mar research

The mar345 Program Manual

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The ***mar345*** Program Manual

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Written by Dr. Claudio Klein

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1. Introduction

The program ***mar345*** is a fully menu driven graphical user interface (GUI) for collecting and displaying images on a ***mar345*** imaging plate system.

The program is provided as binary executable for several computer platforms and operating systems:

- **Silicon Graphics**: IRIX 5.x, 6.x
- **Digital**: Compaq Tru Unix 4.x, 5.x
- **Linux**: RedHat 5.x, 6.x, SuSE 6.x

1.1 Computer Requirements

- Motif 1.2.x shared libraries (except Linux).
- 8/16/24/32-bit colors X-windows terminal with 1280x1024 pixels.
- Standard Helvetica and Symbol fonts.
- 96 MB RAM memory or more.

1.2 Environment

The program relies on definitions of the following environment variables:

- **MARTABLEDIR** Location of the scanner specific calibration files **mar2300.XXX** and **mar3450.XXX** and the corresponding configuration file **config.XXX** (where XXX = MAR_SCANNER_NO).
- **MAR_SCANNER_NO** Three digit serial number, e.g. 049.
- **MARLOGDIR** Location of the log output files.
- **MARHELPDIR** Location of interactive help files.

The program relies on the correct network setup, i.e. the **mar345** scanner must be accessible by **ping** and **telnet** with IP-address 192.0.2.1.

For a description of the setup of the ***mar345*** software suite, see the "***mar345 Installation Guide***".

2. Running *mar345*

2.1 Command Line

The program ***mar345*** should be started by just typing "*mar345*". The program, however, understands the following command line options:

mar345 **[-h] [-colors N] [-def XXXX] [-host HOST] [-keep] [-more N] [-noxf] [-port PORT] [-setd]**

The command line options are:

-h Print a usage summary

-colors N Use N colors for drawing images.
Default: take N from configuration file.

-def XXXX When starting the program, go to scanmode XXXX where XXXX is 1200, 1600, 1800, 2000, 2300, 2400, 3000 or 3450.
Default: stay in current scan mode.

-host HOST Connect to host HOST.
Default: take HOST from configuration file (usually 192.0.2.1)

-keep Spiral images will be saved on disk.
Default: do not produce spiral files, only transformed images.

-more N Log output level with N=0, 1, 2 or 3.
Use more > 0 only in case of hardware problems.
Default: N=0 (compact output)

-noxf Spiral images will not be transformed into Cartesian images. The program then requires much less memory, but images cannot be displayed.
Default: Do transform spiral images.

-port PORT Connect to host HOST via socket port PORT.
Default: take PORT from configuration file (usually 4441)

-setd The user may redefine the distance detector to crystal from within the program.
Default: Redefining the distance is disallowed..

2.2 Input Files

The program ***mar345*** requires the following input files to work properly:

a) $MARLOGDIR/mar345.dat
The program continuously saves edited parameters into this file. It is nice to find the program in the same state where you left it at startup. However, if mar345.dat cannot be found, program defaults will be used.

b) $MARTABLEDIR/config.XXX
XXX is a 3-digit serial number. This file contains essential scanner specific information. For the scanner to produce valid data it is essential to have this file with all entries corresponding to valid parameters for the scanner. The program ***mar345*** will use program defaults if this file is not available.

c) $MARTABLEDIR/mar2300.XXX
XXX is a 3-digit serial number. This file contains flat-field corrections and the geometry table for transforming spiral images into Cartesian images for all scans at 0.15 mm pixelsize. This file is scanner-specific and required to do scans in 0.15 mm pixel modes. The typical size of this file is 73 MB.

d) $MARTABLEDIR/ma3450.XXX
Same as mar23000.XXX but used for all scans at 0.10 mm pixelsize. The typical size of this file is 103 MB.

See Appendix A and B for more information about input files.

2.3 Output Files

The program ***mar345*** writes all relevant messages to standard output but it also produces several types of log files, depending on the configuration. Since log files can be important to look at in case of software or hardware problems, the program creates different versions of log files named:

1.) **$MARLOGDIR/log/mar.log.X** (always)
2.) **$MARLOGDIR/spy/mar.spy.X** (configuration file entry: **USE SPY**)
3.) **$MARLOGDIR/lp/mar.lp.X** (configuration file entry: **USE STATS**)

where **X** is a number running from 1 to 99. All log files reside in the subdirectory assigend by the logical variable MARLOGDIR. In this directory, there is also a file called "last.log" that contains only the version number of the latest (i.e. current) log file and a soft link of **mar.log** to the latest mar.log.X file in subdirectory log. Accordingly, soft links are also set to files mar.spy and mar.lp if configured..Up to 99 copies of the log files will be kept and then cyclically overwritten.

The contents of the different types of log files are as follows:

1.)	**mar.log:**	All messages on the terminal output.
2.)	**mar.spy:**	Native mar345 controller messages. These messages become very important in case of hardware problems. Therefore, **USE SPY** should always be set. Note, that these files can become very large in size, so sufficient disk space should be available in $MARLOGDIR (up to 100 MB in total).
3.)	**mar.lp:**	Some image statistics like minimum, maximum and average intensity. Normally, these values are not of much interest, so **USE STATS** should rather be the exception.

2.4 Basic Concepts and Rules

The program has to perform different tasks:

- Allow user input (i.e. change data collection parameters, analyze images, etc.)
- Send commands to the scanner.
- Receive information from the scanner
- Transform spiral images into Cartesian images.
- Display transformed images.

User input is done via the graphical user interface (see chapter 3).

Communication with the scanner is realized through an Ethernet interface. Usually, the host computer features a dedicated Ethernet card for communicating with the scanner. Host computer and scanner are linked via a so called "cross-over cable", i.e. a special RJ-45 type cable that allows for directly connecting 2 computers without the need of a hub.

Transformation and data display requires some memory as well as CPU-time. Typically, ***mar345*** keeps the equivalent of 2.5 images in memory. When using 3450x3450 pixel images this corresponds to **75 MB**.

Data collection should always have **highest priority**. However, there is no real protection against abuse of the computer by other processes. In particular, memory consuming data processing jobs can cause drops in performance of the workstation to such a degree that nothing else will work. Also network I/O can severly degrade the host computer performance, e.g. when processing data across NFS-mounted disks!

2.5 Starting Up

Create a new window for running the program and type: "*mar345*". Do not run the program in the background and do not use this window for other purposes. The program will send important output to the window and you don't want to miss it.
At start up, the program will tell you something like:

```
============================================================
         Program      :  mar345
         Version      :  2.0.8 (Feb 16 2000)
         Scanner no.  :  049
         Scanner mode:  345 mm @ 0.15 mm
         Started on   :  Wed Feb 16 15:09:08 2000
         LOG  file is:  /home/mar345/log/log/mar.log.58
         SPY  file is:  /home/mar345/log/spy/mar.spy.58
         STAT file is:  /home/mar345/log/lp/mar.lp.58
============================================================
```

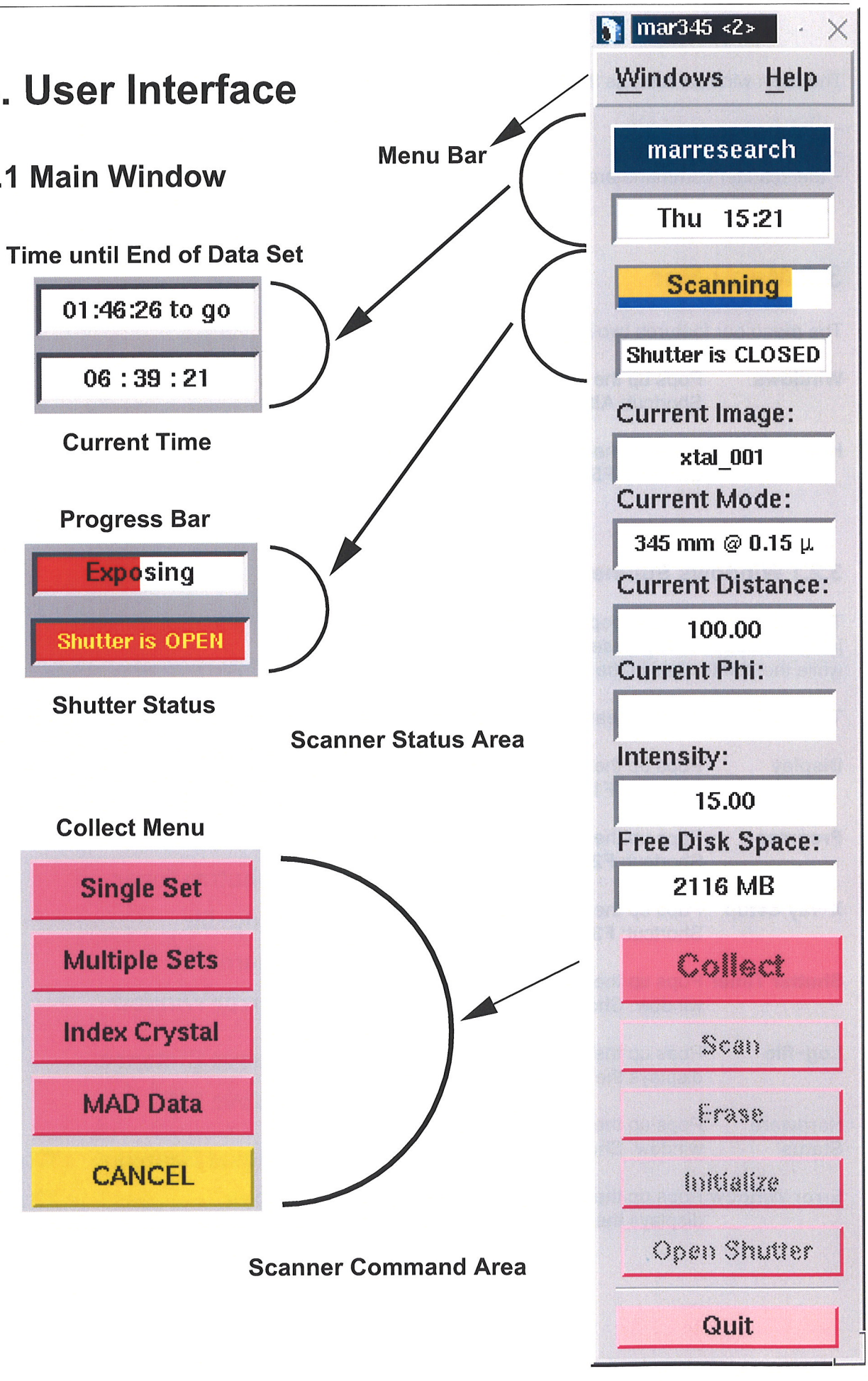
It will also tell you if it is able to talk to the scanner. If environment variables are not set you will be notified. Next, three windows will be created and automatically placed on the screen: a startup window, the mar345 main window and an empty image display window.

If the scanner is not turned on at all, by invoking program mar345 on the command line, you will not get any feed back. This is because the program tries to open a network connection to the scanner and the program will sit there and wait until the scanner starts talking to it.

