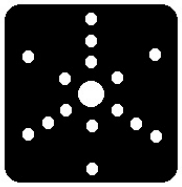
The NorthStar Real-Time Orientation System

Program Manual for MS-Windows Systems

Version 5.0
(Windows 32-bit)

Release: August 5, 2004



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Preface

The MultiWire Laboratories NorthStar system is the culmination of many years of experimentation, development, and testing. We are proud of our achievement and we would like to thank you for purchasing this system. We hope that you will find the system accurate, easy to use, and worthy of telling others about! We also hope that you will let us know of any errors you may find and/or any enhancements you would like to see.

Space For Your Notes

Table of Contents

1. Introduction

The MWL110 real-time back-reflection Laue camera system and NorthStar program make orienting single crystals very simple. NorthStar, a menu driven program, provides real-time viewing of a Laue x-ray pattern for dynamic imaging as the crystal is rotated in the x-ray beam. Well defined images can be collected for a few seconds and then displayed, with the program allowing for the storage and retrieval of these images from floppy (or hard) disks.

The NorthStar program also provides analysis routines which you may use to determine the crystal orientation from a Laue pattern. The program can assign Miller indices (HKL) for both cubic and non-cubic systems. A limited starting list of angles between planes is consulted to start the indexing procedure. When the indexing procedure is complete and the orientation matrix known, a data report can be issued with a list of the angles between planes and their angular distance from the x-ray beam direction.

Lastly, the NorthStar program can take the resultant solution and generate a stereographic projection of that orientation. The stereographic projection can be manipulated through various rotations to allow viewing of other orientations. In all cases, the display screen output (images, indexed results, etc.) can be directed to the printer, thus eliminating the need of x-ray film to record the images while also providing a fast written printout of the orientation information including the sample name, date, etc.

With the 32-bit version of NorthStar (running on Windows 2000+), the NorthStar system has been redesigned to operate ‘cooperatively’ with the Windows operating system. Networking (e.g. file and/or printer sharing) is now transparent and will no longer (normally) impact real-time image acquisition.

1.1. System Interconnection & Setup

The MWL110 system consists of a multiwire proportional counter, high speed readout electronics in a NIM instrument bin, a data acquisition board, and the NorthStar system software residing in a dedicated IBM-compatible personal computer.

During operation, a Laue pattern is digitized through an interface board residing within the MWL Model 3 Time-to-Amplitude Converter/Pile-Up-Rejector Module found in the NIM bin. A 2-meter cable connected to this board brings the digital data to an acquisition circuit board installed in one of the computer's internal bus slots.

During the MWL110 system configuration, the NorthStar software is installed and the system is fully tested. Because the system's computer is setup specifically for the needs of the NorthStar software and hardware, caution should be used when considering adding unrelated software or interface boards. Should you have any questions, please call us first...

1.2. Shipping Contents

Upon receipt of your MWL110 Laue Camera, you should inspect the contents to ensure the following is present. Should any of these items be missing, please call us immediately.

a) Real-time Laue Camera and NIM Bin electronics.
b) Si100 reference sample
c) Computer system (interface and software installed).
d) Program security key (HASP), installed on the printer or USB port.
e) This manual.
f) CD-ROM containing installation software.

Please note that it is your responsibility to keep periodic backups of the data and program files as they have been installed (and/or created) on your harddrive. Backing-up your data is an important aspect of maintaining your computer system.

1.3. Printer Setup

Printers are installed through the Windows' Print Manager. This allows you to use a variety of output devices with NorthStar. Please refer to your Windows' manuals to install your printer if you have not already done so previously.

Note that when printing, use the Print Setup facility under Windows to set your print quality. Also, should you wish to include NorthStar windows in your own documents, the graphical windows under NorthStar have special menus allowing you to save the images as bitmap files for later retrieval. The system PrintScreen key is also active, and when depressed, will give you the option of printing or saving the full-screen image as a bitmap.

1.4. Windows Notes

This release of NorthStar is designed to work under Windows version 2000 Pro. It will *not* operate under a lesser version of Windows. Should you wish to upgrade your

Windows version (as future versions become available), please contact MultiWire Laboratories first to obtain advice and an upgrade of the NorthStar software.

Where error tones are mentioned in this text, the generation of such is dependent on having the Windows facility setup to produce different tones for different conditions. Please refer to your Windows manual for further information on configuring the sound output of your system.

1.5. Getting Started Quickly

Although it is strongly recommended that you read through the rest of the manual before using the system, a quick reference section has been supplied in the appendices, starting on page 33, that can be removed (e.g., for lamination) and used to get you started. In addition, a Si100 reference standard has been included to practice with and employ when diagnosing orientation problems. Please note that NorthStar is simply a tool to assist you in analyzing a particular crystal sample. Certain steps must be followed in order to consistently obtain a unique solution in your work.

Throughout this manual, illustrations are included of the actual program as it is operated. These illustrations have been made, for the most part, using the same data from which the histogram file SI100a.HS2 was created. This histogram file can be called up and used for tutorial and/or verification purposes as desired.

NOTE: NorthStar cannot be run from the installation disk. Also, a file called 'readme.txt' is included in the directory you install the program which contains any last minute changes to this manual. You may want to take a minute and check its contents before proceeding.

2. The MWL110 Interface and X-ray Generator

The NorthStar software is an integral part of a much larger system that includes the x-ray generator and the MWL110 Real-Time Back-Reflection Laue Camera System (detector and associated electronics and orientation stages).

Because the x-ray generator is equipment procured separately from the remainder of the system, the operation of such cannot be covered within the scope of this manual.

Likewise, the MWL 110 system's operation and maintenance is documented in a separate manual. During the installation of the system, training is provided to cover the operation and collection of data. Should additional training be required, please contact MultiWire Laboratories for more information.

3. A NorthStar Tutorial

3.1. Starting up the System

Power-up the MWL110 system, then the PC. Start up Windows (if it is not already running), then select the 'NorthStar' icon.

Figure 1. Menu Bar

3.1.1. The Startup Display and Accessing the Menu

After the program has started up, the program's work area will now be visible. At this point, the screen will be blank (solid color) with a bar across the top with text labels. This bar is considered the 'menu bar.' Moving your mouse pointer into this region will cause the menu under each descriptor to drop down. As the mouse moves over each menu function, it becomes highlighted. Clicking on the left mouse button then selects this function.

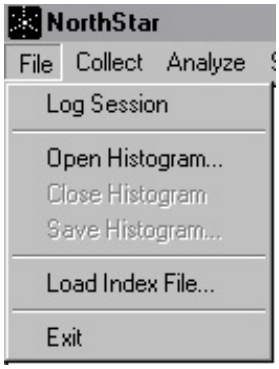

Figure 2. File Menu

Give it a try, allowing yourself to get used to this method of accessing the various menu facilities. As a reference, each of these menu facilities are described in the following section. Menus that appear 'grayed' are disabled until later actions dictate their accessibility.

3.1.2. The Windowed Displays and Forms

Within the NorthStar system, when information is needed from you or a message is generated, an interactive 'box' will pop up. This box is called a dialog (or form) and will carry instructions on its usage. One such example is the program 'About' form that appears when the menu item HELP-ABOUT is selected. Another example is the parameter entry form which we will explore shortly.

On these forms, when multiple 'buttons' appear, you may notice that one may have thicker borders than the rest. This is considered the 'default' button, and may be accessed by pressing <enter> at your keyboard.

As we progress further, various 'windows' will appear on your screen. These windows are used to contain data or graphics depicting the actions be undertaken. One such example is the window that appears when you are viewing real-time data.

3.2. Setting up your System Parameters

Now that you have gotten familiar with getting around the program, you will need to set up the various system parameters that will govern how the collected image will be treated.

3.2.1. The Index File

Move to the FILE menu and select INDEX FILE. A file selector box will appear showing all choices (matching the *.idx description), with the currently loaded file specified in the upper right. By default, the system loaded NICKEL1.IDX. Should a different index file be desired, move the mouse to the name and either double click on the name, or click once on it then on the OK button.

The index file contains a set of angles (0 to 60 degrees) between two planes of different Miller indices for a specific crystal system. As mentioned previously, NorthStar starts up initially with an angle file called "nickel1.idx". Other index files can be created on demand using the INDEX GENERATOR utility. See the appendix on 'Creating Index

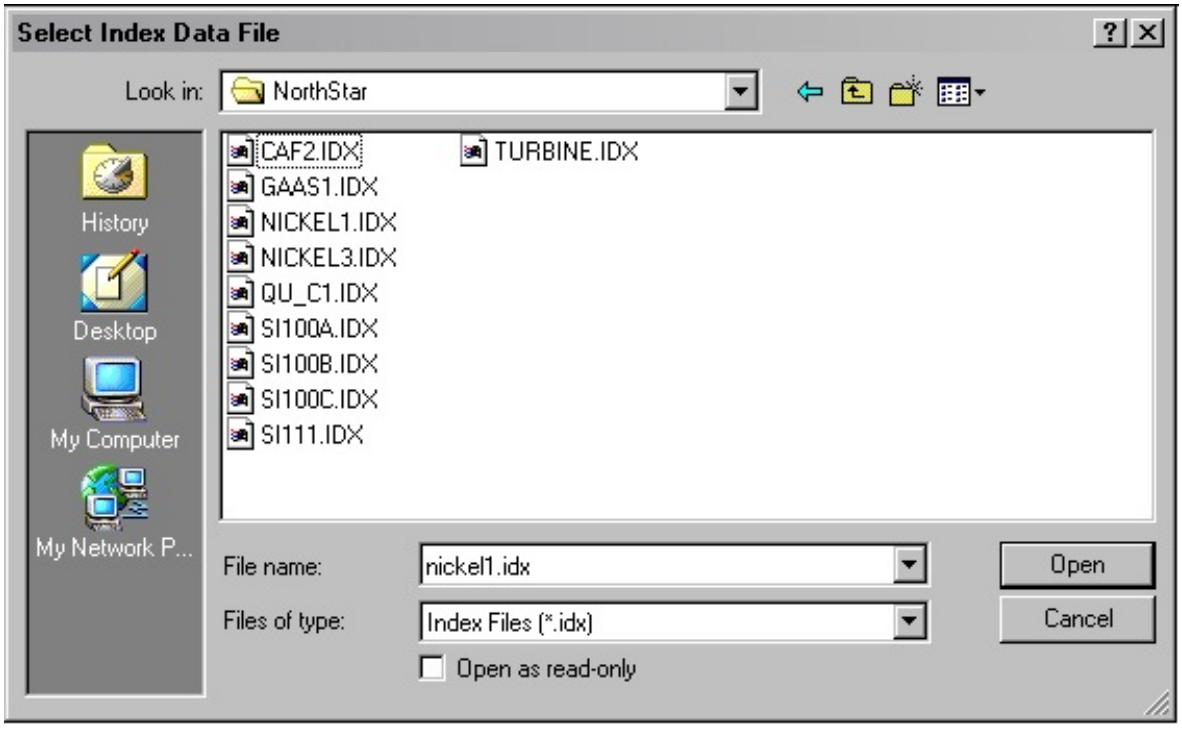

Figure 3. File Select

Files' (page 43) for more information on creating your own custom index files. Each

session will automatically load the index file you last used for convenience (as will bringing up a previously saved Histogram).

