Introduction to DataScan and Jade on the Scintag PADV System

(prepared by James R. Connolly, for EPS400-002, Introduction to X-Ray Powder Diffraction, Spring 2003)

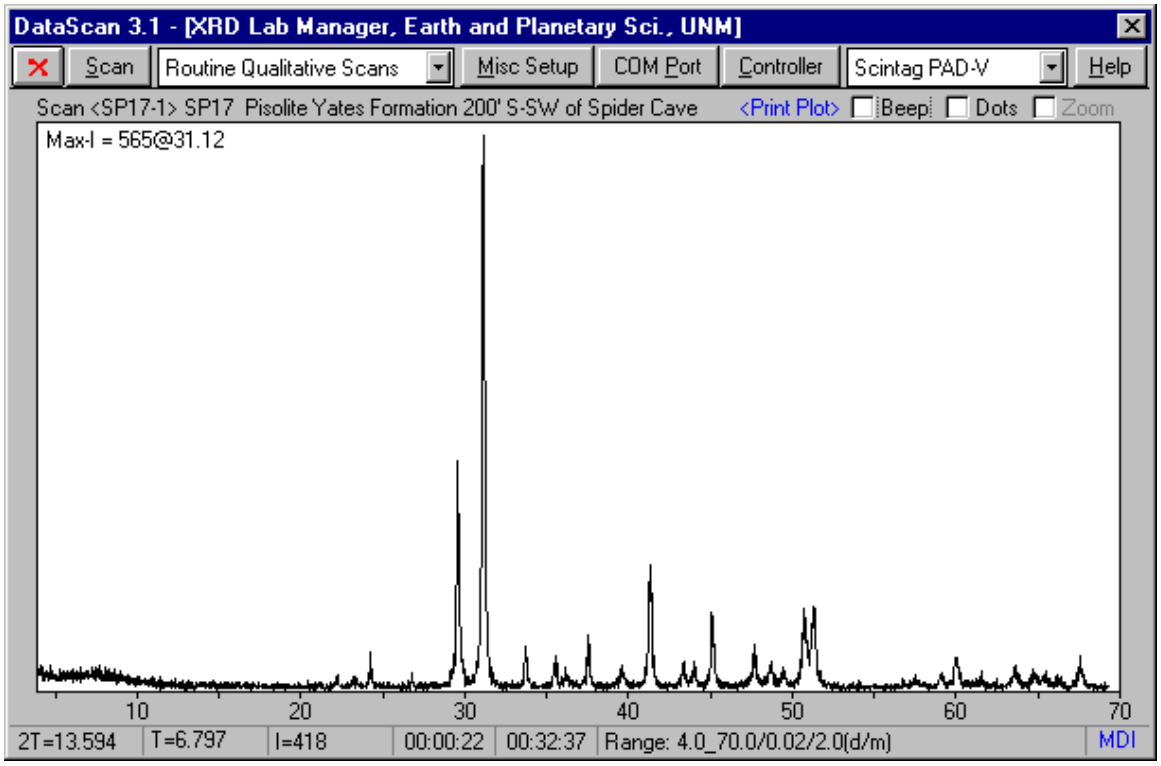
Introduction

In the last 15 years, the development of sophisticated and easy to use software for data collection and analysis has made sophisticated analysis of X-ray powder diffraction data accessible to anyone with the ability to operate a personal computer. In many cases the software is so easy to use that analysts run the risk of using it as a "black box" to obtain answers not warranted by the data.

The material in this section is concerned specifically with the software installed for use with the Scintag PAD V system in the X-ray powder diffraction laboratory in the Department of Earth and Planetary Sciences at the University of New Mexico. As of this writing, this software is DataScan 3.1 (for data collection) and Jade 5.0 Plus (for data analysis) from Materials Data, Incorporated (MDI). MDI software is written by experts in X-ray diffraction and is relatively user friendly. Jade, in particular, is extremely powerful and well worth the time and energy spent learning to use master its many and varied capabilities.

Most of the material in these sections is abstracted from MDI's documentation.

Data collection with MDI's DataScan 3.1



Above is the DataScan 3.1 interface Window referred to in the following sections.