When the scanner is turned on, the scanner controller will start very quickly basic network services, so a ping to the address of the scanner (usually 192.0.2.1) will work within 10 seconds after turning the scanner on. However, before starting communication with the program mar345, the scanner must do first some initialization, i.e. drive the scanning head to its default position (scan mode 2300) and lock the plate. Only when the plate is successfully locked ("cling!") program ***mar345*** can start talking to the scanner. You may, however, start the program first and then turn on the scanner. The program really waits until a connection can be established.

3. User Interface

3.1 Main Window



The main window controls the most important scanner functions. It consists of different areas:

- a menu bar
- the scanner status area
- the scanner command area

3.2 Menu Bar

The menu bar features two buttons:

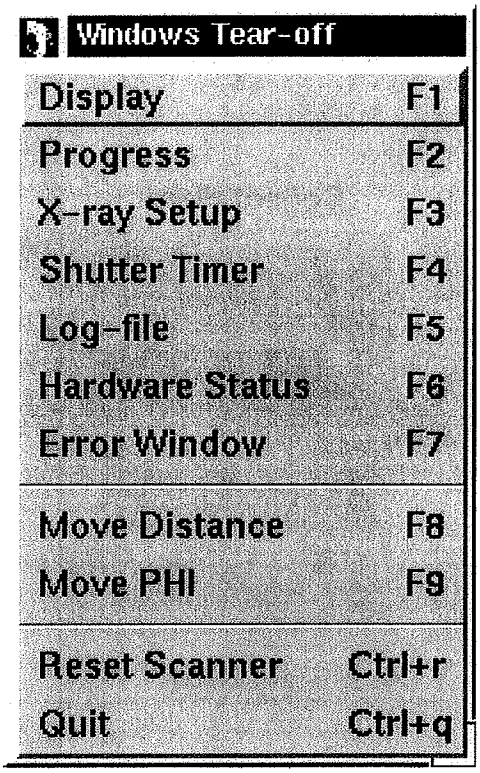
Windows Pops up the ***Windows*** submenu (3.2.1). Shortcut: **Alt+w**.

Help Pops up the ***mar345-Help*** window. Shortcut: **F5**.

3.2.1 Windows Submenu

The Windows submenu pops up if the "Windows" button in the menu bar was pressed or if **"Alt+w"** was pressed while the pointer was in the main window.

The Windows submenu features the following buttons:



Display Pops up the ***mar 345-Display*** window. Shortcut: **F1.**

Progress Pops up the ***mar345-Progress*** window. Shortcut: **F2.**

X-ray Setup Pops up the ***mar345-Setup*** window. Shortcut: **F3.**

Shutter Timer Pops up the ***mar345-Shutter Timer*** window. Shortcut: **F4.**

Log-file Pops up the ***mar345-Help*** window and displays the current log file. Shortcut: **F5.**

Hardware Status Pops up the ***mar345-Hardware Status*** window. Shortcut: **F6.**

Error Window Pops up the ***mar345-Error*** window and displays the current errors. Shortcut: **F7.**

Move Distance	Pops up the ***mar345–Distance*** window. Shortcut: **F8.**
Move Phi	Pops up the ***mar345–Phi*** window. Shortcut: **F9.**
Reset Scanner	Reboots the scanner reboot. Shortcut: **Ctrl+r.**
Quit	Quits program. Shortcut: **Ctrl+q.**

3.3 Scanner Status Area

The status area provides at all times all necessary information about the current status of the scanner.This part of the user interface changes dynamically according to the current scanner operation. It features the following items:

Item	Description
marresearch / Time until End	During data collection, this field shows the time it takes to finish all active or queued data sets.
Current Time	Displays local computer time.
Progress Bar	If the scanner is performing an operation, the progress of this operation will be displayed with a colored progress bar and an appropriate text string.
Shutter Status	Shows the state of the local X–ray beam shutter (open or closed).
Current Image	Shows the name of the current image leaving out the directory and file name extension.
Current Mode	Shows the current scanmode of the scanner.
Current Distance	Shows the current distance of detector to crystal.
Current Phi	Shows the current position of the PHI axis.
Intensity	Displays the current intensity reading of the selected ionization chamber.
Free disk space	Shows how many MB of disk space are available on the disk where the current image will be written to.

Under normal conditions, the program retrieves status information from the scanner once a second. The time and the free disk space will be updated less frequently.

Note: Timing is a crucial issue when operating the scanner. If the computer is very busy doing other computations, the internal clock of the program will work slower. A good check for excessive computer activity is if the X-windows server is not able to repaint the user interace at a reasonable speed.

3.4 Scanner Command Area

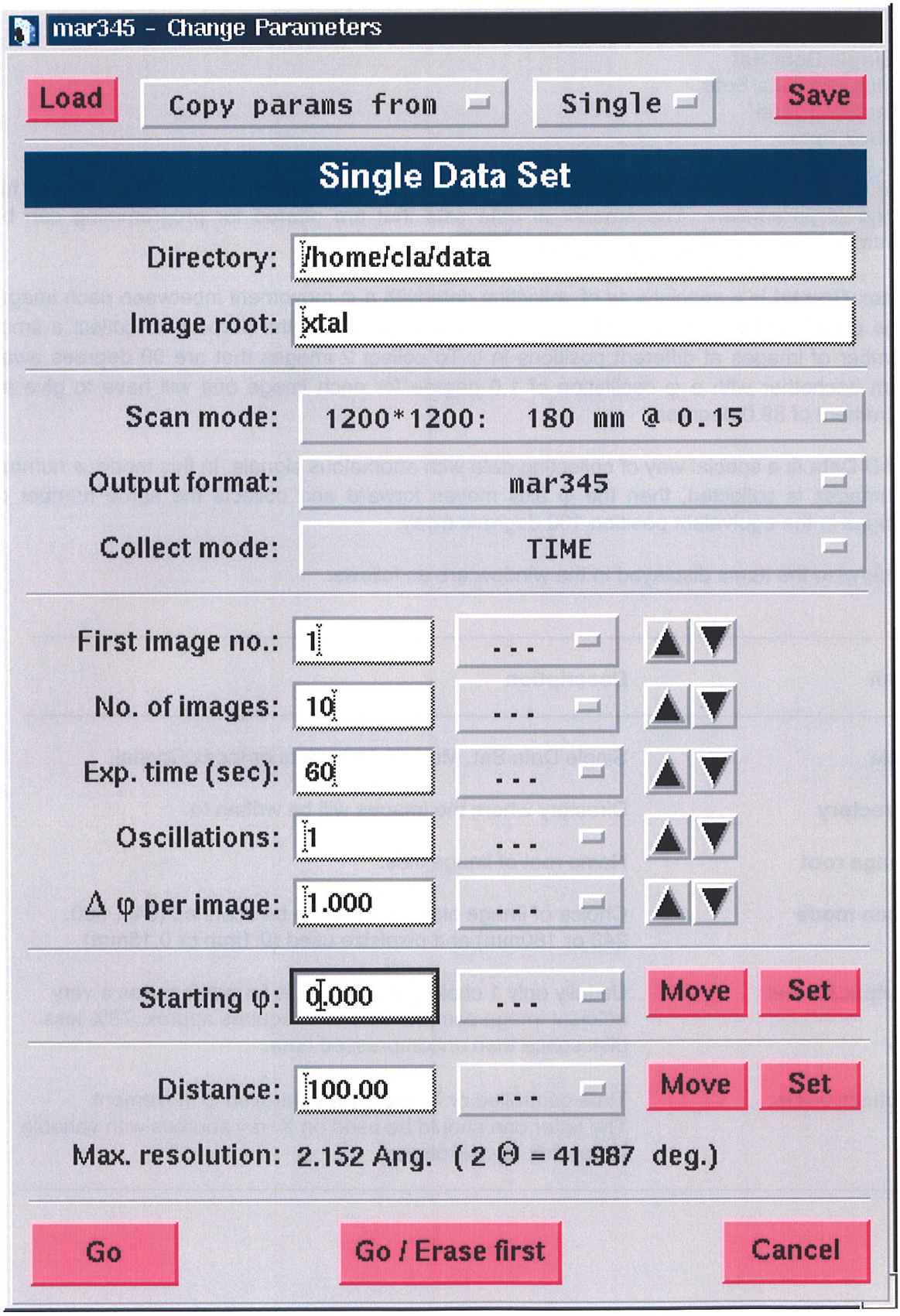
The buttons in the command area can be used to send commands directly to the scanner or to pop up further windows, i.e. the ***mar345-Scan*** and ***mar345-Change Parameters*** windows. The functions of the individual buttons are:

Button	Description
Collect	Changes layout of the button choices, i.e. the ***Collect Menu*** buttons are displayed.
Scan	Pops up the ***mar345-Scan*** window.
Erase	Immediately starts to erase the imaging plate. Erasing is identical to doing a scan, but no data are taken.
Initialize	The scanner will move to its distance reference position (usually at the far end of the translation stage). This distance initialization may have to be done if the scanner looses the information about the distance for some reasons. The reference positions are taken from the configuration file. The detector movement has to be confirmed. The configuration file will be reread when pressing this button.
Open Shutter	Opens (or closes) the local X-ray beam shutter.

And in the ***Collect Menu*** there are:

Single Set	Pops up the ***mar345-Change Parameters*** window for programming a single data set.
Multiple Sets	Pops up the ***mar345-Change Parameters*** window for programming up to 64 data sets.
Index Crystal	Pops up the ***mar345-Change Parameters*** window for programming a small number of images to be used for indexing a crystal.
MAD Data	Pops up the ***mar345-Change Parameters*** window for programming a data collection typical for anomalous and/or MAD data.
Cancel	Returns to the original layout.

3.5 Editing Data Collection Parameters



The ***Change Parameters*** window is used to program data collection parameters. The window comes in 4 slightly different flavours, depending on the button choice in the ***Collect Menu***:

- **Single Data Set**
- **Multiple Data Sets**
- **Index Crystal**
- **MAD Data**

The difference is, that in **Multiple Data Sets** one can program up to 64 data sets with the full range of parameters. The amount of data sets that are offered for programming can be controlled by the configuration file (entry **SETS**).

Index Crystal is a special way of collecting data with a φ movement inbetween each image. This φ movement is denominated "φ increment" and serves the purpose to collect a small number of images at different positions in φ.To collect 2 images that are 90 degrees away from eachother with a φ oscillation of 1.0 degree for each image one will have to give an increment of 89.0 degrees.

MAD Data is a special way of collecting data with anomalous signals. In this mode, a number of images is collected, then the φ axis moves forward and collects the same number of images in the equivalent position 180 degrees away.

Otherwise the items displayed in the window are as follows:

Item	Description
Title	Single Data Set, Multiple Data Sets or Index Crystal.
Directory	Directory where the images will be written to.
Image root	Name root of image files.
Scan mode	Choice of image plate diameter to be scanned (345, 300, 240 or 180mm) and pixelsize used (0.1mm or 0.15mm)
Output format	Usually only 1 choice: mar345. This format features a very efficient image compression that requires approx. 70% less disk space than uncompressed data.
Collect mode	Time controlled or X-ray dose controlled φ movement. The latter one should be used on X-ray sources with variable X-ray flux (synchrotrons).

Table continued from previous page.

Item	Description
First image no.	Image number of first image. Range is 1 through 999.
No. of images	Number of images to be collected. Range is 1 through 999.
Exp. time	Exposure time in seconds. In DOSE mode, the actual time may be different from the desired exposure time.
Oscillations	Number of φ–oscillations per image. One oscillation is stronlgy recommended for exposure times < 15 min.
Δ φ per image	φ movement per image.
Starting φ	φ position to start data collection.
Distance	Distance crystal to detector.