3.2.2. The Data Parameters

Move to the COLLECT menu, activating the drop-down submenus. Move down the various choices to SET PARAMETERS and click on it using the left mouse button. A large 'form' will appear in the middle of the screen with different fields in which to enter applicable setup data.

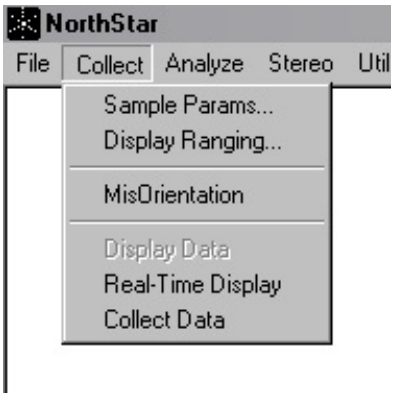

Figure 4. Collect Menu

Additionally, along the bottom are 'buttons' that dictate what the program will do with the entered data.

You may want to try entering various parameters into the 'form' at this time, noting that to move from field to filed, the TAB key is used. Each entry field is explained in detail in the 'System Parameters' section, beginning on page 29. Alternatively, pressing the F1 key brings up on-line help for all parameter fields.

3.2.3. Logging the Session

There is a logging facility built into the program that you may want to enable before proceeding. It is accessed under the FILE menu, and its purpose is to record the events occurring during a session. Such events are written to a file in ASCII (text) format which can be printed (or brought into a word processor) at a later time. Data logged the individual activities selected, solution matrices and a copy of the data report if selected.

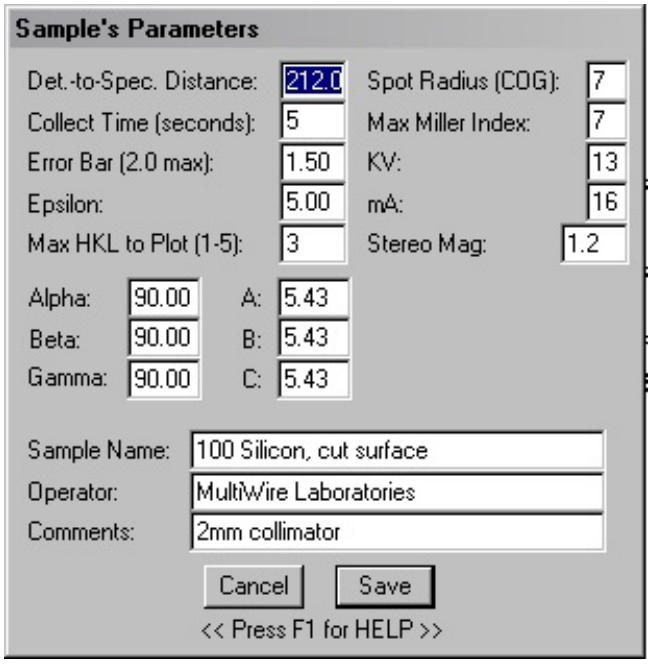

Figure 5. System Parameters

Each session creates a unique log file name of the format "sesXXXXX.log", where the XXXXX is a numerical sequence.

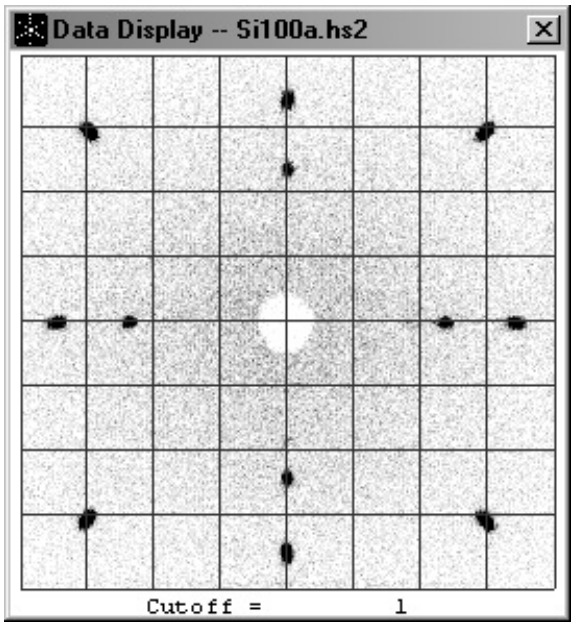

Figure 6. Data Display

3.3. Collecting an Image

The system has now been setup for the crystal specimen to be analyzed. Make sure the x-ray generator and the MWL110 system is ready, position your crystal specimen (e.g. the Si100 reference standard included), then open the x-ray shutter.

3.3.1. Real-Time Viewing

Move to the COLLECT menu and select the REAL-TIME DISPLAY function. You should be able to view the crystal structure in real-time. Try moving the orientation stages to shift the crystal through the x-ray beam along different axes. If the image is weak, use the number keys 0 through 9 to change the persistence levels. Note also that the display is tri-toned, with the darkest shade representing the highest incidence of x-ray events and the lightest shade the lowest.

Note the ease in which you are manipulating the crystal to the plane desired -- this is the beauty of the REAL-TIME facility; being able to setup the crystal exactly the way you need it in seconds, without using expensive film.

Once the crystal is positioned in the manner desired, press the <ESC> key to terminate the real-time mode. Because the real-time mode does not collect any data, we now want to go into the collect mode. Based on the sharpness of the image for the crystal just viewed however, you may first need to adjust the collect time (ref; SET PARAMETERS) to ensure a good pattern for analysis later.

3.3.2. Collecting a Time-Integrated Image

Return to the COLLECT menu, and this time, select the COLLECT DATA function. A small box will appear in the center of the screen and will start 'ticking' off the percentage of time elapsed per the data collection time you have set.

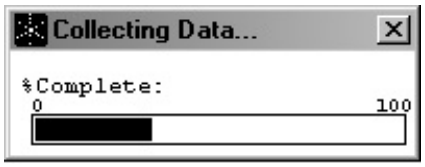

Figure 7. Collecting Data

Should you wish to stop collection early -- either to check the progress during long collection sessions or to perform other functions -- press the <ESC> key. When you are ready to collect data again, select the COLLECT DATA menu once more. A 'dialog' form will appear asking you if you wish to re-start where you left off or begin anew.

Once you have finished collecting data, the program will automatically display the results.

While viewing this image, the 0 through 9 keys can be used to change the 'cutoff' level -- this being a scaled value related to the number of events at each location required before the data is plotted to the screen. To get the mouse back and move on, press the <ESC> key.

Figure 8. Analyze Menu

3.3.3. Saving and Recalling the Image

Now that we have collected and displayed data for this crystal specimen, we can save a copy of the Laue image for later reference. To do this, move to the FILE menu and select SAVE HISTOGRAM. A file selector box will appear in which you can then enter the filename you wish to save the image under. By default the file name suffix is 'HS2' (short for 'Hstogram v2), but any name can be specified. When the image is saved, a copy of the current parameters (as you have entered) are attached to the image. This is so that when you 'load' that image in the future, you will automatically load the parameters it was collected under as well.

On that same note, you may want to try re-loading the image you just saved. Select OPEN HISTOGRAM under the FILE menu, and enter the filename desired in the file selector box that appears. Once the image file is loaded, the program will automatically put up a viewing window showing the image.

3.4. Selecting Index Points (Spots)

At this point you should have valid data loaded, either through the COLLECT DATA or OPEN HISTOGRAM facilities. There are probably several potential 'spots' in your data we can use and now we must identify the ones we want to use to the program. We do this through the ADD POINTS command under the ANALYZE menu.

When you select the ADD POINTS facility, a similar window to what we have been working with is displayed, but this time, the mouse is active. As you move the mouse into the window, the normal 'arrow' pointer becomes a cross hair. Move the cross hair over each point you wish to use, then press the left mouse button. A bell tone will sound with each point selected (and accepted).

Should you enter an invalid point, you can press <ESC>, then use the DELETE POINTS function to remove it. You could also use the ERASE ALL POINTS function to delete all points entered and start fresh.

During the spot selection process, the 0 through 9 keys are active to change the cutoff. This allows you to get the best definition of the point. Internal to the program however is a weighting algorithm that will find the spot's peak automatically, as long as you've selected some portion of the spot itself. This routine works well for small to medium size spots, but not on large, diffuse spots.

To finish the ADD POINTS (or DELETE POINTS) activity, press the <ESC> key.

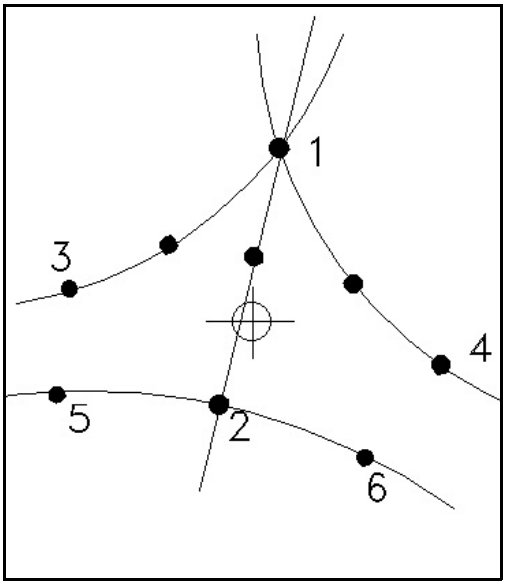

Figure 9. Sample Spots

3.4.1. Rules for Point Selection

1) The first 2 spots selected are critical to the way the indexing algorithm functions, while spots 3 through 'N' are only used to confirm the "orientation matrix" generated from spots 1 and 2.
2) To pick spots 1 and 2, choose points that are believed to be of low Miller index[1] and are greater than 5 cm apart (if they are too close together, there will be a larger error in forming the orientation matrix).
3) Spots 1 and 2 *must be represented (listed) in the index file* (the HKL for spots 3 through 'N' are generated by the program's algorithm). If indexing problems arise, use the TEST OUTPUT command to examine the angles in question and compare them to the selected index file's contents.

[1] Low index spots have two characteristics: (a) the spots lie at the intersection of many crossing hyperbole, and (b) the spots have a 'clear zone' around them with no immediately adjacent spots.

3.5. Finding the Orientation Solution

Under the ANALYZE menu is the function FIND HKL. This function takes the spots you have selected to this point and attempts to find a valid solution. Before selecting this command, re-check your parameters (ref. SET PARAMETERS menu) to ensure this specimen is properly represented.

Once you have re-checked the parameters describing your specimen, select the FIND HKL sub-menu. The program will generate orientation matrices internally and test the validity of all spots you have selected (for a more detailed discussion on what the system is doing during this time, see the appendix on the Indexing Algorithm, page 35).