DataScan 3.1 is a 16-bit Windows program. The only significant limitation this imposes is that no more than 8 characters (and no spaces) are allowed for file names. The program communicates with the Scintag PAD V goniometer by means of a standard RS-232 serial interface. This is a single bit-stream interface and if it is interrupted it is possible to lose

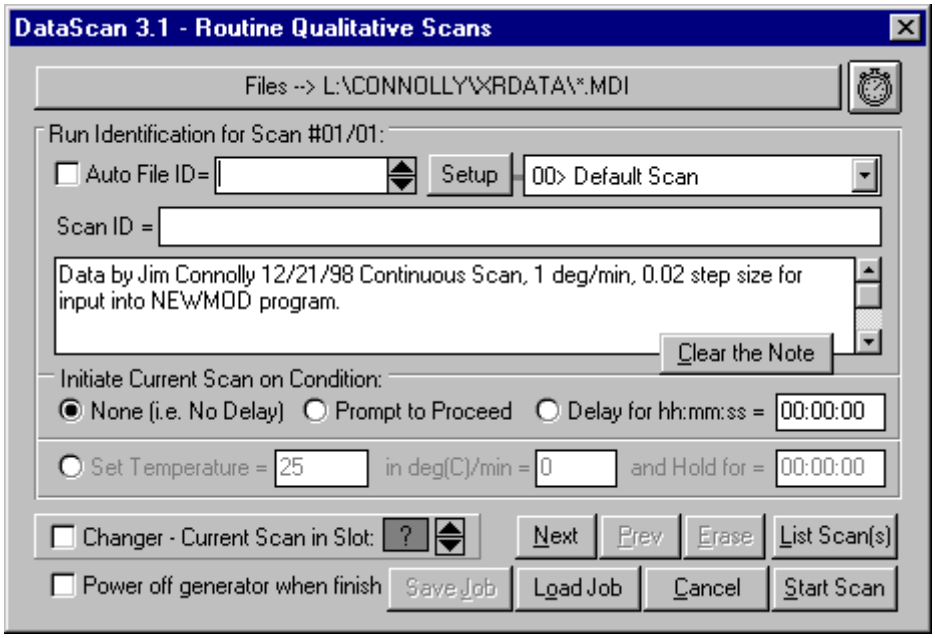
communication with the diffractometer causing data collection to fail. With recent configuration changes in the system, this is now a rare (but still possible) occurrence.

The DataScan Interface and Data Collection Setup

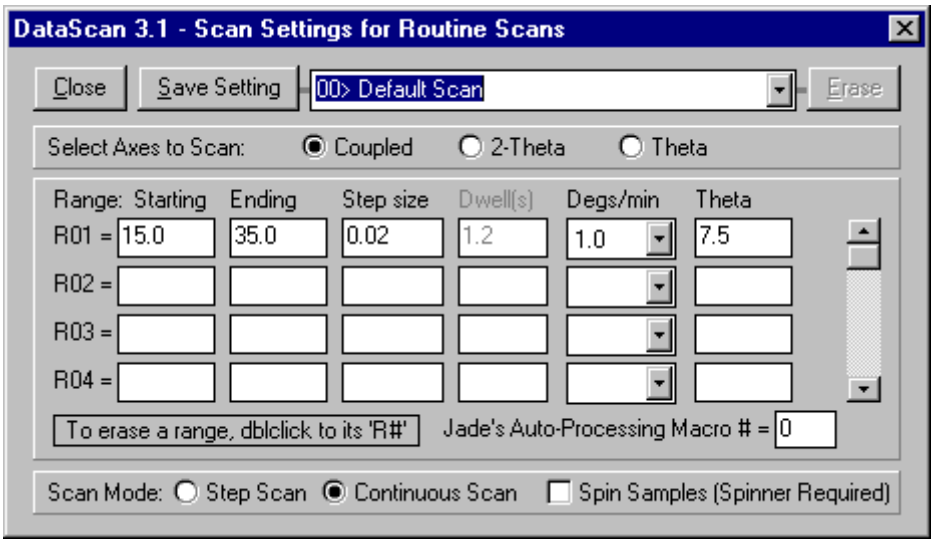
Data collection and operation of the diffractometer is through a series of dialogs called up through the buttons at the top of the main program window as shown on the previous page. Details of operation may be found in the XRD Lab Procedures Manual (or "XRD Cookbook") in the laboratory. The manual is also available at http://epswww.unm.edu/xrd as an Acrobat PDF file.