For convenience, the program calculates the maximum resolution possible from the chosen distance and the chosen scan mode (image plate diameter).

The image names are created according to the following convention:

directory / root_TYPE_XXX.extension

- **TYPE** is:

not used	in ***Single Data Set*** mode	e.g. /images/zeo_001.mar1200
1, 2, 3 or 4	in ***Multiple Data Set*** mode	e.g. /images/zeo_1_001.mar1200
INDEX	in ***Index Crystal*** mode	e.g. /images/zeo_INDEX_001.mar1200
A or B	in ***MAD Data*** mode	e.g. /images/zeo_A_001.mar1200

- **XXX** is a three digit image number like 027,
- **extension** is:mar1200, mar1600, mar1800, mar2000, mar2300, mar2400, mar3000 or mar345 for ***Output format*** "mar345", depending on the ***Scan mode*** chosen.

In ***Index Crystal*** mode **"First image number"** is replaced by "φ **increment"** (see above). The starting image will always be 001 and the following images will have numbers that will be calculated from their φ–position relative to image number 001 according to:

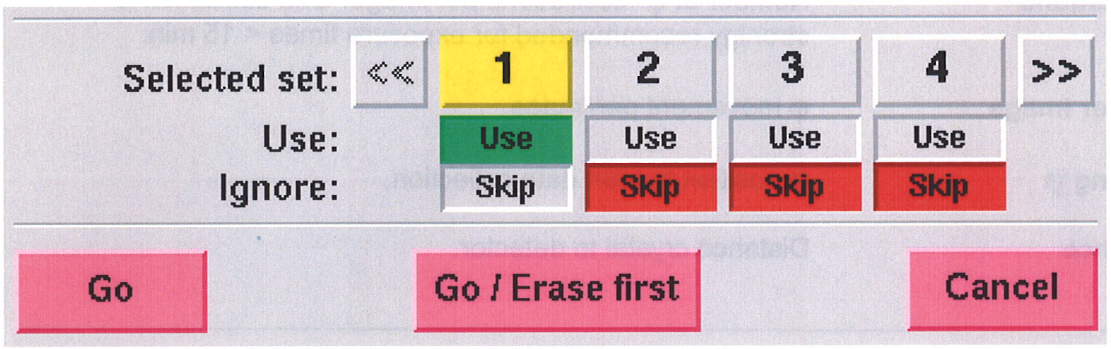
$$XXX = i * \varphi \text{ increment} / \Delta\varphi + 1 \qquad (i=0,1,2,3...)$$

e.g. with φ increment = 90.0 and Δ φ = 2.0, XXX = 1, 46, 91, 136, etc.

In ***MAD Data*** mode "**No. of images**" is replaced by "**No. of φ blocks**" and a field for entering the number of images per φ block. It is supposed that one wants to collect a number of contiguous images at a certain position and then the same wedge of data 180 degrees away. It is not such a good idea to collect only single images at one φ position since the detector will have to move φ very often and that takes time. Finally one ends up with 2 contiguous data sets A and B, both covering the same φ range but differing by 180 degrees.

For your convenience all text fields are followed by a menu with preset values. The menus can be activated by using the left mouse button. Most of the option menus are followed by up and down arrows that will increment or decrement the currently displayed values by one unit.

In ***Multiple Data Set*** mode, the following buttons are added underneath the"Distance" field:



You may toggle between different data set parameters by pressing the corresponding "**Selected Set**" button. The currently selected set will be highlighted and the title string at the top of the window will also tell you which of the sets you are programming.
Even if you have edited one of the data sets, you don't actually have to use it. The "**Status**" of a programmed data set can be set to "**Use**" (green) or "**Skip**" (red). Default is: "**Skip**".

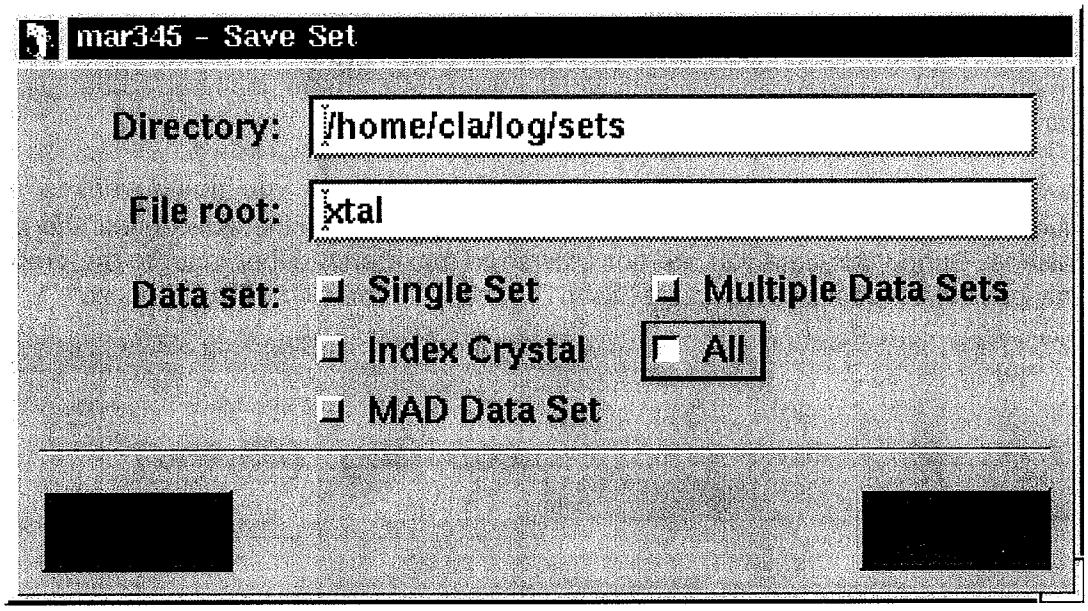
When more than 4 programmable data sets are configured (entry "SETS" in the configuration file) one may move forwards and backwards to the next or previous 4 sets using the **>>** and **<<** buttons, respectively.

Note 1:
All changes are saved automatically to file **mar345.dat** in directory **MARLOGDIR** and are available the next time ***mar345*** is used.

Note 2 (synchrotons only):
Since wavelength varies on synchrotron sources, the configuration file should contain the keyword:
wavelength variable
In this case, there is an additional input field for the used wavelength underneath the "**Distance**" field. Make sure that the correct wavelength is entered, since this information is written into image headers and programs like ***marView*** rely on it!

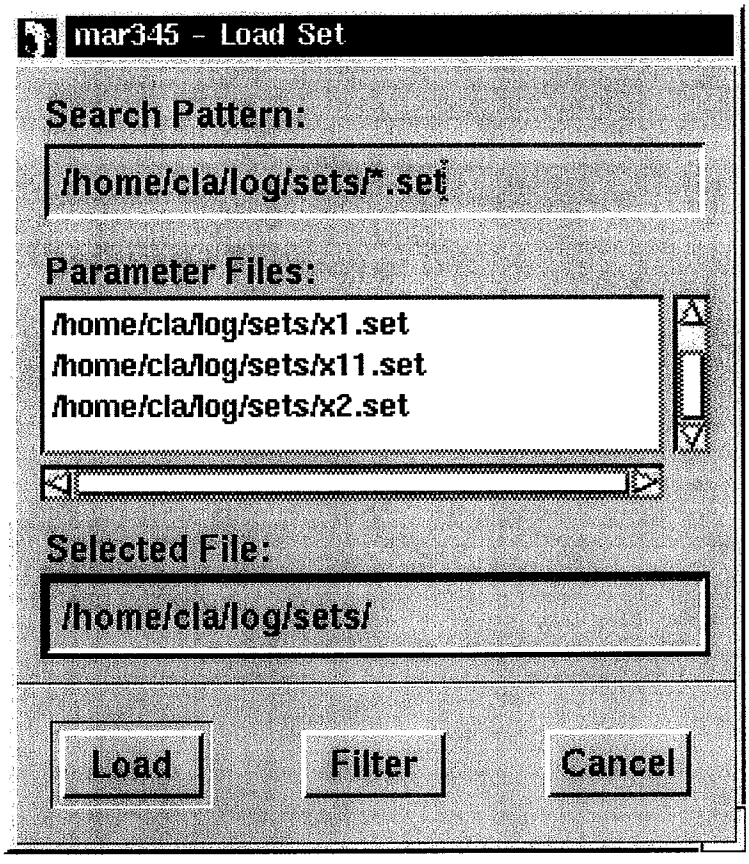
3.6 Loading and Saving Data Collection Parameters

Crystallographers often collect data of a certain crystal type in always the same way, i.e. using a certain oscillation range, a certain distance, etc.It is therefore useful to store a typical set of data collection parameters to a file and retrieve the parameters when desired. To save parameters, press the **"Save"** button in the ***mar345–Change Parameters*** window.



One now has the choice of saving only some sets of programmed parameters or all of them. By default, the files to be saved will be written into directory $MARLOGDIR/sets. The filename will always be File_root.set.

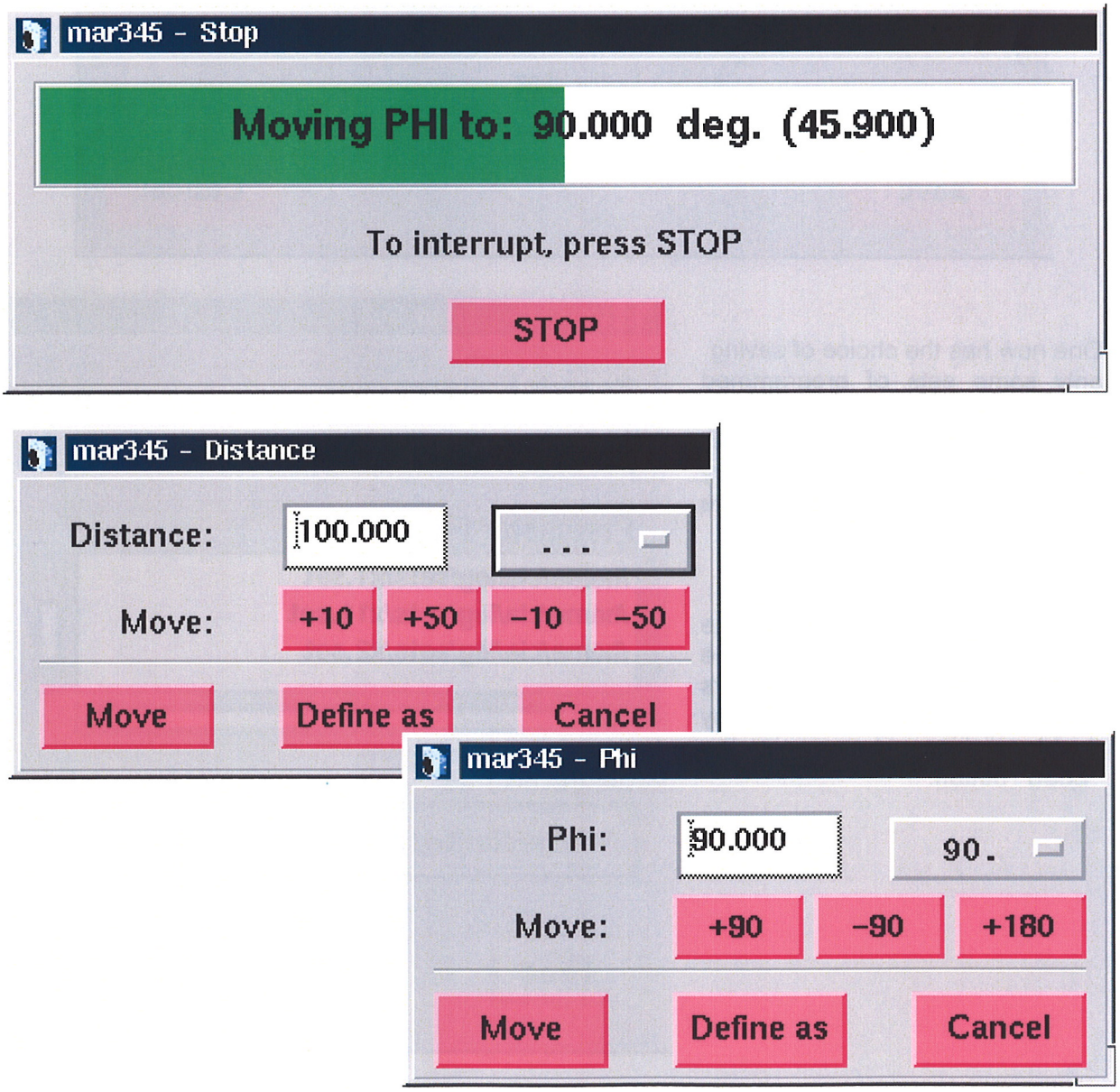
To retrieve parameters, press the **"Load"** button in the **mar345–*Change Parameters*** window. Select a file by double–clicking or by pressing the **"Load"** button.