If a solution is found, a new window will be drawn, with each spot represented by a point and the solution's HKL above each. If the solution doesn't seem correct, try reducing the MAX MILLER INDEX parameter value so that only lower indices are considered.

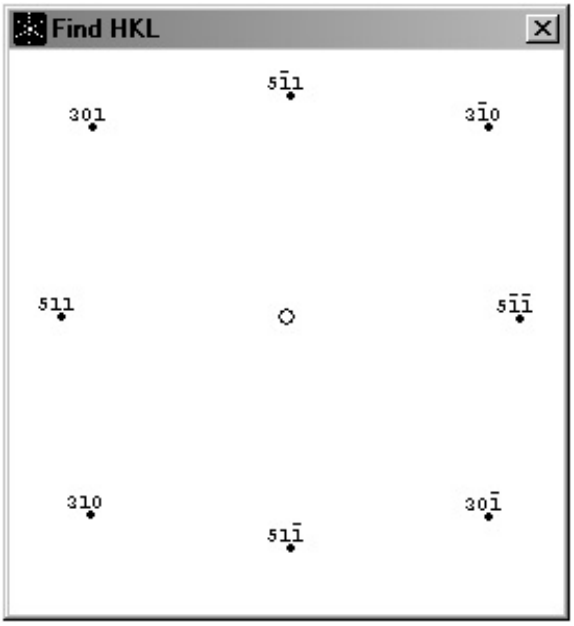

Figure 10. Find HKL Window

3.5.1. Matrix Reporting

NorthStar reports the 3x3 orientation matrices of a successful solution to the session's log file. To enable this data output, the Menu '/File/Log Session' must be enabled (checked). A file called 'matrix.txt' is also created and updated, for each solution found, with the UB matrix and associated parameters for specialized activities.

3.5.2. Persistent Indexing Problems

There may be several reasons for difficulty in reaching a solution with a particular sample. The following points should be used as a checklist before proceeding.

1) Epsilon, a 'fitting' parameter, should not be less than 4.0 for nice sharp diffraction spots and can be made as large as 6.0 for crystals with bigger or more diffuse spots.

2) Check the Detector-to-specimen distance with a ruler. Usually a paper ruler made from a file card is perfect since it generally won't scratch or damage even delicate crystal surfaces. If a 100 mm distance is desired, then make the paper scale of a length 100 - 78 mm = 22 mm. The distance from the tip of the collimator to the center of the detector is approximately 78 mm.

Figure 11. Report Redirection

3) Check the table of angles between planes to make sure it contains a reasonable number of starting values. If all else fails, try to index a crystal of known orientation (or use the example Laue image file included in your directory called "SI100a.HS2"). Use the TEST OUTPUT menu function to directly compute the angles between selected spots. Then compare these values with their computed values. If the indexed spots stay the same when you add additional planes, then this is a good sign that the orientation is correct.

4) Another possibility is that the spots chosen are not in the indexing table and thus it is not possible for the NorthStar program to get started. Pick another set of low index planes that are far apart spatially and try again. Note that the spots with low Miller index are those that can be observed with the very low generator high voltage and also have no close neighbors.

3.6. Generating Reports

Reaching this point means you've reached a solution with the test image you are using. The report facility provides you with the means of obtaining a hard-copy record of your orientation for record-keeping (documentation purposes.

To select a report, move the mouse pointer up to the ANALYZE menu and select DATA REPORT. A report re-direction form will appear in the bottom right. Choose the printer and / or window output options, then review the accuracy of the data reported. If you do choose the window option, any existing windows will be removed first.

Note that if you'd like a copy of the DISPLAY window with this report, the PRINT WINDOW menu facility can be used (this menu is attached to the selected by clicking on the square in the upper left corner of the window in question).

Alternatively, there is a menu facility (UTILITIES-PRINT PIC W/REPORT) that can be used to automatically tag the image to your printed report!

For the given report output, the 'diff' column indicates the difference (in degrees) between the 'theory' and that of the 'exper'(imental) or observed angle for each pair of planes. This variance is summarized in the 'Quality of Fit' (QF) figure. Ideally, a QF as close to zero is desired. If the QF figure is too large, your Detector-to-Specimen distance may be incorrect.

The optimal Detector-to-Specimen Distance is reported just below the QF figure. This value can then be manually entered into the sample parameters facility (and the report re-requested) to better refine the final solution and its resultant report.

Data Report

```
Detector to specimen distance: 212.0 mm
Alpha, Beta, Gamma = 90.00 90.00 90.00
A, B, C = 5.43 5.43 5.43,  Epsilon = 5.0
Error bar = 1.50 degrees,  Noise Cutoff = 5 (1)
Conditions of 13 KV and 16 mA,  Collect time = 5 sec
Hist File: Si100a.hs2
Index file: SI100A.IDX
```

Angles between planes(degrees)	theory	expmnt	diff
01) 3 0 1 and 02) 3 0 -1	36.86	36.78	-0.08
01) 3 0 1 and 03) 3 -1 0	25.84	25.63	-0.20
01) 3 0 1 and 04) 3 1 0	25.84	25.84	0.00
01) 3 0 1 and 05) 5 -1 1	13.16	13.15	-0.00
01) 3 0 1 and 06) 5 1 -1	31.56	31.66	0.09
01) 3 0 1 and 07) 5 -1 -1	31.56	31.29	-0.27

Figure 12. Report Window

3.7. Stereographic Projections

Now that we have a valid solution and a report in hand, the stereographic projection facilities still need to be explored. There are two separate functions to the stereo facility; STAND-ALONE and LAST POINTS.

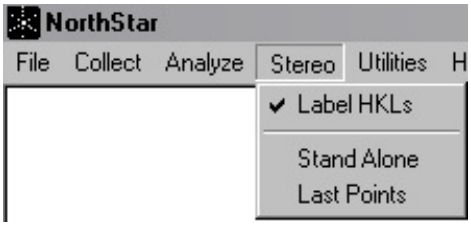

Figure 13. Stereo Menu

The Stereo projection window (STAND-ALONE or LAST POINTS) are sizeable to get a larger image on your screen. To size the window, use the size box at the upper left of the Stereo window. Move the Stereo window by dragging its caption bar. There is a maximum size restriction and screen position imposed however, which should be quite obvious once you try it. This is to ensure the Stereo window's aspect ratio is maintained and that it does not block other windows later on. One last item; if you use the PRINT WINDOW facility, the larger the Stereo Projection is (window-wise), the better the resultant print quality.

3.7.1. Stand Alone Projections

The STAND-ALONE facility is used to generated a stereographic projection based on the entered a, b, c, alpha, beta, and gamma parameters. The base (or HOME) position use Elizabeth Wood's standard orientation as based on the '001' reference, except that the x-axis is reversed to keep the projection in the perspective of the back-reflection system. The STAND-ALONE facility does not require points to be entered nor a valid solution to be found. However, if a previous solution has been found before entering this facility, FIND HKL will need to be selected again before proceeding to the LAST POINTS stereo projection.

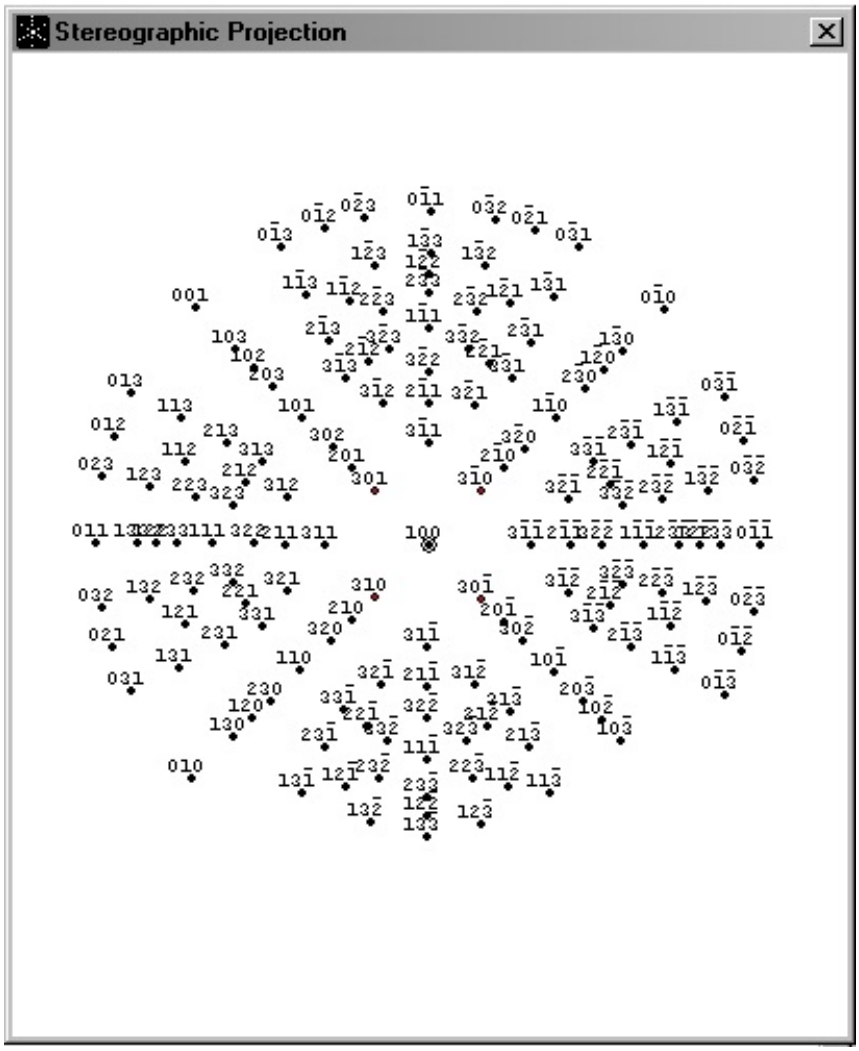

Figure 14. Last Points Projection

3.7.2. Last Points Projections

A stereographic projection of the orientation just determined, using FIND HKL, can be obtained with the LAST POINTS feature.

Selecting this function causes the program to generate a stereographic projection using the orientation matrices generated under FIND HKL. Only indexes falling within the MAX HKL parameter value will be plotted in order to preserve readability. Should this value be too high, HKL label overwriting may occur so you may want to turn that OPTION off.

Planes correlating to those entered (i.e., under FIND HKL) will appear in a different color to facilitate ease-of-distinction. Note that --like the STAND-ALONE projection-- the stereo image will be plotted with the x-axis inverted to keep the projection in the perspective of the back-reflection system.

3.7.3. The Stereo ROTATE & MOVE-TO Functions

After the projection has been plotted, a Stereo PLOT form will appear in the bottom right should you desire manipulating the projection further. This feature allows one to bring any diffraction plane into the orientation's center plane for purposes, say, of determining proper specimen 'slicing' angles.

The dialog contains three 'edit-able' boxes, one for each axis, the movement indicated by the 'arrowed' figures above the boxes. Enter the desired value (in degrees, positive or negative) in the respective axis's edit boxes for which you wish to move the projection.

