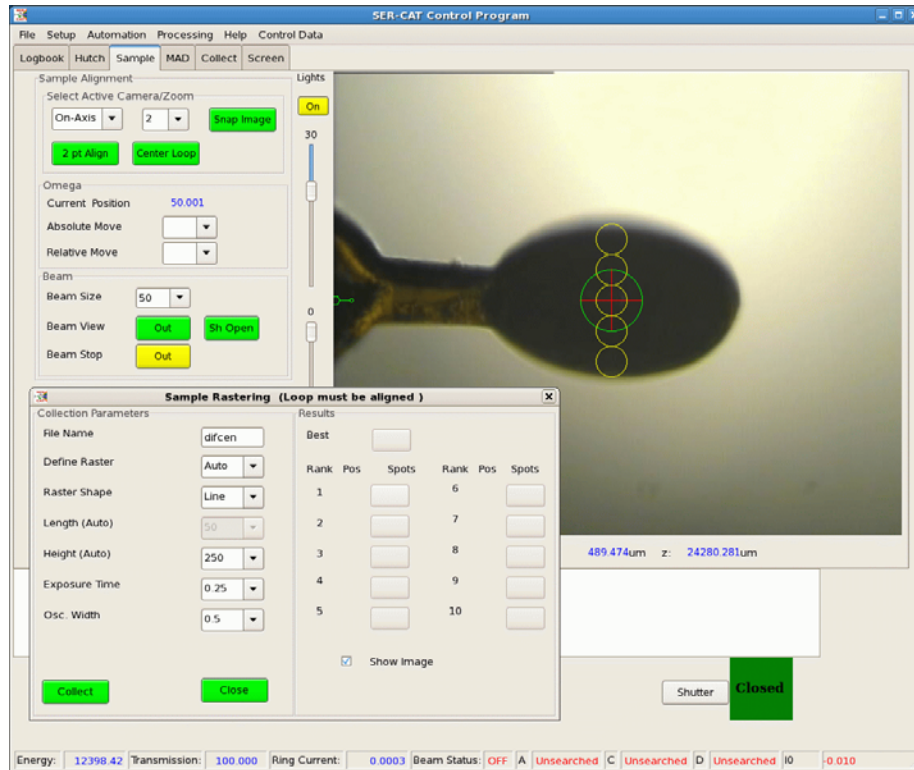
Figure 3. This image shows an automated line with a vertical range of 250 microns.

The length (horizontal) and height (vertical) of the roi can be changed by selecting different values for the appropriate pull down menu.

Figures 2 and 3 show yellow circles, of the current beamsize, where a data frame will be collected. Yellow indicates that the data frame is waiting to be collected.

Note: On 22ID, the beamsize can be changed after the definition of an roi has been established. The program will automatically redefine the current range suing the new beamsize.

Defining a User ROI

This method can define an roi that is not centered on the red cross hair. The roi can be a line, rectangle, parallelogram, or 3D. After the raster shape is chosen for a User defined raster, the user will be prompted in the gui and the standard out of Sergui to click in the sample display.
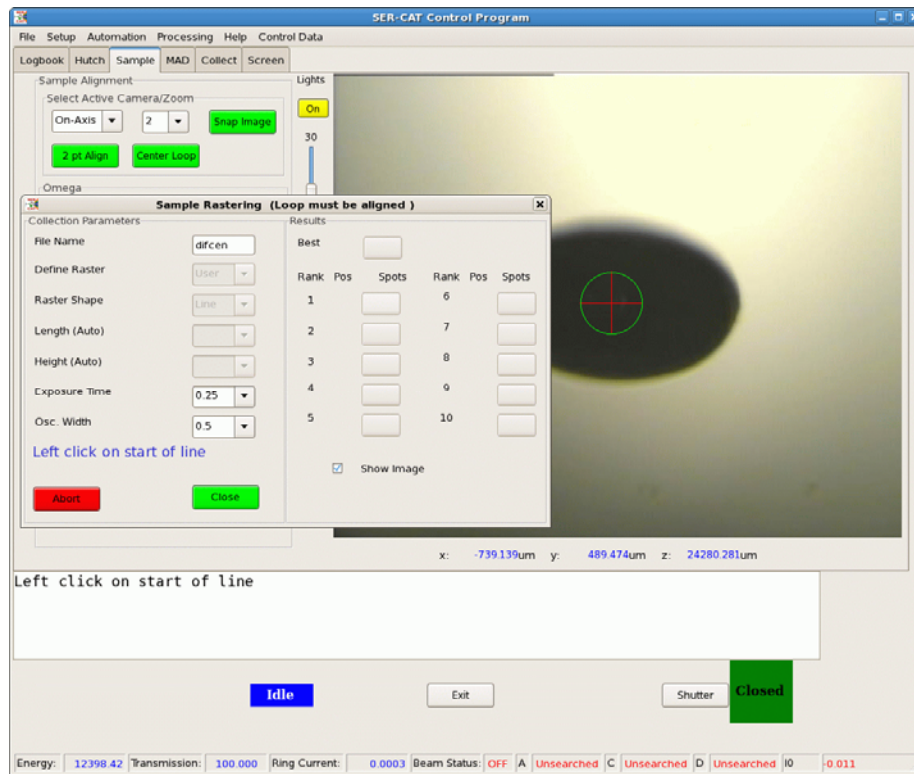