3.7 Moving Distance and Phi

The detector position and the φ axis can be moved by pressing buttons in the ***mar345–Change Parameters*** window. One can also get separate windows for moving "φ" and "**Distance**" by pressing the corresponding status fields in the scanner status area of the main window and/or by activating the corresponding choices in the menubar of the main window. "**Starting** φ" and "**Distance**" are both followed by two additional buttons. Pressing "**Move**" will tell the scanner to move the detector or the motor to the desired position. "**Set**" will redefine the currently known value. This can be dangerous in case of the detector movement, so for the distance this button works only if the program has been started with the command line argument "**–setd**".

In any case, confirmation of the desired action is required. If you really want to move Distance or φ , the ***mar345–Stop*** window pops up and stays on the screen until the action has finished. During this time you are not allowed to make any further input to the program. The only possible action is pressing the "**Stop**" button in the ***mar345–Stop*** window.



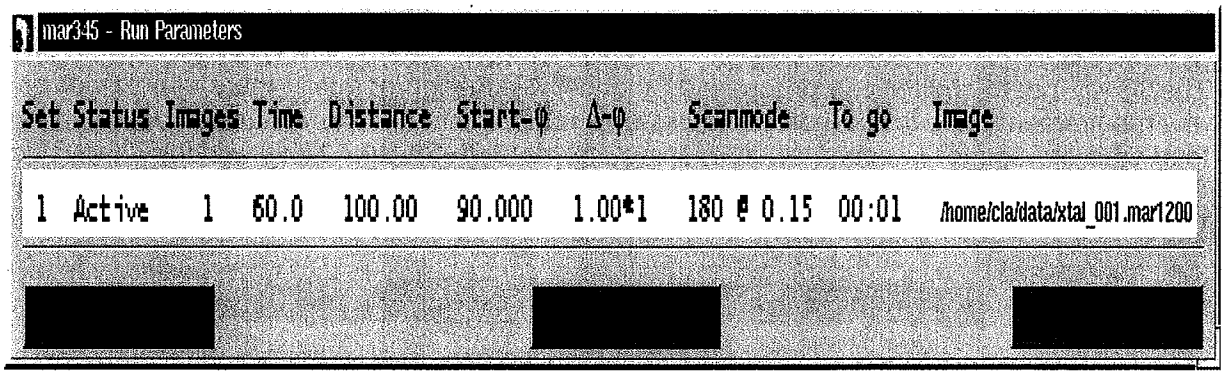
3.8 Starting Data Collection

Data collection can be started by pressing the "**Go**" or "**Go/Erase first**" button in the ***mar345–Change Parameters*** window. It is a good idea to always let the plate clean first before actually starting the data collection.

In **Multiple Data Sets** mode, before actually sending the command to the scanner the ***mar345–Run Parameters*** window will pop up. This window gives an overview ofthe currently programmed data sets. The buttons in the lower part of the window come with different layouts:

Mode	Left	Center	Right
Before data collection	**"Go"** really start	**"Change"** reedit parameters	**"Close"** Close window
During data collection	**"Abort NOW"** Aborts exposure	**"Stop AFTER IMAGE"** Stops after current image	**Close** Close window

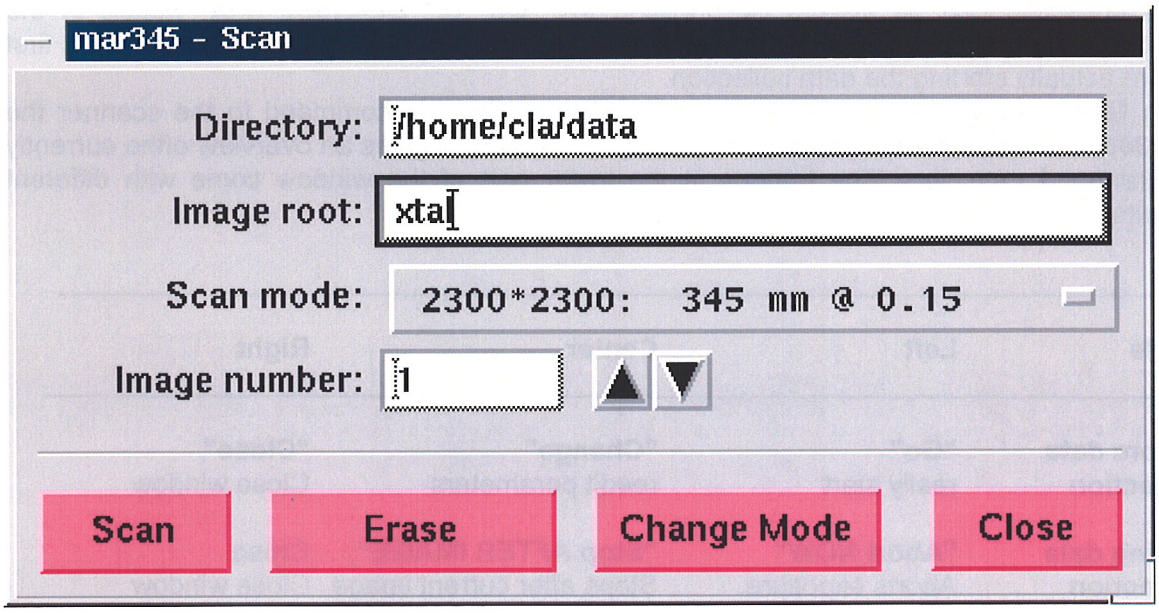
To start data collection you will have to press the "**Go**" button in this window. During data collection the ***mar345–Run Parameters*** window monitors the progress of the data collection. The window can be opened by selecting the "**Progress**" option in the "**Windows**" submenu (see 3.2.1). Active data sets are highlighted. Start–φ and Image will be updated. The number of oscillations is given by the multiplier in the Δ φ field. If the scanner is idle, this window cannot be obtained.



3.9 Stopping Data Collection

Data collection can be stopped by pressing the "**Stop**" button in the main window or by pressing the "**Stop**" or "**Abort**" button in the ***mar345–Run Parameters*** window. If the scanner is scanning or erasing the imaging plate, this cycle will always be finished. Pressing "**Abort**" in this moment will be the same as pressing "**Stop**". Otherwise, "**Abort**" closes the X–ray beam shutter immediately and stops φ or distance movement.

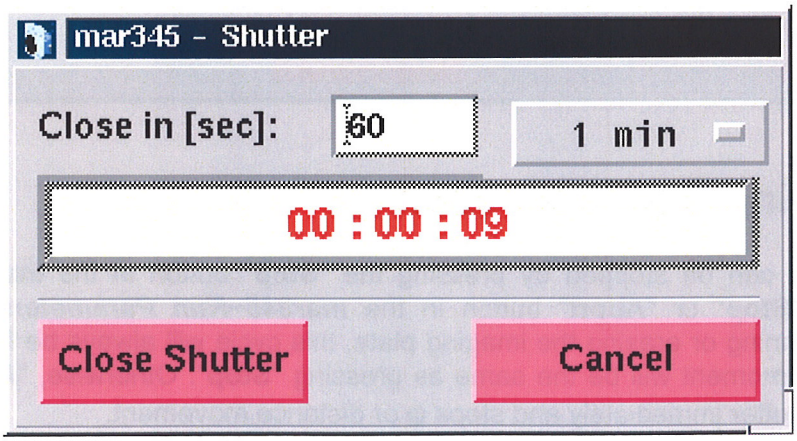
3.10 Single Scan



A single scan can be done by pressing the "**Scan**" button in the main window. The ***mar345–Scan*** window pops up. The directory, image root, image number and scan mode can be selected. The output format always is "***mar345***". Press "**Scan**" to start the scan A scan is always followed by an erase. Instead of a scan one can do an erase cycle. "Change Mode" only drives the scanning head to the desired position.

3.11 Shutter Timer

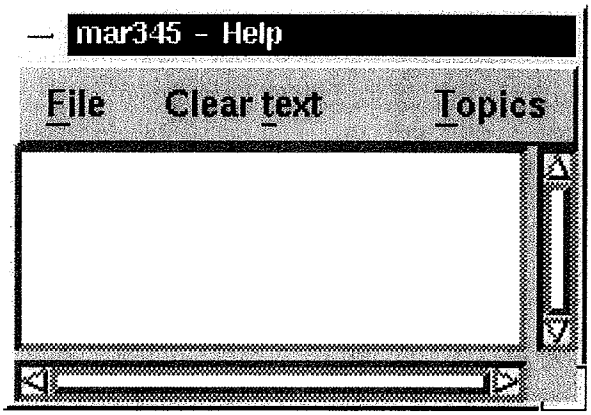
The X–ray beam shutter can be operated manually, although normally there should not be any requirement to do this. When operating the shutter manually it can be useful to know how long time the shutter is open. When opening the ***mar345–Shutter Time***r window (shortcut: **F4**) the program starts counting how long time the shutter is open. One may enter a closing time (in seconds). When this time period has elapsed, the shutter closes automatically.



3.12 Getting Help

Interactive help can be obtained by pressing the "**Help**" button in the menu bar of the main window or by pressing the **F5** key.