Four buttons also appear, one to initiate the 'rotation' based on values entered, one to reset the projection to the HOME or initial position, one to move the current projection directly to a plane of choice (MOVE-TO), and the last to 'Cancel' the rotation interaction.

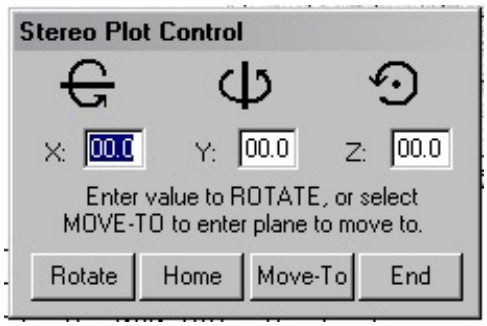

Figure 15. Stereo Plot Control

When using the MOVE-TO facility (reference the MOVE-TO button), negative ('bar') indices are entered with a 'minus' sign preceding the desired index. There are no limitations on the +/- index entered (i.e. 0 through 9 are all valid), however, the sequence of indices entered must match the plane of interest.

When the projection is shifted to the plane of interest, the numerical boxes are updated to show the total X, Y, Z rotation from the starting (or HOME) position. This feature can be especially helpful when attempting to determine how much a specimen must be rotated in order to get a desired 'cut.' Note that when a 4-Miller index sequence (HKIL) is

employed, *only* the H, K, and L components are to be entered. As a move-to rotation is an x, y sequence, the reversal of that move-to is not always possible. In this case, the use of the HOME button is preferred and will return the projection back to its initial position.

Stereo projection hard-copies may be obtained through the PRINT WINDOW facility attached to the STEREO window (upper left corner box of the projection's window).

When a 'Last Points' stereographic projection is requested and some subsequent rotation is applied, the software reports this on the graphic print out of that window if such a printout is requested. This should help identify a stereographic projection that has been rotated from the solution point.

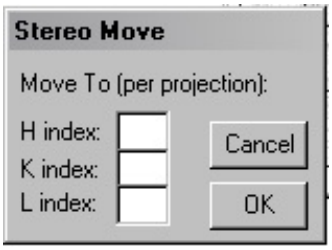

Figure 16. Stereo Move-to Control

3.8. Shutting Down the System

Now that our tour is over, how does one shut down the system? Move the mouse pointer to the FILE menu and select EXIT. Exit Windows (and shut down the PC) as desired. Then power down the x-ray equipment and MWL110 electronics.

Figure 17. Menu Bar

4. Menu Reference

Note, under various functions, other menu facilities may become disabled (titles become light gray). This is to prevent interaction when data, etc. may not be available due to the current actions underway.

MENU SUB-MENU and Function
v v

4.1. FILE

The FILE menu group provides general system functions, including the commands to save and retrieve Laue picture information.

LOG SESSION - turns on or off logging of an NorthStar session. When on, the menu has a 'check' mark beside it. Each time this is selected, a new log file (or session) is begun.

OPEN HISTOGRAM - Use the Open command to retrieve Laue pictures that have already been saved on disk. Activating this menu feature brings up a dialog box that allows you to select the desired file. Point with the mouse to the desired file name and then click on OK or double click quickly on the file name directly.

Once a valid Laue picture file has been selected, the file will be loaded and the image will be displayed in a window on the screen automatically. Further manipulation of the image follows those available under the DISPLAY DATA menu command.

CLOSE HISTOGRAM - Select the Close command to clear Laue files loaded with the Open command from the program's memory. This should be done before loading different Laue files from disk so that the data is properly cleared.

SAVE HISTOGRAM - The Save command permits storage, onto disk, of a picture that has just been collected with the MWL110 detector. Selecting this command brings up the item selector box.

To save data under a different file name, simply backspace over the default name and type the desired name. Some examples of satisfactory file names are: SILICON2.HIS and Q15K_2.HS2[2].

The second example represents a convenient notation to simplify file storage. The name represents a quartz file (Q) that was collected at 15kV (15K), the second (_2) in a series.

The file is written to disk in a binary form to conserve space. The program also appends the Parameter's information to the file thus keeping collection information with its Laue picture. Together, the 256 by 256 16 bit/pixel picture file and the Parameter's data yield a file of approximately 129K bytes[3].

INDEX FILE - Load an index file. Use this feature when you need to load an indexing file other than the default (or when you want to check what index file is already loaded).

Loading an index file also resets some of the system parameters so you will want to recheck these through the SET PARAMS menu.

To create your own index files, see the appendix on 'Creating Index Files' (page 43) for more information.

EXIT - Exit the program back to Windows. All parameters are saved on exit automatically.

4.2. COLLECT

This group of commands provides control over the collection and viewing of dynamic real-time back-reflection Laue patterns.

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[2]The .his file suffix is employed for the 8-bit (old-style) histograms, while the .hs2 file suffix is employed for the new 16-bit histograms.

[3]The old-style (256x256x8-bit) histograms were approximately 65K bytes in size.

SAMPLE PARAMS - The Sample Parameters command allows the user to specify various attributes concerning the analysis of Laue patterns, as well as information related to the collected data. This information is also appended to the image during storage (see the SAVE HISTOGRAM command).

To enter text in a field, point and click with the mouse in the desired field or press the tab key until the cursor appears in the appropriate field. Backspace if necessary to remove old information and enter the new data from the keyboard. If all data is correct, select the OK button with the mouse, otherwise select CANCEL and the newly-entered information will be ignored.

See the section on Parameters for detailed descriptions of each field and their usage (page 29).

DISPLAY RANGING - Selecting the Display Ranging Menu brings up a dialog box that allows you to select between conventional key-driven persistence / cutoff driven displays and logarithmically-scaled displays. Under each type, there are entries that help tailor the selection to your tastes.

The Cutoff Key method uses the keys 0-9 to select the appropriate cutoff values based on the Cutoff Multiplier (explained below). This method has been retained for those used to being able to change the cutoff level. The Log10 Scaling method scales the log of the individual histogram cell value against the gray scale range (0-255). The 0-9 keys are no longer used (scaling is automatic). A shift value and threshold point may be specified if you wish to shift the grayscale of the log10 scaled image. See the program's help facility for further information.

MISORIENTATION - The MisOrientation menu provides the means to analyze across crystal grain boundaries or bi-crystals. It is intended for Cubic systems only.

When you select "MisOrientation", you will be asked to orientate the specimen on each side of the grain boundary. Following orientation, the differences in orientation between the two will be calculated. This report contains the orientation differences between the two crystals or across the boundaries, in terms of delta x, y and z. You will then be given the option of having this report directed to the screen, printer, or both. Note that the "MisOrientation" report is automatically logged (if logging is

enabled) and a report prefixed with the job number will be placed in the working directory.

REAL-TIME DISPLAY - The Real-Time Display command displays a live-time Laue pattern on the screen per the detector, specimen, and generator's current configuration. Any parameter varied during this display (x-ray voltage, crystal position, etc), will be instantly seen on the screen itself.

This function provides a method of orientating the specimen in real-time to the correct position so that an ensuing COLLECTION command can be given. During the orientation (or viewing), the 0 through 9 number keys may be used to change the persistence of the display. Pressing the <ESC> key terminates the function and returns the mouse to your control.

COLLECT DATA - The Collect command collects Laue pictures, in real-time, directly into computer memory. During the collect period, the image is not displayed on the screen, so it is important that you have correctly orientated it first using the REAL-TIME function.

This form of data collection gives the clearest image of the diffraction pattern. Integrating for a few seconds of time is all that is usually necessary. In very weak signal applications or when collecting Laue patterns from very tiny crystals, you can integrate the image for several minutes to obtain better results.

You can change the data collection time using the SET PARAMS command. If in doubt, first try an initial value of 10 seconds. Select the COLLECT DATA command to begin the collection procedure. A time line will appear showing a START and FINISH point.

DISPLAY DATA - Select the Data Display command to display either the Laue pattern last collected or the image most recently loaded from disk.

The computer displays the Laue image as a 256 by 256 array of 8-bit/pixel intensity information (values ranging from 0 to 255). Data Display plots all pixels with values greater than the specified cutoff

level. This cutoff level is adjusted by pressing the 0 through 9 keys while viewing the display.[4]

This same cutoff level will be employed during the ADD and DELETE POINTS function.

As with the REAL-TIME DISPLAY command, pressing the <ESC> key terminates the display function and returns control to your mouse.

4.3. ANALYZE

The Analyze menu group contains commands to index the Laue patterns. These operations are only enabled once an image has been gathered with the COLLECT DATA command or recalled from disk with the OPEN HISTOGRAM command.

ADD POINTS - Use Add Points to enter spot coordinates in preparation for calling the indexing command, FIND HKL. When this function is selected, the current image is drawn on the screen and the mouse is then used to select each spot.

The first two spots selected are very important because NorthStar uses them to form a trial orientation matrix which it will then test against the remainder of the spots used during the indexing process. The orientation matrix is a 3 by 3 matrix that contains all the information necessary to specify how the crystal is positioned relative to the incoming x-ray beam.

Generally, a minimum of four to six spots (*the maximum is 25*) should be entered to achieve unique results. Spots are sequentially selected by moving the cross-hair over the desired spot and clicking once with the left mouse button. A center of gravity input routine automatically finds the peak position, even if

[4] Each cell of the histogram data can be up to 65536 counts deep (16-bit value) but only the first 8-bits are used (256 counts deep). A 0 value is white while a 255 value is black when displayed. The cutoff value (0-9 key during display) is used to elevate the values of these cells to make them less or more visible by the following formula: display_value = cell_value * (cutoff_mult - (cutoff_key * (cutoff_mult / 10))) where the value 10 indicates the potential cutoff steps (0..9)

the mouse pointer misses the true peak position by several pixels. Duplicate entries are ignored, and a 'beep' tone will be generated for each point accepted. Should you need to change the cutoff level to discern between points, the 0 through 9 keys can be used as under the DISPLAY DATA command.

When you have entered all desired points, press the <ESC> key to end the ADD POINTS action.

DELETE POINTS - Delete Points reverses the action of the ADD POINTS command and uses the same control format. Delete one or several spots from the list of points by centering the cross hair on the spot(s) and clicking the left mouse button. Exit by pressing the <ESC> key (as in the ADD POINTS facility).

Note: You should use the ERASE ALL POINTS command if you want to clear all the points.

ERASE ALL POINTS - The Erase All Points command removes all previously selected points from the list of points used in indexing.

SAVE POINTS - Selecting the Save Points command writes to disk all points selected with the ADD POINTS routine. This ASCII file is primarily used as a tool for troubleshooting should problems with a set of points arise. It is also compatible with MultiWire's EZORIENT software package.

FIND HKL - Find HKL is the heart of the NorthStar program. This command assigns Miller indices (HKLs) to the diffraction spots selected with the ADD POINTS command.