From right to left, the buttons are:

- **Controller:** Used routinely prior to data collection to verify the angular position of the specimen and detector, and calibrate these positions as necessary. Primarily used by the lab manager for configuration of the diffractometer including establishment of default operating parameters.
- **COM Port:** Not accessed during routine use. Used during initial installation for setting communications parameters for the serial interface with the diffractometer.
- **Scan Type Pull-down:** For most general data acquisition, "Routine Qualitative Scans" is chosen in this box. Some other specialized scan types are available and listed in the next section.
- **Misc Setup:** These are program parameters set by the lab administrator. Items set here include: Display colors, anode in use, goniometer parking position, a variety of display options, the "data save" interval, and the data file format used for routine qualitative scans.
- **Scan:** This pulls up the primary dialog for the scan type selected. A sample window is shown with the different entries described below:



- **Files:** Click this bar to select location where data will be saved. Default is the local (C:) drive. Correct location is the user's network folder (L:\username using your network username).
- **Clock Icon:** After all parameters are setup, clicking the clock will estimate the total time required for data collection.
- **File ID:** Enter a file name here, no more than 8 characters, no spaces.
- **Setup:** Click this button to configure parameters for the scan. The following dialog will come up:



Items configured here include:

- **Scan Axes:** Coupled is the standard Bragg-Brentano θ - 2θ coupled scan, and will usually be used. In a 2-theta scan the specimen (θ) is fixed throughout the scan (and manually entered) and the detector (2θ) varied; this is sometimes used for thin films and specimens where a fixed low θ value is required. In a Theta scan, the detector (2θ) is fixed and the specimen (θ) varied through the scan; this is virtually never used for routine work.
- **Scan Mode:** Choose a step-scan or continuous scan. The step scan mechanically moves specimen and detector by fixed steps, counts only while at that step and then moves to the next step. The continuous scan moves specimen and detector continuously
- **Range Settings:** Include Starting and Ending angles, Step-size, Dwell (time spent at each step in seconds), Degrees/min scan speed, Starting Theta value. If Step Scan is selected the Dwell time in seconds per step is entered and the Degs/min setting is grayed out (and calculated by the program). If Continuous Scan is selected, Degs/min is set by the operator and Dwell time calculated by the program.
  Multi-Range scans may be selected and included in a single data file. Jade will automatically read these data files and display the multiple

ranges as overlays. Multi-range scans are not generally exportable easily to other programs.
Step vs. Continuous: In general, Step Scans should only be used for scans with dwell times of more than 3 to 5 seconds per step. The main reason for this is that accurate step scans require mechanical stability during counts which is difficult to achieve with very short dwell times and step sizes of less than 0.05°.

- **Save Settings:** Allows users to save standard settings with a unique name for use in later data collection sessions.

- **Scan ID:** Free-form Field for description of sample, up to 80 characters included as part of the "header" in the data file.
- **Note Box:** Free-form field up to several hundred characters included as a separate note (.not) file. This is not an intrinsic part of the data file, but can be accessed and printed by Jade if available in the same folder as the MDI data file.
- **Initiate Scan:** Initiates how scan starts when the "Start Scan" button is pressed. For one-at-a-time specimens, "None" is selected and scan starts immediately. "Prompt to Proceed" may be selected for a sequence of pre-programmed scans with the prompts allowing for quick manual change of specimens. If desired, start time may be delayed by a specific amount of time after "Start Scan" is pressed.
- **Changer:** Operates a sample changer if available. Our PAD V is a single-specimen manual-change system.
- **Power off Checkbox:** For systems where DataScan controls the high-voltage power supply, this will power-down the generator after the run. This is not functional on our system.
- **Next, Prev, Erase, List Scan(s):** Each job can include more than one scan. Next adds a new scan to the job, or shows the next one if it is already configured; Prev. displays the previous scan in the job; Erase deletes the current scan; List Scan(s) shows a list of all scans in the current job. By default, Next duplicates the previous scan, thus it is easy to make unwanted multi-scan jobs. List Scan(s) will let you check for this and remove scans you don't want in your job list.
- **Start Scan:** Starts the scan following instructions in the Initiate Scan settings.