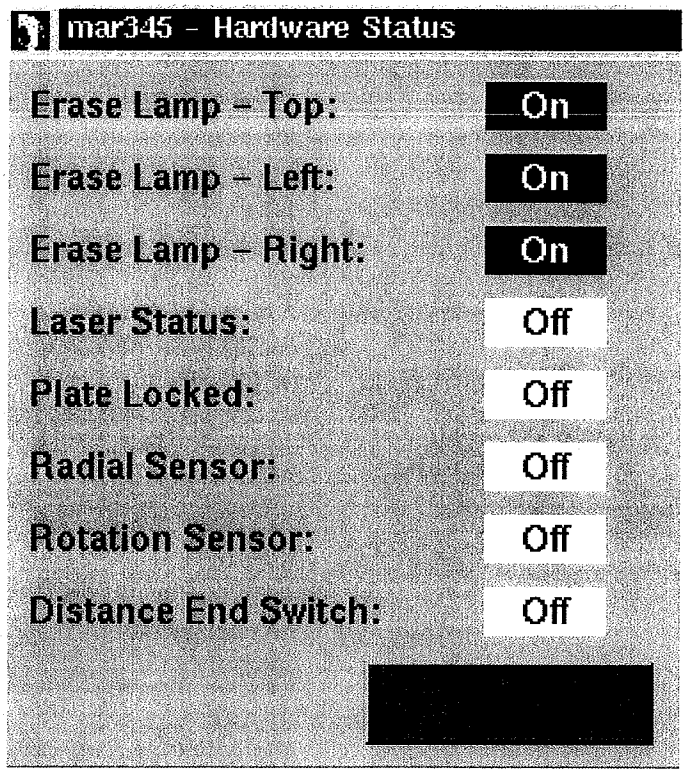
In the ***mar345–Help*** window, a help topic should then be selected from the "Topics" submenu (shortcut is: Alt+t).



3.13 Hardware Status

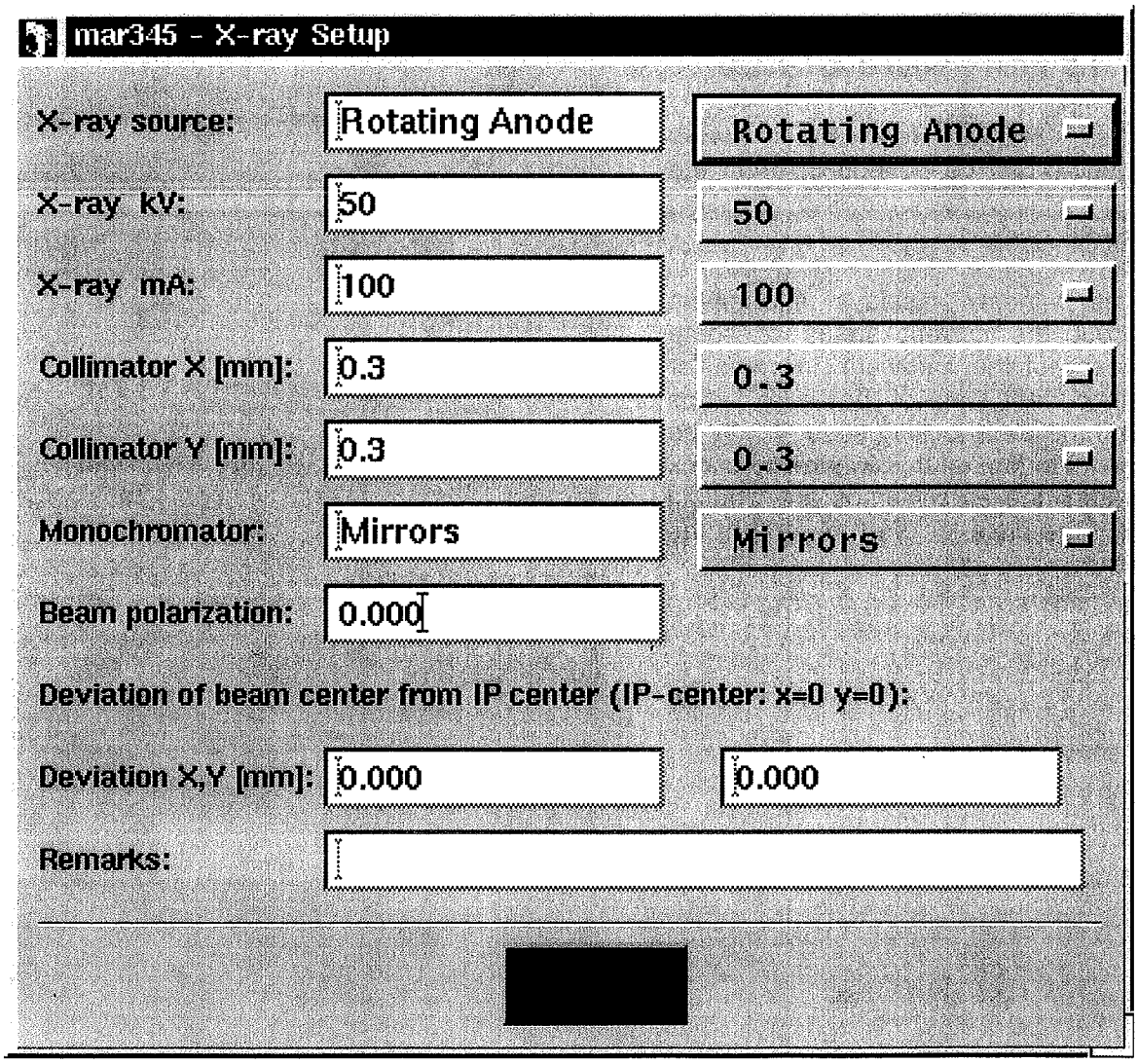
The ***mar345–Hardware Status*** window can be popped up from the main window menubar or by pressing the **F6** key.

This window displays information about the current status of some pieces of the hardware, in particular the current state of the erase lamps and the plate locking state. It may be useful to look at this window to check wether the erase lamps are working or if the plate locks at the end of the scan.



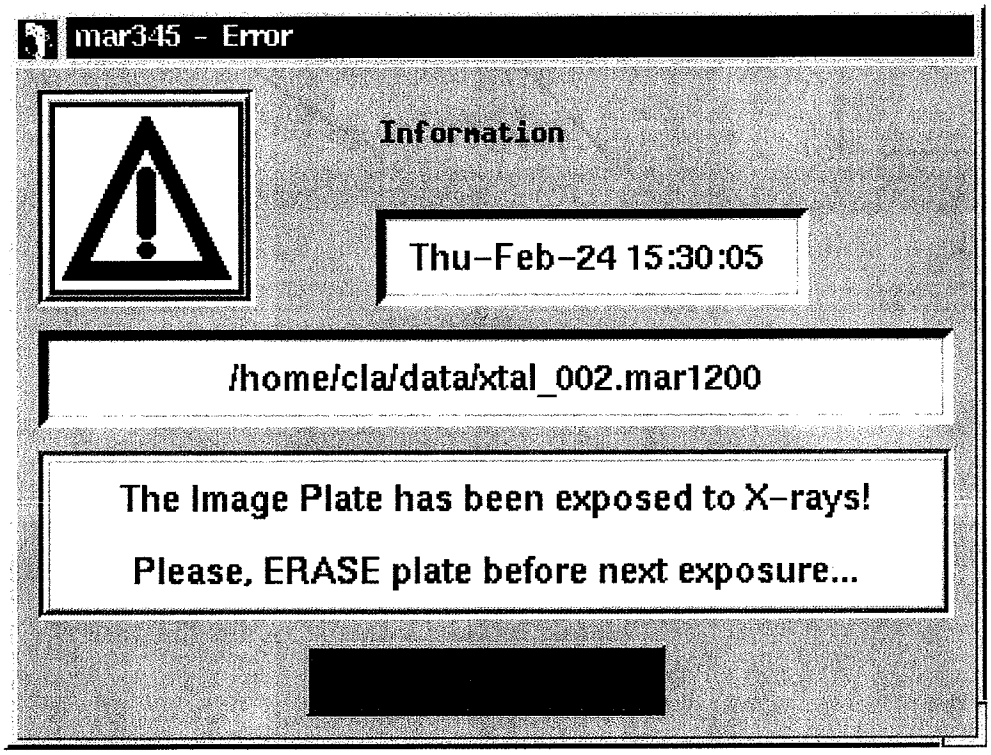
3.14 X-ray Setup

When producing images during data collection many parameters concerning the current experiment are automatically written into the output image headers, so this information can be retrieved later on. This is most relevant for parameters like the distance and the goniometer positions. It might, however, be useful to add also some information about the state of the X-ray source. Unfortunately, the program ***mar345*** does not have knowledge about the generator and collimator settings, so this information must be entered manually. For this purpose, open the ***mar345-X-ray Setup*** window. This window can be popped up manually from the main window menubar or by pressing the **F3** key. All information given here is really not essential but it may help later on to track down problems during data processing.
The center of diffraction is supposed to be a physical constant (for one data set) and is valid for all scan modes, regardless if working at 0.15 or 0.10 mm pixelsize. This is why the center should not be entered in absolute pixels or millimeters referring to an origin in the lower left corner but as a deviation from the center of the image plate. These values should be given in mm, not in pixels, and can become negative. Negative x deviation means that the center of diffraction is left of the IP-center. A negative y deviation would be underneath the IP-center.



3.15 Errors and Warnings

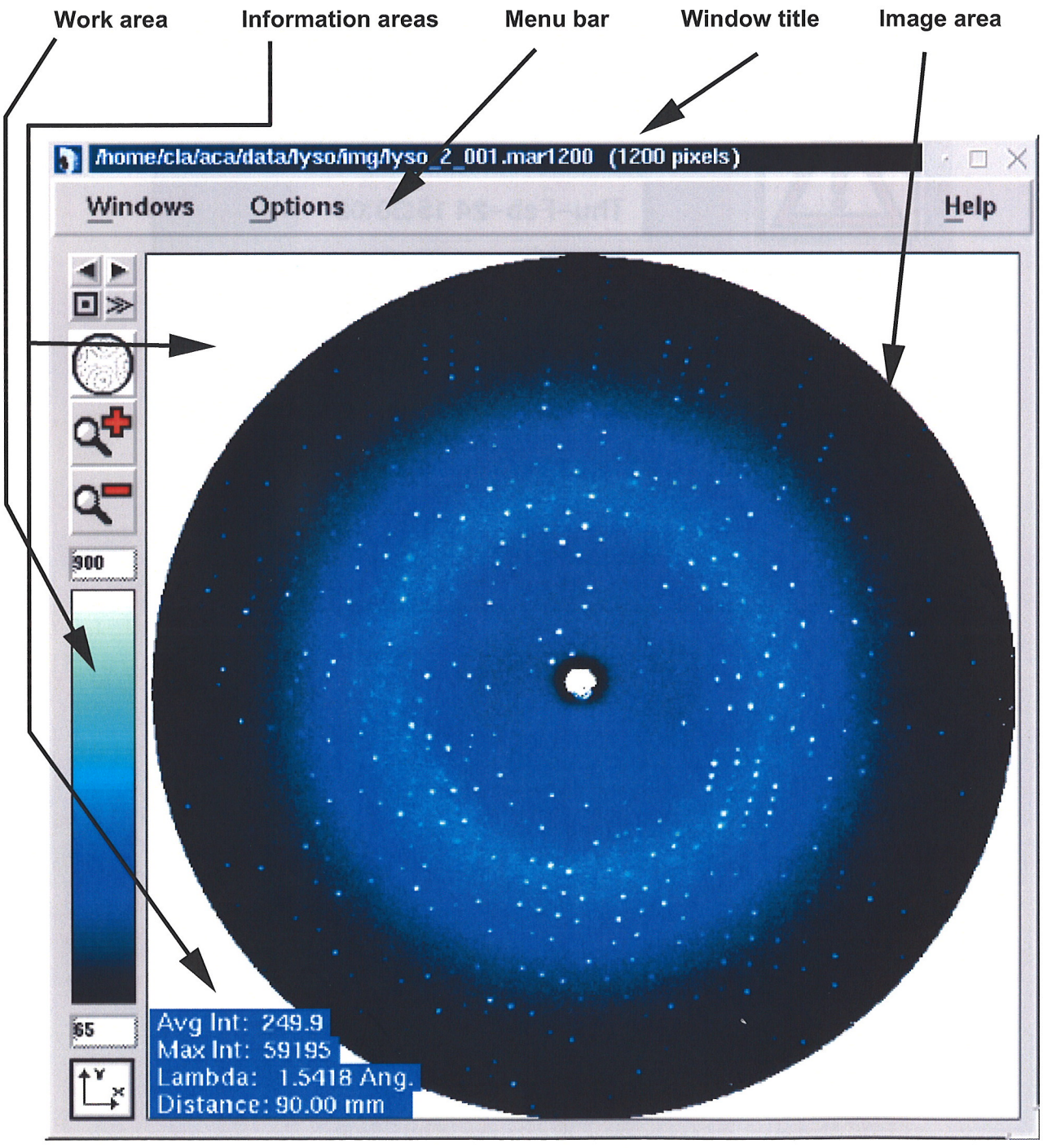
During operation, i.e. data collection or other tasks, the scanner itself or the program ***mar345*** might produce error messages or warnings. All relevant messages are displayed automatically in the ***mar345-Error*** window. This window can be popped up manually from the main window menubar or by pressing the **F7** key. Some warnings and errors may have an obvious solution if they are not related to the scanner hardware. For latter ones, please refer to section **Troubleshooting**.