The routine requires a valid index file for the system being analyzed. This index file contains a starting list of angles between planes and is used to identify the first two points you have selected. In addition, the data parameters must be correct for this sample, with a special emphasis on the following:

* Maximum Miller Index (e.g. 7).
* An Epsilon value (e.g. 5.0).
* An Indexing Error Bar (e.g. 1.5).

If you experience problems indexing the pattern, see page 11 for additional considerations to check.

Once the index solution has been found, a window will appear with the selected points and the Miller indices labeled.

TEST OUTPUT - Select the Test Output command to display the raw x and y pixel location of peaks selected with ADD POINTS, as well as the angle between spots calculated for a given Detector-to-specimen distance (you may change this distance using the SET PARAMETERS command). As with DATA REPORT function, you can select the output to be directed to a window, the printer, or both.

DATA REPORT - Once you have achieved the desired indexing of the Laue pattern using the FIND HKL routine, use the DATA REPORT command to create a summary of the indexed pattern. This report can be directed to your printer, a report window, or both. We recommend that you use the report window output ONLY when you are indexing 8 or fewer points due to limited window space.

The generated report contains information about the calculated and experimentally determined angles between planes as well as the entered parameter data such as sample name, date, etc.

4.4. STEREO

The STEREO menu provides a 3-dimensional projection and rotation facility for the crystal system you are currently working with.

LABEL HKLs - This command enables or disables labeling of HKLs during plotting. Note that when more than two Miller indices are being plotted under standard magnification (e.g. 0.8), overwriting of the labels may occur.

STAND-ALONE - Select the Stand-Alone command to generate a stereographic projection plot based on the current system parameters. This projection is centered on 001 based on Elizabeth Woods discussions. This command is useful for obtaining a reference projection or for educational purposes and is not indicative of the current data you have collected.

LAST POINTS - Following a successful FIND HKL operation, this function becomes available. The function, when selected, will generate a stereographic projection of the crystal you are working with, based on the points selected and the data parameters

entered. The maximum Miller index plotted is under the control of the value you have entered under the SET PARAMETERS command.

NOTE: Under both types of projections, a projection rotation control panel appears that allows you to further rotate the projection as desired.

4.5. UTILITIES

The UTILITIES menu provides commands to augment the data collection and reporting process.

DETECTOR CALIB - This function should only be used under guidance from MultiWire Laboratories. It is designed to calibrate for any detector non-linearities and thus the improper use of such can affect subsequent data analysis.

The calibration value is entered in the calibration dialog as a value between 90 and 110, representing a percent change in the y-axis speed (100 = no adjustment). Note that this value is determined when the system is first setup and calibrated at MultiWire Laboratories so we highly advise you calling us for that value before entering one arbitrarily.

PRINT PIC W/REPORT - Select this command when you desire a copy of the LAUE image to be 'tagged' with the REPORT function's data output. Note that the image window must remain on the screen for this function to print the window (as it uses the PRINT WINDOW facility).

DISPLAY GRID - The Display Grid On command causes a reference grid to appear in the Real-Time and Data Display windows. If the window is already being displayed, the display must be re-activated in order for the grid to appear.

3-MILLER INDICES - The 3 Miller Indices command forces all output in the FIND HKL and STEREO windows to use either standard HKL notation, or HKIL notation -- where 3-Miller Indices is the default. Selecting this menu will toggle the setting between 3 and 4-Miller Indices (where I = -(H + K)).

INVERT IMAGE - The invert command causes the Display Data function to show the collected data in an inverted gray scale representation.

INDEX GENERATOR - Brings up a parameter box in which to enter the desired crystal system's parameters. Following entry, the program will then generate an index file (*.idx) to those specifications, for subsequent use. See the appendix on 'Creating Index Files (page 43) for more information.

OMLIST ANGLE GENERATOR - This is a supplemental angle generator that takes a list of indices of interest, in multiple segments, and produces the appropriate angles.

The "infile" should have a header section like that of a standard angle file that includes a,b,c, alpha, beta, and gamma. Following this should be the planes of interest, in an interest list format; but each interest segment must be separated by "99 99 99". The entire list should be terminated by " 0 0 0". Comments may follow the data but should be separated by a tab and a '#'.

This file can be the result of previously generated intermediate files (temp.tmp) as produced by ANGGEN. Sample files are included with the suffix "*.om2". The resultant (.idx) file produced by OMLIST is formatted for direct use as an index (or angle) file by the NorthStar program. See the appendix on 'Creating Index Files (page 43) for more information.

4.6. HI-RES

The "HiRes" menu group contains functions to calibrate and check the performance of the system.

CALIBRATE - The procedure involves orientating a specimen normally and collecting an image. At the end of collection, and removal of the display window (via the <esc> key), a dialog box will appear to prompt you to select a reference spot.

You should then rotate the specimen 180 degrees and collect a pattern once more. Again, at the end of collect/display, a dialog box will prompt you to re-select that spot at its new position. After

you have entered the new position, another dialog box will appear giving you the delta and gamma factors for the reference as well as the previous values. You are then prompted as to whether you want to keep the old values or update the parameters with the new value.

The delta and gamma calibration factors are used in the "Use Calibrate" function.

USE CALIBRATE - Select this option to check the system calibration. A check mark will appear beside the menu when it is active. To disable this option, select the menu item once more and the check mark will go away.

The check procedure involves orientating a specimen normally and collecting an image. At the end of collection, and removal of the display window (via the <esc> key), a dialog box will appear to prompt you to select a reference spot.

After you have entered the new position, another dialog box will appear giving you the delta and gamma factors for the misalignment.

4.7. HELP

The HELP menu provides access to the program and system help facilities.

CONTENTS - Selecting CONTENTS brings up a Help index for most NorthStar subjects. Note that pressing F1 (except from within those areas noting the use of same), brings up this same function.

HOW TO USE HELP - This menu calls up Windows' system-wide Help.

ABOUT - Selecting this menu function shows the 'About' form containing program revision notes.

4.8. Window Menus

These menu items are found under the SYSTEM MENU attached to certain graphical windows like STEREO, COLLECT, etc. To select them, move the mouse to the box at the top left of the window in question.

PRINT WINDOW - causes the window to be printed at the printer. A Form Feed is automatic.

SAVE WINDOW - causes the window to be saved, in standard bitmap format After selecting the menu item 'Save Window' -- you will be prompted for a filename and once entered, the program will convert the image and save the file as directed. The images saved can be loaded into any image processing software application that works with standard bitmap formats.

4.9. Special Keys

PRINT SCREEN - At any time, the “PrtScr” key may be used with the NorthStar application; and when pressed, you will be asked if you want to print or save the current screen to a file (in bitmap format). If you are requesting this during an interactive dialog, the image will still be captured but you may not get the prompt until after you have responded or exited the dialog.

Space For Your Notes

5. The System Parameters

The SET PARAMETERS command brings up a form containing several fields that must be completed for a crystal to be indexed. These fields are described below.

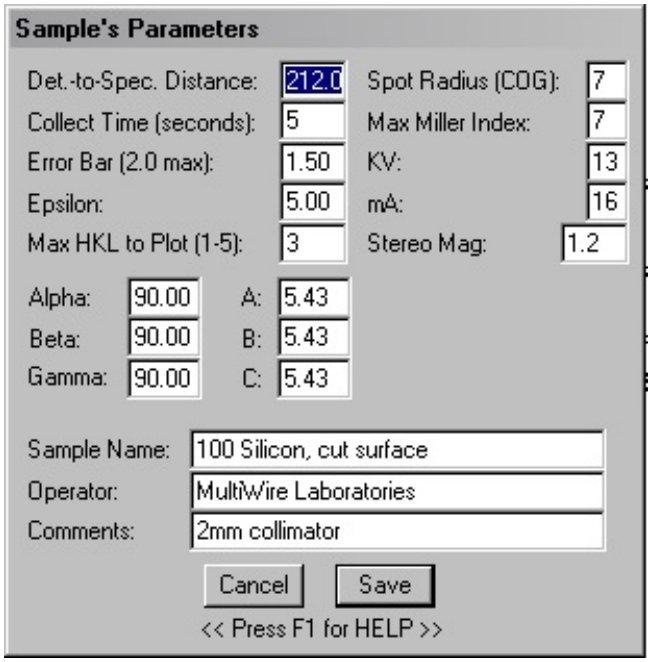

Figure 18. Set Parameters Dialog

5.1. Specimen Data

Det-Spec Distance: [Detector-to-Specimen Distance] Enter the distance from the center of the detector to the crystal for the specimen being analyzed.

Collect Time: When the COLLECT DATA function is called, this will be the period (in seconds) over which the data will be collected. 300 Seconds is the maximum collect time that can be entered.

Error Bar (0.01 to 2.0 Degrees): A tolerance (+/-) from which the calculated angles between the first two spots selected are compared to those angles in the index file. Typical values are 1.0 to 1.5 degrees.

Epsilon: Epsilon represents an internal 'fitting' factor used when comparing the remaining spots. If the image being analyzed has sharp spots, a value of 5.0 is usually sufficient. For larger, more diffuse spots, use a value of up to 6.0.

Spot Radius (COG): The Spot Radius is a figure used to determine the Center Of Gravity (COG) of a selected spot. It is measured in pixels around the selected area (as defined by the center of the cross-hair). The typical value of '7' should suffice must applications unless the image is heavily blurred. Use it cautiously, returning to the default value (7) if problems persist.

Max Miller Index: This is the maximum Miller index that will be considered during the search for a solution. If this value is too large, a secondary solution (of higher-order indices) may be found first. Start out with a value of 5 or 7 if you are unsure. The allowable range is 1 to 15.

Cutoff Mult: This value provides a means of extending the range of the cutoff value used during the display of collected or saved data. Each displayed cell of the histogram data can be up to 256 bits deep. A 0 value is white while a 255 value is black when displayed. The cutoff value (0-9 key during display) is used to elevate the values of these cells to make them less or more visible by the following formula: display_value = cell_value * (cutoff_mult - (cutoff_key * (cutoff_mult / 10))) where the value 10 indicates the potential cutoff steps (keys 0..9). Presently the Cutoff Mult may be from 1 to 50, with 20 being the default value.

KV, mA: These are for documentation purposes only and are typically used to note the x-ray generator voltage and the tube current settings for this particular specimen.

Sample Name, Operator Name, Comment Fields: Allows entry concerning the sample and the operator for data collection purposes.

5.2. Stereo-Specific

MAX HKL to Plot: To generate a stereo projection, tables of HKLs up to some max limit of h or k or l are required and computed here. Each time MAX is changed, a new table is computed. Allowed values are 2 - 5. Note that when 4-Miller index sequences are specified (i.e., HKIL), the 'MAX HKL' restriction will be applied *only* to the HKL components. On the same note, when a LAST POINTS stereographic projection is requested, this limitation will preclude any plane from being represented that has an H, K, I, or L component outside of the restriction range.