As soon as the scan starts, the 2θ vs. intensity trace is written to the DataScan window. The window will automatically adjust the intensity scale for the trace as data are collected.

The bottom line of the Window keeps count of the current 2θ and θ positions, intensity, elapsed and total time and the scan parameters.

Specialized Types of Scans Available in DataScan

Routine Qualitative Scans are used most routine data collection; setup parameters are discussed in the previous section.

Area Scans (Peak Integration) are specialized scans done around specified peak locations to determine integrated peak areas. These are generally used for production control or

detection of known trace phases in a sample. Data is output as a .DAT file specifying the peak position and the total integrated counts minus background counts. There are two scan modes: In "Summit Search" mode peak location is specified with a ± range around it; the software scans to locate the peak within the defined interval and then does determines the peak shape and does the calculation. In "Fixed Range" mode the range to be scanned and scan rates are specified for a range containing the peak of interest; the peak summits are located in the range and intensities calculated.

External Quantitative Scans can be used to enable quantitative analysis by comparison with a set of standard calibration curves obtained on standard materials. This is an optional feature that we do not have.

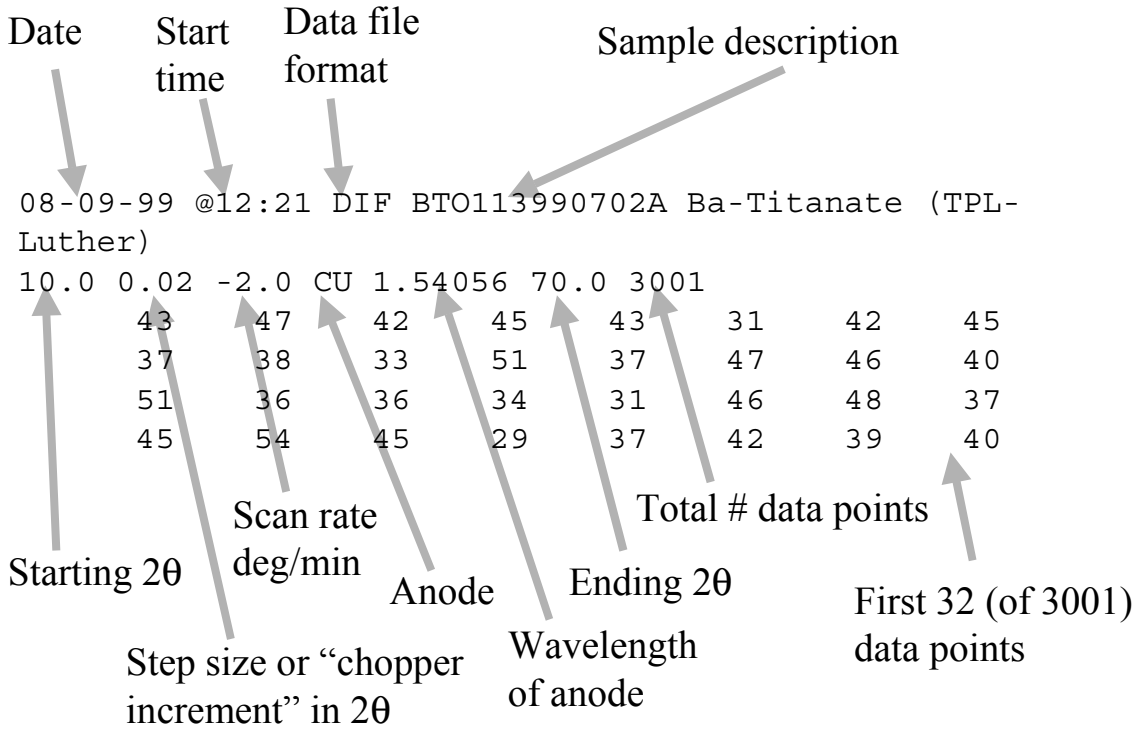
Residual Stress Scans are used with Jade to analyze strain. This is another optional feature that we do not have.

Reflection and Zero Scans: These are scan types are accessed through the Controller and are used by the lab manager and do a quick scan of the 100% lines for a number of standard materials in coupled mode for use in angular calibration and setting optical zero of the goniometer.