4. Image Display

4.1 Display Window

The image display window controls the most important display functions. It consists of different areas:



4.2 Menu Bar

The menu bar features the following buttons:

Windows Pops up the ***Windows*** submenu (see 4.2.1). Shortcut: **Alt+w**.

Options Pops up the ***Options*** submenu (see 4.2.2). Shortcut: **Alt+o**.

Help Pops up the ***mar345-Help*** window.

4.2.1 Windows Submenu

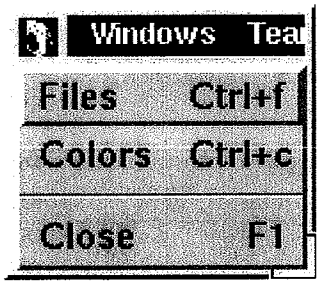
The Windows submenu pops up when the "**Windows**" button in the menu bar was pressed or if **"Alt+w"** was pressed while the pointer was in the main window. The submenu is a so called "tear-off" menu.

The Windows menu features the following buttons:

Files Pops up the ***mar345-Files*** window.
Shortcut: **Ctrl+f**

Colors Pops up the ***mar345-Colors*** window.
Shortcut: **Ctrl+c**

Close Closes the display window..
Shortcut: **F1**



4.2.2 Options Submenu

The Options submenu pops up when the **"Options"** button in the menu bar was pressed or if "Alt+o" was pressed while the pointer was in the main window. The Options menu features the following buttons:

Show/Hide resolution rings Toggles display of resolution rings
Shortcut: **Ctrl+r**.

Show/Hide statistics Toggles display of image statistics. The statistics about maximum intensity and average intensity in the image as well as the wavelength and distance are normally displayed in the lower left corner of the image area.
Shortcut: **Ctrl+a**

Do not/Keep view Normally, if a new image is loaded, the program displays the entire image and also calculates the best color scheme. If you want to look at all images in the very same way, select "Keep view". Shortcut: **Ctrl+v**

Do not/Keep color scales

Normally, if a new image is loaded, the program recalculates a new color scheme. If you want all images to be displayed in the same way, select "Keep color scales"
Shortcut: **Ctrl+k**

Reset colors

Recalculates colors and redisplays the image.
Shortcut: **Ctrl+t**

Turn On/Off 3D-plot

Toggles 3-D representation of magnified areas of the image. Available only at zoom factors > 4.
Shortcut: **Ctrl+d**

Next image

Load the next image, i.e. increment image number by 1.
Shortcut: **Ctrl+n**

Previous image

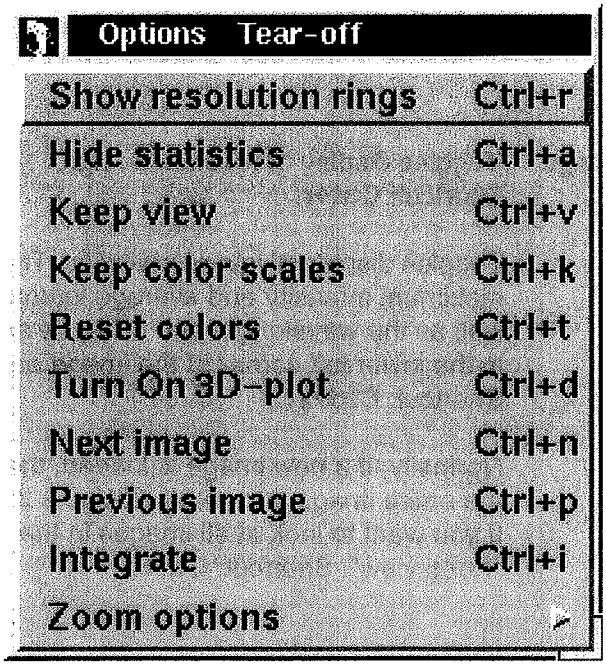
Load the previous image, i.e. decrement image number by 1.
Shortcut: **Ctrl+p**

Integrate

Pixels in the image area are integrated and the results are displayed in the upper right corner of the image area.
Works for zoom factors >= 1 only.
Shortcut: **Ctrl+i**

Zoom options

Pops up a menu with 3 choices that affect the way the image looks at zoom factors < 1. If one pixel on the monitor corresponds to more than one pixel in the image, the program will take only one image pixel to display and ignore the neighbours (n'th pixel) or take the average of the neighbours or their maximum, respectively.
Note, that "N'th pixel" mode is faster than the others, since no calculation is involved.



4.3 Image Area

In this area, the image is displayed. With the pointer (3-way mouse button) several additional functions can be accessed.

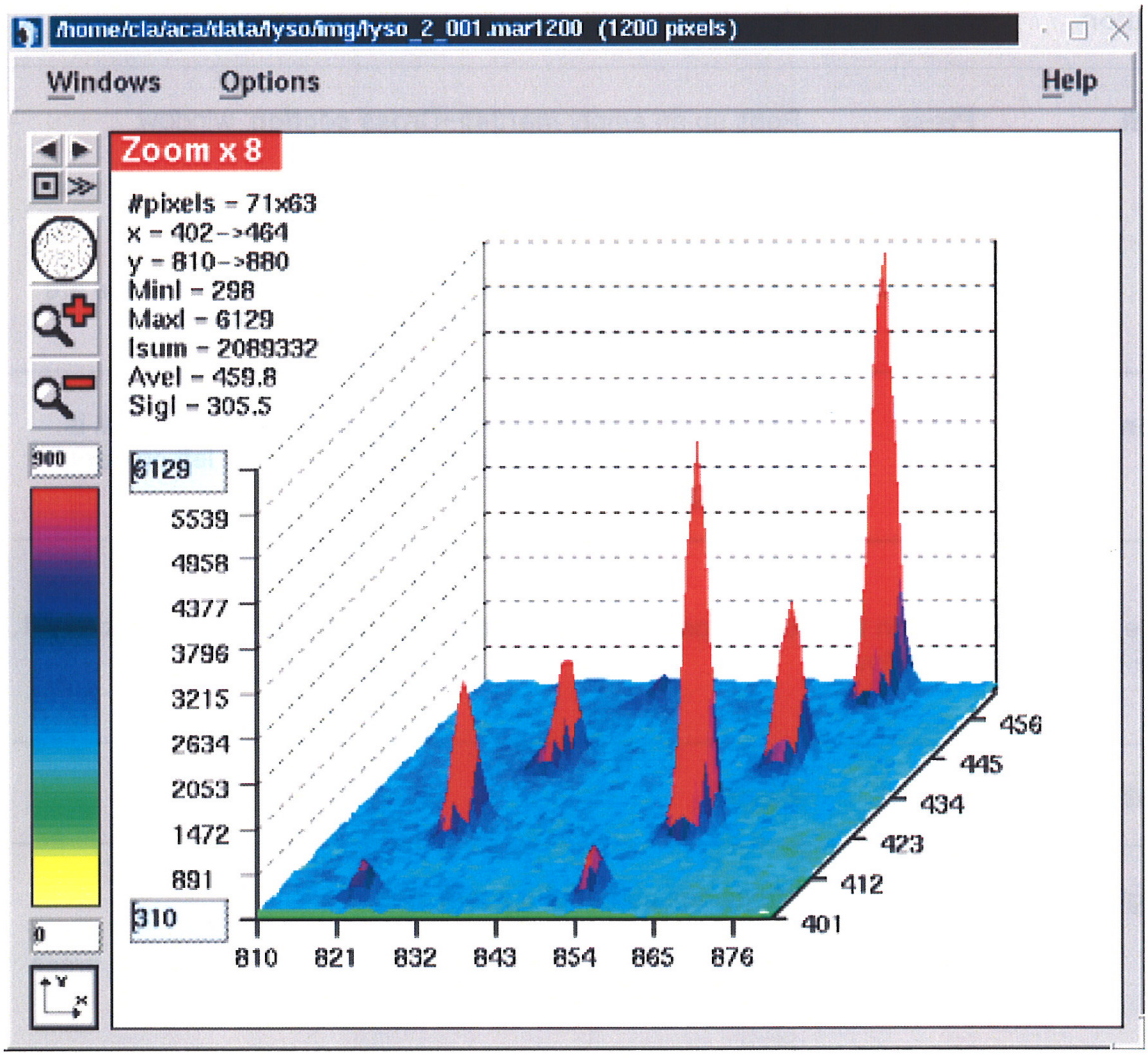
Button	Action	Result
Left	**Press**	Pops up an empty ***mar345-Cross section*** window
	Drag	A red line is drawn from the position of the first mouse press to the position of the last mouse press.
	Release	The (interpolated) intensities of the pixels along the line are displayed in the ***mar345-Cross section*** window.
Center	**Press**	The x,y-coordinate, intensity and resolution of the pixel is displayed in the information area in the upper left corner of the image area.

The right mouse button functions depend on the current zoom factor. At **zoom factors < 1**, the behaviour is as follows:

Button	Action	Result
Right	**Press**	Marks one corner of a zoom area.
	Drag	A red box is drawn from the position of the first mouse press to the position of the last mouse press.
	Release	The pixels contained in the red box are displayed in the "Image Area". The magnification factor depends on the size of the box and the size of the window.

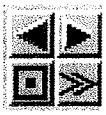
At **zoom factors >= 1**, the currently displayed magnified part of the image will be **recentered** at the position where the right mouse button has been pressed. By this method, one can move around in the image by always recentering at new positions.