Stereo Magnification of Plot: The stereo projection's image size can be changed with this function (the window size does NOT change however). If a particular area is overwritten by too many HKLs, then the central region can be magnified with this function. Default value is 0.8, i.e., the natural design value. To double the scale of the output, try mag = 2.0. A value of 0.80 is an ideal setting for most applications as it shows the entire sphere. On the other hand, a setting of 1.8 gives a point-spacing relationship nearly identical to that of the points in the 'FIND HKL' window. Please note that this value does not change the window size however, rather it simply allows the magnification (or compression) of planes close to the center.

Alpha/Beta/Gamma, a/b/c: Entry of angles between, and the lengths, for each axis. These fields allow you to define the type of crystal system you are using. It should be noted that these parameters are loaded automatically with the index

file and that the Alpha, Beta and Gamma variables are limited to 0 < x < 180.0 degrees.

5.3. Buttons

SAVE Button - saves the new parameters you have entered.

CANCEL Button - aborts the parameter entry, discarding any changes.

Space For Your Notes

Appendix A. Quick Reference Guide

This section provides a quick-reference summary for the use of the NorthStar system. It can be removed from this manual, laminated, and kept close at hand for your convenience. The page number references provided allow quick access to the applicable tutorial sections. Note that a similar reference is included in the 'on-line' help, accessible by the F1 key while the program is running.

Step 1: Power up the MWL110 electronics, the x-ray generator, and the PC. Position the crystal specimen on the orientation stages in front of the detector's collimator. Start up Windows, then select the 'NorthStar' Icon to start the program. (page 5).

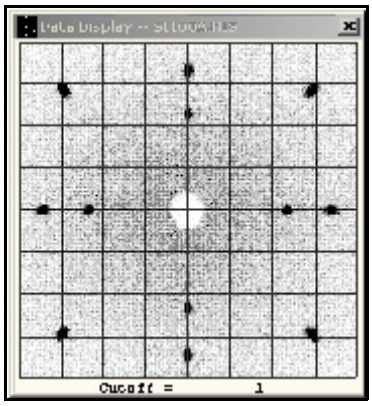

Figure 19. Data Display

Step 2: Open the MWL110's shutter, then select REAL-TIME DISPLAY under the COLLECT menu. Orientate your specimen to the desired position while watching the real-time display window. Use the 0-9 keys to change display persistence. When satisfied, press the <ESC> key to terminate the real-time mode. (page 8).

Step 3: Select SET PARAMETERS and enter the specimen's information and enter the desired collect time (page 6). Then, check that the correct index file is loaded via the INDEX FILE menu (e.g., NICKEL1.IDX for cubic crystals). Lastly, select the COLLECT DATA function to let the program collect the specimen's data. When the data collection is finished, the image will be displayed automatically.

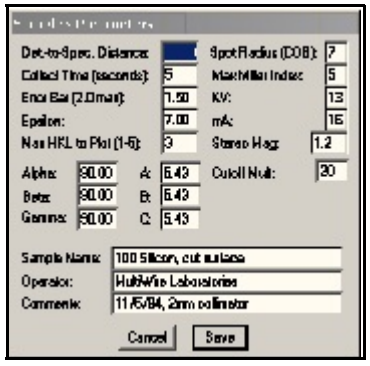

Figure 20. Sample Parameters

Step 4: Close the MWL110's x-ray shutter. Move to the ANALYZE menu and select ADD POINTS (page 9). Using the mouse, select 4 to 6 spots, using the rules discussed in the 'Tutorial' section of this manual. Press the <esc> key to terminate spot addition.

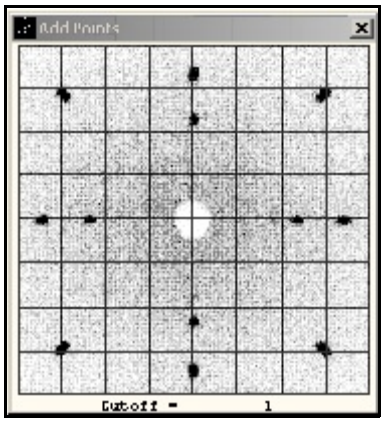

Figure 21. Add Points

Step 5: Select the FIND HKL function under the ANALYZE menu to see if a solution can be found (page 11). If a solution is not found, see the section on Indexing Problems in the Tutorial section of this manual (page 11). If the solution is found, select DATA REPORT under the same menu to view or obtain a hardcopy of the results (page 12).

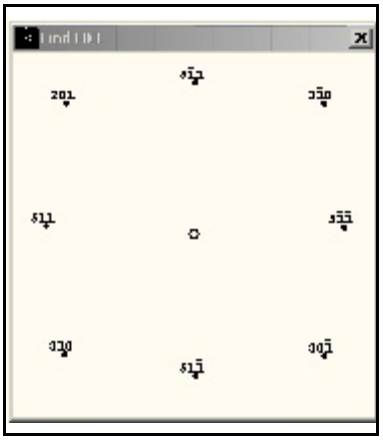

Figure 22. Solution Found!

Step 6: As desired, you can now select the LAST POINTS function under the STEREO menu to view a stereographic projection of the specimen just orientated (page 13). Use the MOVE-TO feature to bring the selected HKL to the center (i.e., into the orientation).

Step 7: Exit the program using the EXIT option under the FILE menu. Power down all equipment (page 16).

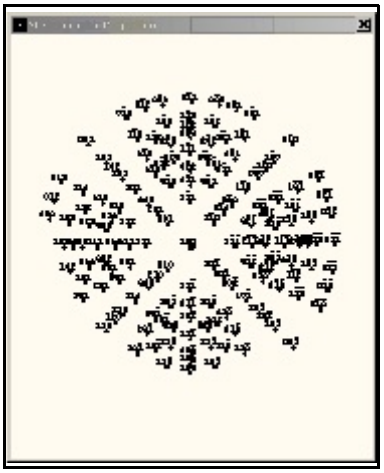

Figure 23. Stereo Projection

Appendix B. Indexing Methodology

The NorthStar program employs an algorithm based on orientation matrix methodologies to determine the solution for a given set of entered spots (planes). In NorthStar, an orientation matrix is constructed from the first two spots you have selected. The orientation matrix is most accurately made for spots that are far apart (i.e., spanning 1/2 the image size or more). Once this matrix is formed, the information about the remaining spots can be readily derived. This algorithm is discussed in the following paragraphs in order to provide a better understanding of the program's actions.

B.1. The Indexing Algorithm

The orientation of a single crystal can be described by an orientation matrix UB, a 3 x 3 matrix that contains information about the crystallographic unit cell (a, b, c, alpha, beta, gamma) and how it is aligned relative to a reference coordinate system. The orientation matrix is the link between the Miller indices in reciprocal space and the diffraction vector in real space. Once the correct orientation matrix is found, all the (orientation) information is at hand to describe how the crystal is aligned with respect to the x-ray beam.

The diffraction vector for a given Laue spot can then be constructed from the coordinates of the spot observed in the back-reflection image, given the orientation matrix, UB. If the Miller indices in reciprocal space are represented as a column vector:

$$H = \begin{bmatrix} h \\ k \\ l \end{bmatrix} \quad (1)$$

and the x,y,z coordinates in real space (cubic, right-handed) of the diffraction spot are expressed as:

$$X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

(2)

then:

$$X = UB * H$$

(3)

This is the fundamental equation governing the mathematics of this part of the computer program.

The UB matrix can be constructed if the coordinates of two spots in the detector image is known (say X1 and X2), along with their corresponding Miller indices (say H1 and H2).

Equation 3 may be inverted so that an H vector is calculated from the X coordinates of the spot position, i.e.

$$H = [UB]^{-1} * X$$

(4)

As mentioned earlier, a trial UB matrix is first constructed from the two points entered. The angle between these two spots is then calculated and compared to the angles in the index file with respect to the Error Bar's current value. A list of possible HKL assignments is then made for these entries.

The UB matrix is then inverted and H vectors are calculated for each of the remaining spots (planes) using equation 4. If the nearly integer H vectors of less than or equal to the maximum Miller index are recovered in this process, then a SOLUTION has been found.

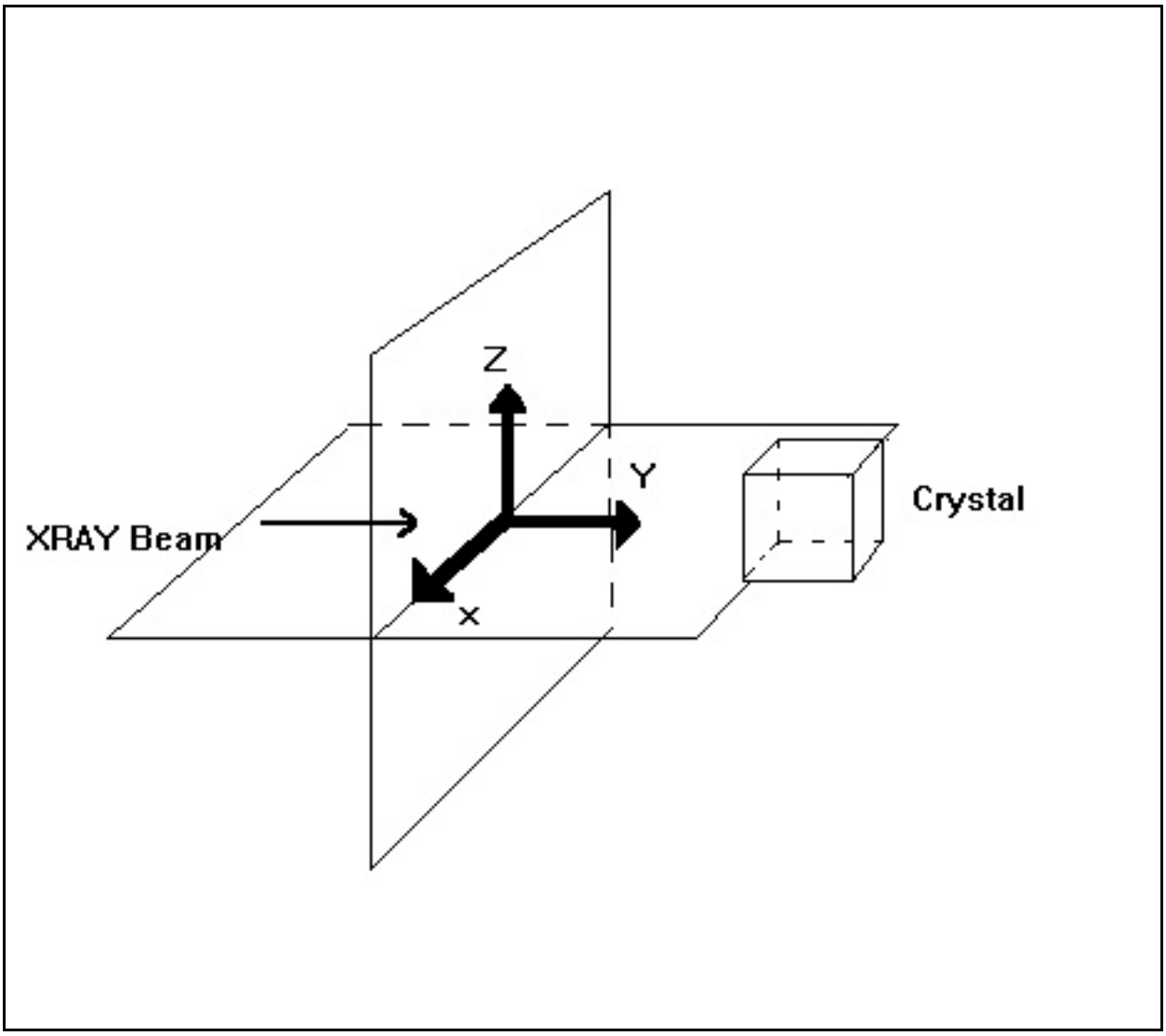

Figure 24. Coordinate System

The coordinate system and general matrix methods follow those of W. R. Busing and H. A. Levy, Acta Cryst. (1967), page 457-464. The polychromatic beam from the x-ray tube is incident along the negative y-axis. The Laue pattern is observed in the x,z plane

by the film. The observed diffraction spots (planes) are assigned (x,z) coordinates depending on their location in this plane.