DataScan Data File Format

DataScan writes data files in the "MDI" file format, and files all have a ".mdi" extension. The file format is basically identical to a standard DIF (data interchange format) file which is a standard 7-bit ASCII text file.

The figure below identifies the parts of the header in the standard MDI data file. A few notes about the format as written by DataScan follow the figure.



- The Scan ID is a free-form text field, starts as the 21st character of line 1 and is up to 80 characters in length
- The date/time stamp is written at the start of data collection. Jade does not use this date in listing and sorting data files. It uses the system date of the data file.
- DIF indicates Data Interchange File format. It may be used by other programs reading the data file, but is ignored by Jade.
- Step size in degrees 2θ
- Scan rate in deg/min. Minus sign indicates continuous scan (not step)
- Wavelength of the anode is whatever is defined in DataScan setup. Jade ignores this number; it reads the anode type and uses the wavelength configured for that anode in program setup.
- # of data points is ([end angle – start angle]/step size)+1. (3001 points in the example above)
- Data block is all data points; data are in counts stored as a long integer
- DataScan may be configured to record data in 8-column rows (the default, as shown above with .MDI extension) or as a single column (configured in DataScan's setup dialog with .ASC extension).

Data Analysis with MDI's Jade 5

MDI's Jade is a very powerful software system designed for XRD powder pattern processing. Some of the operations that can be completed with Jade include:

- Corrections for experimental errors, background and $K\alpha_2$ peaks
- Automated identification of peaks – Integrated and maximum intensity, 2θ
- Access to ICDD's Powder Diffraction File database and overlay of experimental patterns with those from the database
- A variety of printed and digitized data reports in graphical and text formats
- Automated Search/Match of patterns with the ICDD database and manual search match with data retrieval by mineral name, chemistry, or unit cell criteria
- Pattern simulation from crystal data
- Quantitative analysis by reference intensity ratio (RIR) methods using internal or external standard methods
- Pattern indexing and unit cell refinements
- Crystallite size and strain analysis, and residual stress analysis.

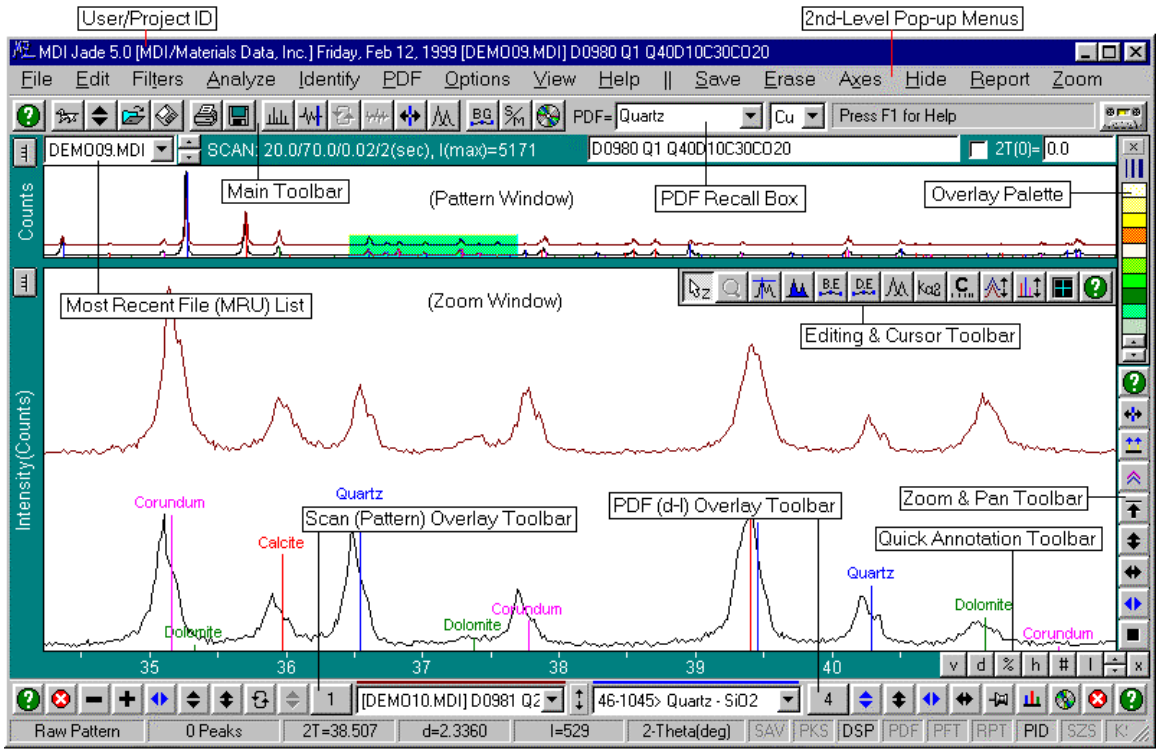
In addition to these main features, there are myriad additional capabilities that make Jade probably the single most powerful tool available for processing and understanding your diffraction data.