At zoom factors > 4 one can obtain a 3−dimensional representation of the magnified portion of the image. For this feature, use "**Turn On 3D−plot**" in the Options menu of view window or toggle this option by pressing **Ctrl+d**. In 3D mode one can still move around within the image by pressing the right hand mouse button, but the recentering corresponds to the position of the 2D display, so this time it is more guessing. In the 3D−plot one may rescale the peaks using the minimum and maximum intensity field on the y−axis of the plot.



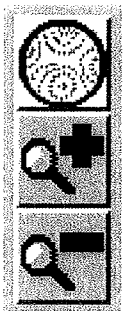
4.4 Work Area

4.4.1 Load Buttons



By pressing the single left or right arrow one can decrease or increase the current image number and load the previous or next image, respectively. The double arrow will continously increase image numbers and continuously load the next image until the stop button is pressed.

4.4.2 Zoom Buttons



By pressing the full image button, the image will be displayed such that it fits entirely into the window. The other buttons will zoom in or zoom out.

4.4.3 Colors

The upper text field has the same function as the "Max"-field in the ***mar345-Colors*** window and the lower text field corresponds to the "Min"-field (see chapter 4.9). Dragging the center mouse button in the color area, the color distribution changes. Try it out to see what happens!. This doesn't work for Rainbow mode (see below) and it doesn't work on 16/24/32-bit color screens, only with 8-bit colors.

4.5 Information Areas

Upper left corner:
When pressing the center mouse button in the image area, the x,y-coordinate, intensity and resolution of the pixel under the pointer is displayed.

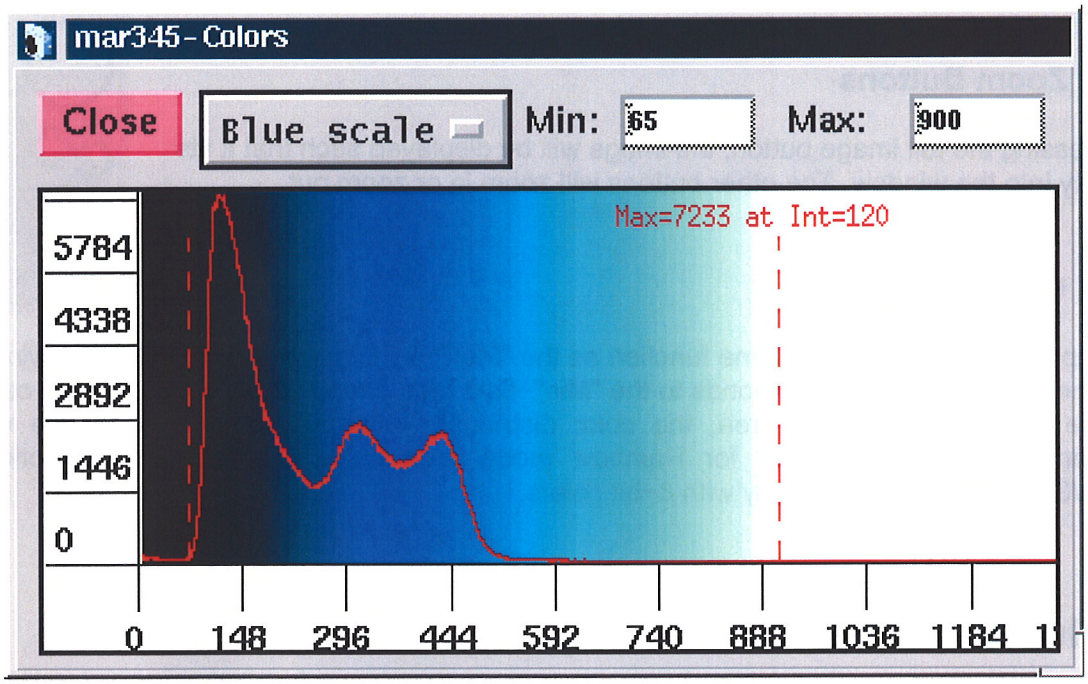
Lower left corner:
Once an image has been loaded successfully, some information (wavelength, distance, maximum intensity and average intensity) is displayed, unless "Hide statistics" was pressed (see 4.2.2).

Upper right corner:
When pressing the "**Integrate**" button in the "Options" submenu (see 4.2.2) the following information is displayed: number of pixels in x and y, maximum, minimum and average intensity, sum of pixel intensities, standard deviation of intensities, average background and mean intensity over background (all relative to the pixels displayed in the Image Area). The background is calculated from a histogram of intensities of a box of 50x50 pixels around the center of the zoomed area. Pixel values > 1000 are not included in the histogram. This option works for zoom factors >= 1.0 only.

4.6 Window Title

In this area, the image name and some parameters extracted from the image header (total number of pixels along x, number of pixels with intensities larger than 65535) are displayed.

4.7 Colors Window



In this window, colors may be modified. The window provides a drawing area showing a histogram of intensity values found in the image, i.e. intensities are on the horizontal axis and frequency of the corresponding intensities are on the vertical axis. The histogram is used to distribute colors or greyscales. The program tries to use 64 colors. All pixels with intensities larger than the value given in "Max" (right dashed bar) or smaller than the value given in "Min" (left dashed bar) are drawn in one color. The remaining colors will be distributed in equidistant intensity ranges between Min and Max.

The following color schemes are used:

Mode	I <= Min	I >= Max	All other pixel intensities
Grey scales	white	black	greys
Blue scales	black	white	blues
Rainbow	white	red	yellow-green-cyan-blue-purple-magenta

The functions of the ***mar345-Colors*** window widgets are:

Grey scales Selection of coloring mode. Alternatives: **Blue scales, Rainbow**.

Min All pixels with intensities <= Min are drawn white (black in Blue scales). The dashed line in the histogram plot moves to the specified value.

Max All pixels with intensities >= Max are drawn black (Grey scales), white (Blue scales) or red (Rainbow). Intensities which are above the saturation limit (128000) are drawn in green. The dashed line in the histogram plot moves to the specified value.

In the histogram plot, the mouse buttons have the following functions:

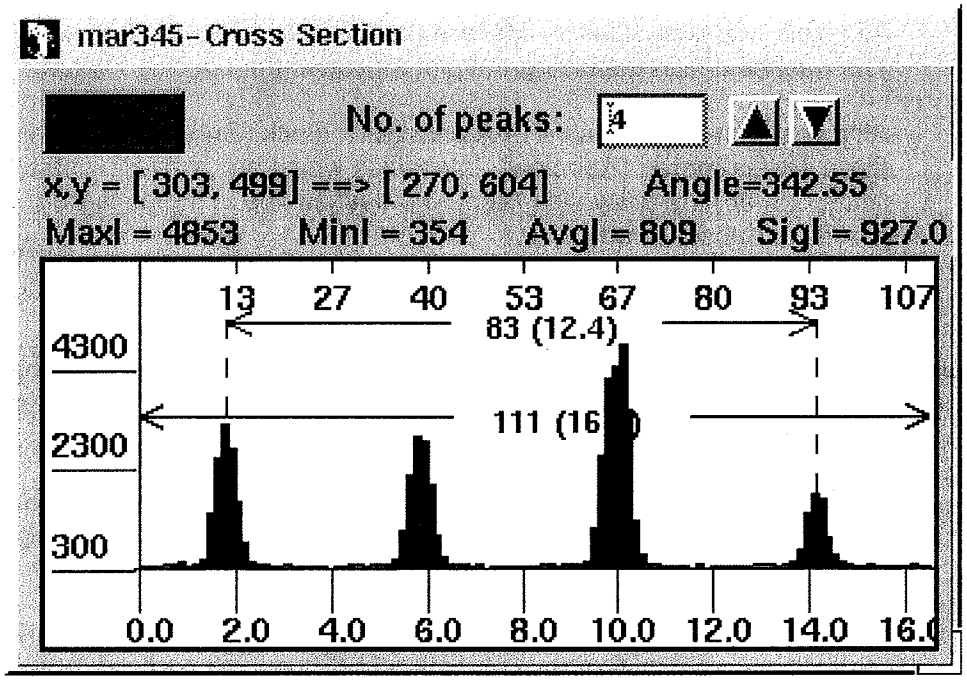
Left mouse button press Places the dashed red line in the histogram plot to a new position marking the minimum. The value in the "**Min**" text field is changed accordingly.

Right mouse button press Places the dashed red line in the histogram plot to a new position marking the maximum. The value in the "**Max**" text field is changed accordingly.

Center mouse button drag Changes color tables. Try it out to see what it really does. This works for grey and blue scales only and for 8-bit color displays only!

Note:
By changing **Min** or **Max** or setting these values with the mouse button the color distribution for the whole image will be recalculated. This takes some CPU-time, so please don't do more than one change at a time.

4.8 Cross-Section Window



This window is used for displaying cross sections through the image. The window can be obtained by pressing the left mouse button in the image area.

The functions for the ***mar345-Cross section*** window widgets are as follows:

No. of peaks

Specifies the number of peaks between the two dashed lines in the plot area of the mar345-Cross section window. Use the arrows on the right hand side of the text field to increment or decrement the value by 1.
When pressed, the real space cell constant is calculated from the distance between the two dashed lines and the number of peaks. The result is displayed in the message area.

Message area

Shows the coordinates of the start and end of the line, the angle with the base line, maximum, minimum, average and standard deviation of the intensities along the drawn line.
When changing the no. of peaks manually, the second line displays the derived cell constant.

The **plot area** of the window shows the following features:

Vertical axis	Interpolated intensities
Upper horizontal axis	Length of line in pixel units.
Lower horizontal axis	Length of line in mm units.
Left dashed red line	Marks the begginning of a measured distance. This line can be moved using the **left mouse button**.
Right dashed red line	Marks the begginning of a measured distance. This line can be moved using the **right mouse button**.
Horizontal red lines	Shows the length of the line in pixels (mm) and the distance between the dashed vertical lines.

The pointer can be used to measure distances by setting the red dashed lines to the desired position along the drawn line. This is particularly useful if you want to measure cell constants. The program features a peak finding algorithm which tries to set the bars on top of the first and the last peak of the plot. In between the peaks the program then looks for other peaks and tries to calculate the best inter−peak distances by assuming a harmonic oscillation. The no. of peaks calculated by the program is displayed in the "No. of peaks" text field. Of course, this value may be modified. The derived cell constants do not take into account any particular setting or symmetry of the crystal but calculates cell constants assuming plain orthogonal axes in reciprocal space.

5. Data Collection

5.1 Strategies

While some general rules apply how to collect data best, a sensible choice of data collection parameters depends on individual circumstances, i.e. crystal quality, beam properties, etc. The following section gives some hints on how to program a data collection:

Distance crystal−detector:
The distance crystal−detector **must** be chosen such that spots don't overlap. It should be chosen such that the highest resolution of the spots is close to the edge of the scanned area, i.e. move the detector back as far as possible. This gives a better Intensity/σ ratio!

$\Delta\varphi$ per image:
The $\Delta\varphi$ **must** be chosen such that spots don't overlap. If the background is large compared to the average spot intensity (i.e. most protein crystals) choose relatively small values (0.5 to 2.0 deg.). The smaller, the better the integration works, but the more exposures you need to get a complete data set.