Figure 4. This figure shows the changes to the gui for a user defined shape.

In the example above, a user defined line has been chosen. Note that the Collect Button has been changed to an Abort button, which will cancel the current process and reinitialize the gui. For a line, the user must left mouse click on the start and end of the line. For a rectangle or parallelogram, the user is prompted for 4 mouse clicks defining the corners of the shape. The Length and Height pull downs are disabled for this method and a new roi must be defined to change the range of the raster scan.

Note: At any time during this process the use can use the Abort button to leave the process of defining the shape of the roi.

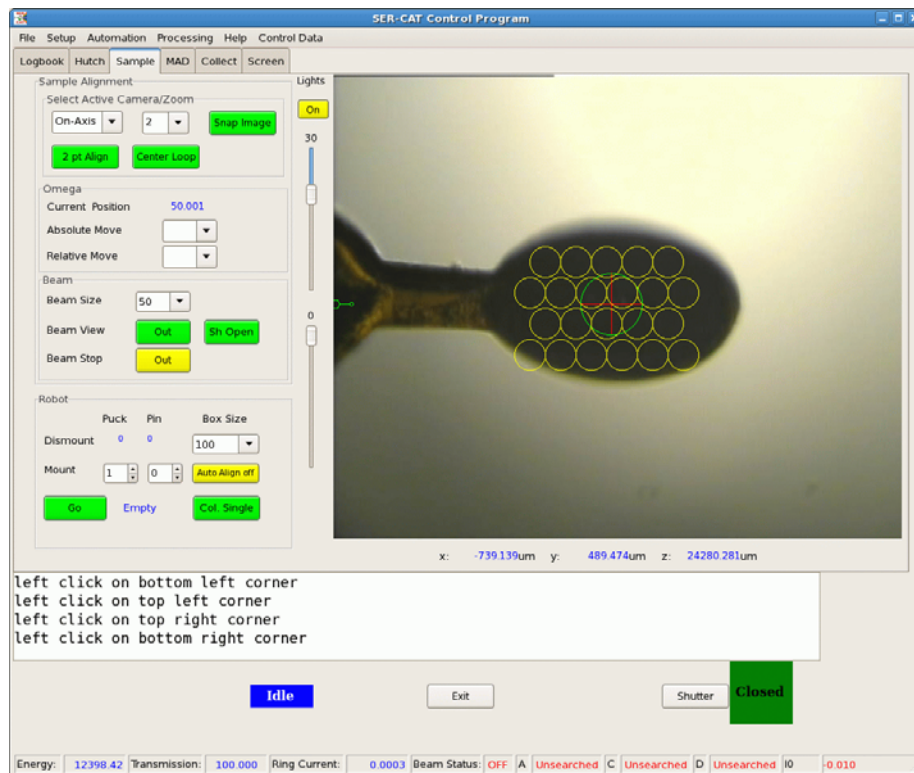Figure 5. This figure show the results of a user defined line.
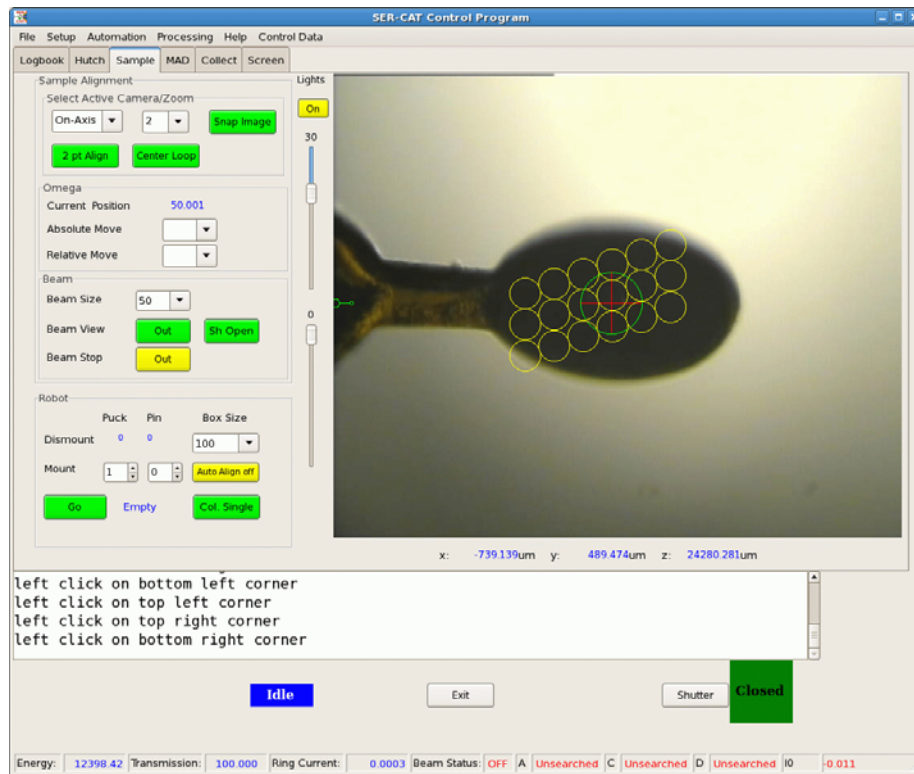