The indexing time depends strongly on the number of starting entries in the index file. This in turn depends on the symmetry of the crystallographic unit cell. Low symmetry crystals require more table entries than high symmetry ones (e.g. cubic systems). A real advantage of this method is that once the proper orientation matrix is found, the indexing of all other remaining spots (planes) is achieved by simple matrix multiplication and is not dependent on how large the Miller indices become. This is in contrast to other indexing programs which expend a large amount of time searching tables for a consistent answer. In this latter case, the number of choices grows very quickly when Miller indices above (say 4) are chosen. The ability to accurately assign Miller indices with this algorithm is dependent only on the accuracy of the measurement of the spot position from the detector's image.

B.2 Crystal Structure Definitions

The following information is presented to clarify the usage in the angle generation facility and in internal calculations.

The designations for the seven different crystal systems are as taken from the International Tables for Crystallography, Volume A (Space-Group Symmetry), Kluwer Academic Publishers, Dordrecht/Boston/London, (1989). Table 2.1.1 on page 13 gives the definition of terms (cubic, hexagonal, ... triclinic).

Elements of X-ray Diffraction by B. D. Cullity, Addison-Wesley Publishing Co, Inc., Reading, Mass. (1956) in table 2-1, page 31 gives an equivalent list of crystal systems and Braviais Lattices. Word descriptions are from this table.

Cubic - Three equal axes at right angles.
a=b=c; alpha=beta=gamma=90 degrees
Can permute h,k,l in any order.

Hexagonal - Two equal coplanar axes at 120 degrees, third axis at right angles.
a=b≠c; alpha=beta=90; gamma=120 degrees
Can permute h and k only.

Trigonal - three equal axes, equally inclined.
a=b=c; alpha=beta=gamma but not 90 degrees

Can permute h,k,l in any order.

notes:

1. Another name for trigonal is rhombohedral.
2. Also a trigonal can also be indexed as hexagonal, but the unit cell is no longer primitive (the smallest possible one) and then you use a hexagonal indexing system.

Tetragonal - three axes at right angles, two equal.

a=b≠c; alpha=beta=gamma=90 degrees
Can permute h and k only.

Orthorhombic - three unequal axes at right angles.

a≠b≠c; alpha=beta=gamma=90 degrees
No permutations allowed.

Monoclinic - three unequal axes, one pair not at right angles.

a≠b≠c; alpha=gamma=90 degrees≠beta
No permutations allowed.

Triclinic

a≠b≠c; alpha≠beta≠gamma≠90 degrees
No permutations allowed.

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Appendix C. Working with High Resolution Mode

The HiRes feature in the NorthStar program is a utility that does not yet communicate with other parts of the software such as MOVE TO, STEREO, etc. It is a little stand alone routine that at the moment, works by itself.

The basic idea is that you first offset the x-ray track horizontally by about 5 degrees (exact value not important) or so that an highly oriented crystal (less than several degrees off) can diffract an oriented Laue spot to an area near the collimator, but off to one side. (The Jack and Translation stage has a curved slot in it to make this easy to do.) If the crystal is rotated in azimuth through 360 degrees on an external precision rotary stage (not supplied by MWL), then the perfectly oriented Laue spot stays fixed in position on the detector surface and doesn't wander off. If the crystal is off-axis a fraction of a degree, however, then when you rotate through 360 degrees, it traces out a small cone. The worse the misorientation, the larger the cone diameter that is traced out by this Laue spot onto the detector surface.

The HiRes feature has you take two images of the same Laue spot (no indexing is involved at this point), one with the sample up (0 degree azimuth) and another with it down (azimuth = 180 degrees). The operator clicks on just this one Laue spot each time. The average of the two readings tells you the center or perfectly oriented position of that Laue spot. The deviation of the observed position relative to the center position gives the misorientation down to the 0.05 degree level in both x and y (gamma and delta angles). This is essentially the Bond Method used on diffractometers applied to our Laue camera. This method works to remove the small non-linearities in the delay lines which cause the 0.25 degree limit in the first place.

In tests with silicon and quartz (really perfect crystals with good strong Laue spots), we actually could see changes down to the 0.03 degree level with a 200 mm film-to-specimen distance. If the signal to noise of your crystal is not as good as silicon or quartz, then the resolution accuracy will suffer slightly.

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Appendix D. Creating your own Index Files

D.1. Overview

Packaged with the NorthStar program is a standard angle index file for the CUBIC system (typically 'nickel1.idx').

Also included with the NorthStar program is a utility, INDEX GENERATOR (located under the UTILITIES menu), designed to allow you to create your own custom index data files and to provide a wide degree of flexibility for your application. Should you wish to customize your angle files, the knowledge and use of a good text editor (NOT a word processor) will be extremely helpful here. Windows' NotePad is quite satisfactory for this purpose (refer to your Windows' manual or Help for further information).

Please note that the specification and creation of index files requires a good level of familiarity with the principles of crystallography.

If you do not feel comfortable with the idea of creating your own index files, *index files for specific systems can be created to your specifications by MultiWire Labs for a nominal fee*. To obtain more information contact the address listed on page 57.

D.2. The Index File Format

An index file consists of three main sections; the header, the angles, and the 'tail'. These are described as follows:

```
  5.4310  5.4310  5.4310
 90.0000 90.0000 90.0000
 505     2   1   1     5   3   3
1316     5   1   1     3   1   0
1316     5   1   1     3   0   1
1326     3   3   1     1   1   0
1419     3   3   1     3   5   1
        . . .
        . . .
5625     1   1   1     5   1  -1
5952     1   0   0     3   5   1
5999     2   1   1     1   2  -1
0000     0   0   0     0   0   0
number of table entries is =   105
```

Block 1. Sample INDEX File Format

a)

The 'header' contains information about the crystal system from which the angles were generated (as specified by you). These include:

LINE 1: a, b, and c parameters (in Angstroms).

LINE 2: alpha, beta, gamma (in degrees).

b) The 'angles' contain the angle and Miller index relationships, one per line. In short, each entry is one line consisting of the following components:

angle * 100 miller index #1 miller index #2

Angle entries may be hand-edited, using a text editor (e.g. the adding or deletion of angles), however, the use of an 'interest list' is the preferred approach (see discussions below). If you do 'hand-edit' the data files, please remember to follow the same format. Also, do NOT use tabs, employ spacing instead. Comments may be added to the file but they must be added *at the end of an existing line* of data. Lastly, there is a restriction as to the total number of angles that can be contained in the file (refer to the section on the angle generator utility below).

c) The last section (the 'tail') contains a terminating 'angle' and index sequence of zeros, followed by one or more comment lines.

D.3. The Interest List File

To ease the creation of index files, an 'interest list' facility has been provided. The primary purpose of the interest list is to specify only the planes you are interested in for generation. An 'interest list' can be extremely helpful in reducing the length of the index file and the planes the NorthStar program must search. More importantly, it is the preferred alternative to hand-editing the output index file and in that sense, it could also be called an 'inhibition list'.

Another application of the interest list is in the restriction of solution considerations to a specific sector of a crystal structure. In order to do this, create a list (using an editor) of planes you are interested lying in the specific sector of interest.

The format of the interest list file is simply one plane per line (3 miller indices, signed as necessary). Comments may be included after the last index; but comments may not begin at the beginning of a line. No special delimiters are required between the 'L' index and the beginning of the comment however.

Sample 'interest lists' have been included to illustrate the format [C_ILIST.TXT (cubic systems) and H_ILIST.TXT (hexagonal systems)] and as a starting point in creating your own data files.

D.4. Hands On

It is wise, before creating your own angle file, to inspect one of the angle data files provided with the system. In order to do so, a good text editor (e.g. Windows' NotePad) will be required.

The 'Index Generator' utility essentially converts your specifications into a list of angles between planes and Miller index relationships. Again, though, I must state that you should have some working knowledge of crystallography before attempting to specify your own angle file.

When the angle generator utility is called up (via the menu UTILITIES-INDEX GENERATOR), it will ask you for a series of parameters that describe your system of interest. These include the following parameters:

-The output filename (prefix only, suffices are automatic).
-Alpha, beta, gamma, a, b, c for the system of interest.
-The maximum Miller index (level) you are interested in (does not affect the 'I' component of 4-Miller index systems).
-The number of planes a restriction angle will be applied to (if any).
-Each plane (with which the restriction will be applied, if any).
-The restriction angle in degrees (if used).
-The name of an HKL interest list file (if one is to be used).

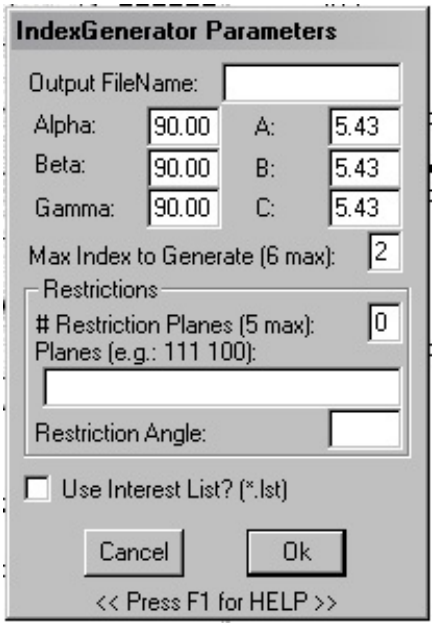

Figure 25. Index Generator Parameters

Note that while filling in these fields, pressing F1 will bring up parameter-specific help for assistance.

Of the parameter fields listed, only one needs additional clarification -- that of the 'interest list.' The primary purpose of the interest list is to specify only the planes you are interested in for generation. Sample 'interest lists' have been included to illustrate the format [c_ilist.lst and h_ilist.lst]). An 'interest list' can be extremely helpful in reducing the length of the angle file and the planes searched during an orientation. More importantly, it is the preferred alternative to hand-editing the

output angle file and in that sense, it could also be called an 'inhibition list' or a better yet, a selection list.