Number of images:
How many images you need depends on the symmetry of the space group and on the setting of the crystal. As a rule of thumb, orthorhombic crystals require 90.0 deg. of data, monoclinic ones 120 deg., triclinic ones 180 deg., trigonal ones 60.0 deg., tetragonal ones 45.0 deg, hexagonal ones about 30.0 deg. and cubic ones about 25.0 deg.. High resolution data collections usually require a wedge of data − say 20 deg. − at another crystal setting because of the blind region.

Exposure time:
The exposure time should be less than 30 minutes, in any case, because of partial decay of the F−centers on the imaging plate. For very weak diffractors which require longer exposure times it is better to scan one exposure after 30 min. and to repeat the same exposure and add the images together later. Otherwise, exposure times should be chosen such that the dynamic range (0:130000) is not exceeded. It is actually best to have maximum intensities considerably less, e.g. 60000.

Number of oscillations:
Best to leave at 1, except when using exposure times larger than 15 minutes.

Scan mode:
Why scan the 345 mm plate if there is not enough diffraction? A 180 mm scan takes half the time to scan, needs 80% less disk space and 80% less processing time!

The decision about what pixelsize to choose is slightly more difficult. In general, the finest pixelsize of 0.1mm is more efficient and yields slightly better data. On the other hand, scans take about 10% longer time and images are larger in size than those taken at the same diameter but in 0.15mm pixelsize mode. So the decision is some kind of compromise.

Output format:
Use of "mar345" format is strongly suggested. A mar345 file typically requires 70% less disk space than a standard uncompressed image file. All major protein data processing packages support this format.

Collect mode:
Use TIME mode unless on synchrotrons.

For **indexing** crystals, usually 2 images that differ from each other by a movement in φ of 90 degrees gives good results. In the case of very small molecules (i.e. cell axes of about 10 deg.) you may not get enough spots from 2 images only.

5.2 Checking Parameters

Before starting a data collection, ***mar345*** makes a consistency check of the input parameters. In most cases the program will tell you if the input parameters really do not make sense. It checks wether files can be opened, if there is enough disk space, etc.

5.3 Errors and Warnings

In case of computer or scanner problems, warning messages will be printed on standard output and in the log file. Very important messages will also be displayed in a special window. Problems fall into 3 categories: fatal errors, warnings and notifications. See chapter **Troubleshooting** for more details.

5.4 End of Data Collection

After having finished a data set, ***mar345*** writes a summary into the corresponding data directory. The summary files come in 2 formats:

- **image_root.SUMMARY** = plain Ascii text file
- **image_root.html** = Ascii-file with HTML-formatting instructions.

These files should be printed and archived.

6. Troubleshooting

Both the computer and the scanner can produce fatal errors and warnings. All messages are numbered. Messages with message numbers < 1000 come directly from the scanner controller and are potentially serious. Message numbers >= 1000 are generated by program ***mar345*** and may be a consequence of a controller error or some other kind of malfunctioning or warning.

If you don't know how to fix a scanner problem, contact *marresearch*. We will usually ask you right away to send us the mar.spy file and the mar.log file where the error occured (see chapter 2.3) since they contain almost all information we need.

The following error messages >= 1000 are produced by program ***mar345***:

No.	Description	
1000	**Message:**	"Error sending command to mar controller"
	Reason:	Network connection to scanner interrupted.
	Action:	Reboot scanner. Check cables. Try "ping mar345".
1001	**Message:**	"SERVO system cannot be INITIALIZED"
	Reason:	Severe hardware problem.
	Action:	Call.
1010	**Message:**	"Waiting for X-rays..."
	Reason:	The X-ray intensity as read from the ion. chamber has dropped below the critical level (see configuration file: INTENSITY MIN xxx). The next exposure starts only after the X-rays are back.
	Action:	Check generator, monochromator or collimator.
1020	**Message:**	"Not enough disk space left on device. Aborting data collection"
	Reason:	Disk full.
	Action:	Clean up disk.
1030	**Message:**	"The Image Plate has been exposed to X-rays"
	Reason:	A running exposure has been aborted.
	Action:	Erase plate and continue.
1040	**Message:**	"X images have been successfully retaken"
	Reason:	Some images had to be retaken due to hardware problems, possibly shutter.
	Action:	Carefully check log file for learning more about the reasons.

Tabel continued from previous page.

No.	Description	
1050	**Message:**	"SHUTTER did not work properly. Abandoning data collection"
	Reason:	X-ray beam shutter damaged or dirty.
	Action:	Check shutter. Open and close it manually. Is it very hard to operate?
1060	**Message:**	"X-ray reading too low ..."
	Reason:	The X-ray intensity as read from the ion. chamber is below the critical level (see configuration file: INTENSITY MIN xxx). The data collection starts only if the X-ray reading is above the configured value.
	Action:	Check generator, monochromator or collimator.
1061	**Message:**	"X-rays reading too high for DOSE mode ..."
	Reason:	The X-ray intensity as read from the ion. chamber shows very large numbers (>100). The work in DOSE mode becomes inaccurate.
	Action:	Turn down gain selector of ion. chambers.
1070	**Message:**	"Could not recover from previous errors after X retries"
	Reason:	Follow up of previous messages.
	Action:	Check previous messages.
1080	**Message:**	"SHUTTER did not open during exposure" or "Shutter did not close at end of exposure"
	Reason:	X-ray beam shutter damaged or dirty.
	Action:	Check shutter. Open and close it manually. Is it very hard to operate?
1090	**Message:**	"Scanner home position (X) differs from Y +/- dy"
	Reason:	Problem with radial movement of reading head.
	Action:	Mail mar.spy. Call.
1100	**Message:**	"Cannot open nb_code!"
	Reason:	File $MARTABLEDIR/mar2300.XXX and/or $MARTABLEDIR/mar3450.XXX are missing or don't have read permission.
	Action:	Check existence of files and permissions.

Tabel continued from previous page.

No.	Description	
1101 1102 1105	**Message:**	"No scan modes found in nb_code ..." "Something wrong with byteorder in nb_code ..." "No suitable scanning mode found in nb_code".
	Reason:	File $MARTABLEDIR/mar2300.XXX and/or $MARTABLEDIR/mar3450.XXX may be corrupted or empty.
	Action:	Check file sizes (73 MB and 103MB). Use command: catmar $MARTABLEDIR/mar2300.XXX to look at the calibration file header.
1103	**Message:**	"Scanner serial number in nb_code differs from config"
	Reason:	The scanner no. in the file headers of files $MARTABLEDIR/mar2300.XXX and/or $MARTABLEDIR/mar3450.XXX are not identical to $MAR_SCANNER_NO. The calibration files may not belong to the scanner.
	Action:	Call.
1110 1111 1112 1115	**Message:**	"Cannot create image file" "Cannot open image file" "Error writing image array" "Error writing image header"
	Reason:	Insufficient disk space or invalid file permissions.
	Action:	Clean up disk or check data directory permissions.
1215/1241 1234 1238	**Message:**	"Cannot OPEN SHUTTER at START of EXPOSURE" "SHUTTER was already OPEN at START of EXPOSURE!" "Cannot CLOSE SHUTTER at END of EXPOSURE!"
	Reason:	X-ray beam shutter damaged or dirty. Otherwise, the manual shutter operation switch mounted on the base may have been left in the "Open" state.
	Action:	Check shutter and manual shutter switch on the base. Open and close the shutter manually. Is it very hard to operate?
1239	**Message:**	"STEPPER error during EXPOSURE!"
	Reason:	Problem with PHI axis movement. Possibly software related.
	Action:	Mail mar.spy file. Call.

Appendix

A. Configuration File

Each scanner has a scanner specific configuration file. This file must reside in directory $MARTABLEDIR and is called config.XXX, where XXX is the three-digit serial number. Please refrain from changing values unless there is good reason to do so. The configuration file is a keyworded Ascii-file. Please refer to the man page **mar345_config_file** for a full description of keywords.

A typical configuration file looks like this:

```
! ____________________________________
!
! Configuration file for scanner no. 120
! ____________________________________
!
! Only modify the following keywords, if desired...
!
DIST                    MIN 75.30  MAX 426.30
!
INTENSITY               MIN  2.0   WARN 20.0
!
USE                     SPY
USE                     STATS
USE                     INCR
USE                     RUN
USE                     HTML
USE                     SUMMARY
!
COLORS                  64
SETS                    4
!
WAVE                    1.541789
MONOCHROMATOR           Mirrors
GENERATOR               Rotating anode
!
NETWORK                 PORT 4441   HOST 192.0.2.1
!
MODE 2300               ROFF 180  ADC 50  AADD -42  BADD -45
MODE 2000               ROFF 180  ADC 50  AADD -42  BADD -45
MODE 1600               ROFF 180  ADC 50  AADD -42  BADD -45
MODE 1200               ROFF 180  ADC 50  AADD -42  BADD -45
!
MODE 3450               ROFF 180  ADC 50  AADD -42  BADD -45
MODE 3000               ROFF 180  ADC 50  AADD -42  BADD -45
MODE 2400               ROFF 180  ADC 50  AADD -42  BADD -45
MODE 1800               ROFF 180  ADC 50  AADD -42  BADD -45
!
!IP-Diameter:           345mm    300mm    240mm    180mm
!GAPS                   89615    78601    63852    49103
! 02.2.2000:  GAPS valid for S/N 120
!
```

B. Calibration Files

Each scanner comes with 2 scanner specific calibration files. These files must reside in directory $MARTABLEDIR and are called mar2300.XXX and mar3450.XXX, where XXX is the three-digit serial number. The file contain flat field and geometrical corrections required for producing Cartesian images out of a spiral scan.

- File mar2300.XXX is used for scans at pixelsizes of 0.15mm (modes 2300, 2000, 1600 and 1200) and has a typical size of 73 MB.

- File mar3450.XXX is used for scans at pixelsizes of 0.10mm (modes 3450, 3000, 2400 and 1800) and has a typical size of 103 MB.

Both files are binary files. They feature an Ascii-file header that can be looked up using program ***catmar***.

A typical output of command "***catmar mar2300.120***" looks like this:

```
Format type: mar 345 ...

============================================================
Line  At byte  Contents
============================================================
  4    (  192)  PROGRAM  improve Version 2.8
  5    (  256)  DATE     Wed Feb  2 12:00:40 2000
  6    (  320)  SCANNER  120
  7    (  384)  PIXEL    LENGTH 75  HEIGHT 150  SUBPIXELS 25
  8    (  448)  PHIOFF   269.970
  9    (  512)  CUTOFF   0.000
 10    (  576)  SCALE    32767.000
 11    (  640)  GAIN     1.000
 12    (  704)  NUMBER   PIXELS 7766361  NEIGHBOURS 25199739
 13    (  768)  MODE     2300 X    0 Y 1149 ROFF    0 SKIP 144
 14    (  832)  MODE     2000 X    0 Y  999 ROFF    0 SKIP 144
 15    (  896)  MODE     1600 X    0 Y  800 ROFF    0 SKIP 809
 16    (  960)  MODE     1200 X    0 Y  600 ROFF    0 SKIP 809
 17    ( 1024)  MODE     2300 PIX 7766361   POS 4096
 18    ( 1088)  MODE     2000 PIX 5956761   POS 17151502
 19    ( 1152)  MODE     1600 PIX 3845618   POS 37076767
 20    ( 1216)  MODE     1200 PIX 2190418   POS 52798207
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