Figure 6. A user defined rectangle

Figure 7. A user defined parallelogram

The versatility of a user defined roi can allow the user to optimize their search pattern to better match the sample geometry or loop shape.

Note: The reasoning behind providing both types of roi definition was based on possible problems with a user's remote connection as well as automation.

Defining an Auto/User 3D Shape

The 3D options for both the Auto and User selection can be used to center your sample using diffraction. In each case a rectangular region will be defined first. After the rectangular region has been collected and processed, the sample will be rotated 90 degrees in omega and a line (identical to the Auto/Line option) of data will be collected. The range of the line will be determined by the software. The lights will be inserted and image analysis software will be used to determine the range of the line that includes the full vertical extent of the loop.

Collecting Data

Once the roi has been defined, the Collect Button will be enabled. Once pushed, the Collect Button will turn into an Abort Button. The Abort Button will terminate the data collection after the current frame and then ask the user if they want to analyze the data that has already been collected. During the data collection, the yellow circles will change color to either Green or Red. Green indicates that there were diffraction spots in the given frame while Red indicates that no diffraction was detected. After the data collection has completed, or an Abort has been continued, the result section of the gui will be enabled an updated and a load raster pull down menu will also become active (this will be discussed in the results section).

Pressing the Abort Button will give the user the option to terminate the entire process immediately, or to terminate the data collection but process the data that has been collected. Continuing with the data processing is useful if a large region has been defined and the sample has been found.
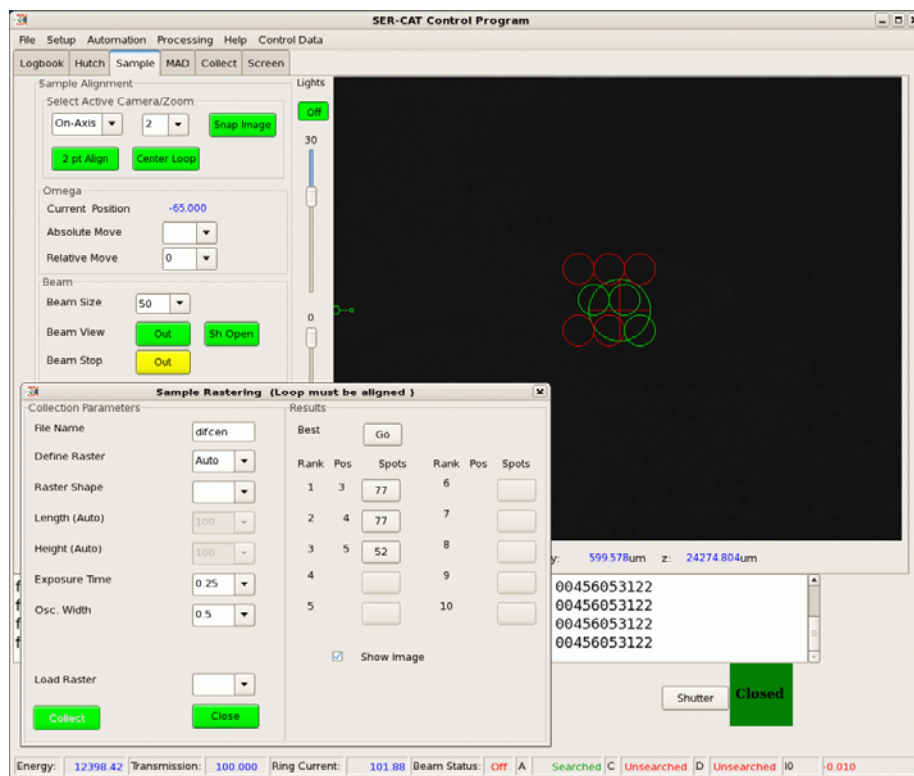