An interest list simply contains a list of indices (or planes) in which you are interested in, *each on its own line*. To create a custom interest list, first examine one of those provided, then use Window's Notepad facility to create your own. One quick method of creating the interest list is to request a STAND ALONE Stereographic projection for the specimen class, then select indices of interest from it as a basis for your list.

After the parameter data is specified, the program will calculate a temporary file of planes ("temp.tmp") – available for your review later -- and then the actual set of angle relationships (along with the appropriate header and 'tail'). Due to the length of processing time involved, the program will also give you an *rough* estimate of the time it thinks it will take to complete the task.

Once the index file has been generated, it is ready for use. However, if a warning message appeared noting that too many angles were generated, the index must be 'thinned' down, using a text editor to remove excess angle entries.

D.5. Combining Index Files

Several data files (as created by the INDEX GENERATOR) can be combined to make one general purpose indexing file. The procedure uses standard DOS or Windows tools as follows:

1) Using Windows NotePad, delete out of each file you desire to combine the top two lines (a, b, c, alpha, beta, gamma) -- be sure to note the content of these lines for addition later. Also delete the lines at the bottom of each of the files that begin with:

"0000 0 0 0 0 0 0"

-- through the end of the file.

2) Concatenate the desired files by the command (Window's Command Prompt facility):

"copy infile1.idx+infile2.idx outfile1.idx"

3) Re-sort the angles in the <outfile1.idx> by the command:

"sort < outfile1.idx > outfile2.idx"

4) Add back in one copy of the data removed in step 1 (updating the line "Number of table entries = XXX" as desired).

D.6. Restrictions

As with any system, some restrictions will apply. In our case, these restrictions are employed to maintain a reasonable search speed within the NorthStar system. The utilities will safeguard against exceeding or violating these limits; but it is good to itemize them anyway:

1) *Maximum HKL that can be generated is 6*. Higher indices can be hand-edited in though.

2) *Maximum number of angles is 1000*. Use the MAX HKL and INTEREST LIST entries to reduce angle count as necessary.

3) *Maximum angle represented = 60 degrees*.

4) *No zero-degree angles can be specified*.

It should also be noted here that the Index Generator automatically generates 3-Miller index sequences for all systems. The NorthStar program will generate the 4-Miller index sequences as necessary (e.g. for FIND HKL, etc), when requested.

D.7. OMList Extended Index Generator

The "OMList Extended Index Generator" utility allows you to create custom index files for the crystal specimen you are working with. Only minimal crystallographic data are necessary. No provisions are made in this generator for removing redundant angle/plane sets.

OmList requires that you create a file in a text editor with an .om2 file name suffix that has the following:

line 1: <a> <b> <c>
line 2: <alpha> <beta> <gamma>
line 3: a list of HKLs, one per line
line n+1: "99 99 99"
line n+2: "0 0 0"

Multiple lists can be concatenated by separating each list with 99's (ref. line n+1), then terminating the file with 0's (line n+2).

Omlist generates a file of angles between planes given a,b,c, alpha,beta, gamma of any unit cell (triclinic included). The file has the same prefix name as the om2 input file, but with the idx suffix. It can then be employed as any other index file. Sample .om2 files are included and located in the program directory for your reference.

Appendix E. File Naming Conventions & Formats

E.1. File Naming Conventions

The NorthStar system creates or employs several file types within the normal course of its operation. These files are listed below in order to identify their purpose. Those file types listed as ASCII content can be viewed with a viewer such as Window's NotePad or a standard word processor, or they may be printed to your line printer.

1) *.IDX = Indexing files {ASCII}

2) *.HIS, *.HS2 = Laue image (histogram) files {Binary}

3) *.LST = Interest lists for the Angle generator {ASCII}

4) SESXXXXX.LOG = Session logging files {ASCII}

5) PARAM.SYS = System / Program parameters {Binary}

E.2. File Formats

The Histogram file contains 2 parts; 1) The histogram itself as an array of 256 x 256 words (16-bit) of data, and 2) The system parameters. The data types and sizes are presented below for the more adventurous of you that may want to create your own post-processing (a sample matlab 'm' file has been included in the installation directory that illustrates reading and plotting a histogram -- "image_his.m"). Note that an 'int' is 4 bytes.

```
Unsigned short      histo[HISTX][HISTY];          (HISTX = HISTY = 256)

struct {

  // user params
  char  spname[52];          // specimen name
  char  operator[52];
  char  comment[52];         // specimen comments
  int   spares1[10];

  // program & histogram parameters
  int   logging;
  int   pscn_flag;
  int   gridf;
```

```
int   hklflag;
int   invimage;   // image inversion flag
int   cursor;     // which cursor?
int   curmag;     // cursor magnification flag
int   drngtype;   // display ranging type
int   spares2[9];

// northstar detector linearity adjustment factors
int   spares25[14];  // residual from 14-point grid cal
float det_yadj;      // detector's error adjustment
int   spares3[9];

// histogram info
UINT  wDIBUse;            // palette type for current histogram (ScanOrient)
DWORD biClrUsed;          // number of colors in image (ScanOrient)
int   hvalmult;           // value multiplier for drawing
int   thresval;   // Nstar; threshold for applying grayscale shift (log method)
int   thresshft;  // Nstar; threshold shift for grayscale (log method)
int   spares4[8];

// analyze / collect params
char  indx_fname[261];
int   persist;          // initial persistance level (key actions)
float errbar;
float detspecd;
UINT  coltim;           // time to collect data for.. (deciseconds)
int   cutoff;
int   maxmind;
float epsilon;
int   mamp;
int   kvolt;
int   spot_rad;         // radius of spot for analysis
float xcal;             // ScanOrient's internal scanner calibration factors
float ycal;

// autodetect variables
UCHAR admxdiam;      // maximum spot diameter to accept
UCHAR admndiam;      // min spot diameter to accept
UCHAR adspare;
UCHAR adduptol;      // for duplication check (range of tolerance)
UCHAR adedexcl;      // peripheral region (edge), don't try to detect here...
UCHAR adcog;         // local COG
USHORT admaxpts;     // maximum nof points to try to detect
int   spares5[8];
```

```
  // stereo params
  int   hkl_label;
  int   maxh;
  float magnify;
  float alpha;
  float beta;
  float gamma;
  float avar;
  float bvar;
  float cvar;
  int   stx;       // sizeable window dimensions
  int   sty;
  int   stw;
  int   sth;
  Int   rpx;
  int   rpy;
  int   rpw;
  int   rph;
  int   spares6[6];

  // northstar calibration variables (hi-res)
  float cald;
  float calg;
  int   spares7[10];

  // northstar interface params
  BOOL  demo;       // for demo usage
  DWORD mispulsefreq;
  DWORD testgenfreq;
  Int   blocksize;
  int   spares8[9];

} SystemParams;
```

Appendix F. System Sounds

Sounds are generated by the application when points are selected, or an error occurs. These sounds are tied to standard Window's sounds, giving you the ability to change them to suit your tastes. To change the desired sound, go to the Window's Control Panel and Select the Sounds item. The sounds impacted are listed below.

Sound Source	System Sound
Point selection, other general sounds	DefaultBeep
Error sound	Exclamation

Appendix G. Upgrading from Pre-v4.0 Versions

Most of the files produced by NorthStar are ASCII (text) based and remain compatible across all versions of NorthStar. However, the HISTOGRAM files (*.his) are binary and have been impacted by changes between versions. This is because histogram files also contain a copy of the current system parameters and the size of the parameter structure has grown as the software evolved. Because of these size changes you may get an error on loading your old histograms. This error simply tells you that the system parameters (tied to the histogram you just loaded) could not be loaded.

How can you use your old HISTOGRAMS? Simply note the params involved with each (using the old version of software or printed reports). Then, using the new version of NorthStar, load the histogram and re-enter the parameters into the SET PARAMS box, then re-save the histogram. Further accesses of that histogram will be problem free.

Appendix H. For Further Reference

General Crystallography:

Cullity, B. D. Elements of Xray Diffraction. 2nd ed.
Reading: Addison-Wesley Pub. Co., 1978.

Sands, Donald. Introduction to Crystallography. New York:
W. A. Benjamin, 1969.

Wood, Elizabeth A. Crystal Orientation Manual. New York:
Columbia University Press, 1963.

Orientation Matrix Discussions:

Busing, W. and H. Levy, Acta Crystal (1967), vol 22,
pp 457-464.

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Appendix I. Problems / Comments

I.1. Common Problems & Error Messages

"Could not locate MWL2000 interface card or driver..." message:
You may need to reinstall the MWL2000 driver and NorthStar software.

"..Software Security Device..." message:
This type of message occurs when the HASP security plug attached to the parallel printer (or USB) port has become loose or misplaced. The software will not run without the proper key (plug) attached.

"Error opening parameter file" message:
The last usage of the system probably used (and specified) a parameter file from another directory or drive that is different from the one you are now starting up in. A new parameter file is created automatically using default values. To avoid losing your settings, do a 'Find' for param.sys and move the original back to the NorthStar directory.

"Error Opening Index file" message:
Message at application startup: The last time NorthStar was run, it used an index file that no longer exists (or has been moved). Load a new index file to resolve this problem.

Message at Histogram load: As above, select a new (current) index file, then save the histogram to save the new file (location).

Real-Time and Collect does not function (realtime menus are enabled):
You may need to reinstall the MWL2000 driver and NorthStar software.

The Display seems "fragmented":
Check that the interface card is seated properly. If the problem persists, connect the test cable and refer to the interface card troubleshooting section for further instructions.

Problems finding a solution:
1) Re-check the angle file to ensure that the correct a, b, c, Alpha, Beta, Gamma values were used for the sample's crystal system.

2) It may be possible that one of the points selected is outside of the range of indices within the angle table. Try another point instead or create a new angle table with a specific focus (on the sample in question and its axis).

3) Verify that the Specimen Distance is correct.

4) Set the ErrBar value to 1.0 (too wide means too many potential solutions to evaluate in the time allotted, too narrow means only a small range of possible solutions are going to be evaluated).

5) Recheck the COG and Epsilon values.

I.2. Problems that cannot be resolved

If an orientation problem occurs, use the SAVE HISTOGRAM facility and provide us a copy of this image file, the index file (e.g. NICKEL1.IDX), and the session's logfile (if used), along with a detailed description of the problem. If possible, use the 'Print Window' and report facilities as well to supplement your description.

I.3. Technical Support

Technical support is provided free of charge for the first 30 days or 2 hours phone support. Beyond this period, a nominal fee must be charged for each support call[5].

[5]We will need to request a PO number for each call. If the call is within warranty, the PO will not be used or charged.

I.4. Suggestions

Comments, Suggestions, etc. about the manual and/or product improvements to the program are welcome. Send them to (or call):

MultiWire Laboratories, Ltd.
165A Langmuir Building
MS 1018
Cornell Business & Technology Park
Ithaca, NY 14850 USA

Phone: 607.257.3378
Fax: 607.257.3201

EMAIL: salesinfo@multiwire.com
WEB: http://www.multiwire.com

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