Figure 8. This figure shows the status of the gui after a completed Auto/rectangle raster.
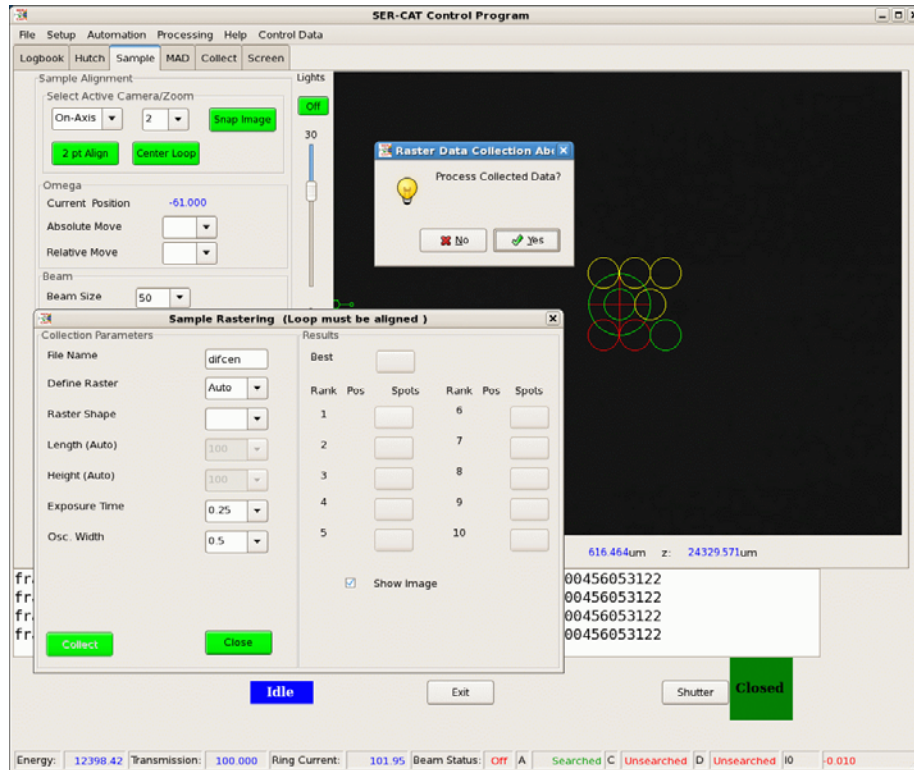
Figure 9. This figure shows and active data collection after the Abort Button has been pressed.

Results

The Results section includes the following:

(1) Multiple buttons for the various ranks of the frames collected
(2) A button for the "Best" position
(3) A check box labeled Show Image.
(4) A Load Raster pull down menu will also become active in the Collection Parameter section.

Result Buttons

The data will be ranked using the number of spots detected as well as the intensity in these spots. The Rank Buttons indicate the rank of each frame in which diffraction spots were detected. The ranking (spots column) is just by number of spots in the frame. The Pos(ition) indicates the frames position in the data collection sequence. If spots were not measured in a frame it will not be ranked.

Pressing an active button will move the sample to the position the data were collected, and if the Show Image check box is active display the image using the program marimage.

Best Button

The Best Button is a weighted averaging of all of the ranked image positions. The Best position will automatically be moved to after a completed raster data collection. Pressing this button will move the sample to the calculated "Best" position.

Show Image

Toggles on/off the displaying of the diffraction images when the Results Buttons are pushed.

Load Raster

The options under the Load Raster pull down menu are the results of the most recent rasters for the currently mounted sample. The naming convention of this section are self explanatory; Auto_AL indicate the results of an Auto/Line. The number of options will increase as different methods of rastering are completed for the current sample. Selecting an option from the Load Raster menu will load the results for that raster into the Results section and rotate omega to the value used for this raster.