The program comes with both Compiled HTML standard Windows help files that are essentially a digital version of the printed manual and provide extremely detailed instructions about virtually all aspects of the program. The Jade help is so good, in fact, that the printed

manual for the newest version (6.1) is very small and largely superceded by the digital versions.

What follows is a very basic outline of Jade 5's capabilities, largely extracted from MDI's documentation. It will barely scratch the surface, but is hopefully enough to help you get started. Hopefully this will get you going. Use the Jade online help to fill in the blanks.

The Jade Interface



Above is an example of Jade's main interface window with most of its main components labeled.

Left and Right Mouse Buttons: Jade makes extensive use of the right mouse button. In general, the left mouse button will execute a command, and the right button will call up some sort of configuration settings for that command. For instance, a left-click on the S/M button will execute Search/Match on the current pattern with the default parameters; a right-click will bring up the Search/Match configuration window.

Zoom Window: The main window Jade is the lower one and is called the ***zoom window*** because it is easily zoomed by stretching a box around an area of interest to examine particular peaks in detail. **The Pattern Window** (above the zoom window) always shows the full pattern with a color highlight indicating the are shown in the zoom window. The zoom windows is where most pattern processing takes place. Many pattern processing operations may be carried out on the whole pattern or restricted to the "zoomed" portion of the window. This includes Search/Match, printing plots or data, etc. The right-mouse button in the zoom window will give you a popup menu of frequently used tasks.

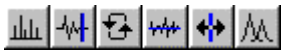
Status Bar: This is the bottom line of the screen, and includes information about the file as processed, the cursor position (2θ and intensity), and a list of all of the Jade file types created for this pattern (most of which can be displayed by clicking on the file extension).

On the figure above, other components of the main Jade interface are labeled; these labeled components are listed and briefly discussed below:

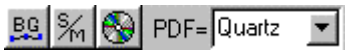
- **User/Project ID:** This is the Windows "Title Bar" for Jade and includes the User Project ID loaded at startup plus the data filename loaded and some of the project description in the data file's header. When Jade starts, saved project IDs are listed – with WindowsNT your project ID is attached to your Username.
- **Main Menu (just below Project ID):** This contains many (but not all) of the commands available on other Jade toolbars is a fairly standard windows menu interface.
- **2nd Level Pop-up Menus:** These additional menu items are not shown by default. Clicking on the two vertical bars will alternately show and hide them.
- **Main Toolbar:** The main toolbar provides quick access to most routine Jade functions. From left to right these are:

  - **Read and Access Files** (first four buttons). Read-in newest pattern, Scroll List, Patterns – Open dialog, and Open from floppy disk.

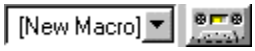
  - **Print and Save** (next two buttons). Print will print whatever is set as the default; use Ctrl-Left click to bring up the Print Setup/Preview dialog. Save saves all the current work to a .SAV file; SAV files can be recalled from the File - Load menu. When you exit Jade and choose to "Save your Work", this creates a SAV file with your username attached to it.



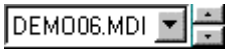
  - **Process and Analyze Data** (6 buttons). In general the left button applies the selected tool in default mode and the right configures it before application. Left to Right these are:
    - Automatic Peak Search (Right click for peak search dialog)
    - Apply Active filter, usually pattern smoothing (Rt. click for smoothing dialog)
    - Swap between raw and derived data (if pattern is not raw)
    - Shows difference between the raw and derived pattern as a "difference" pattern
    - Applies (if available) or builds and applies (if not available) theta calibration curve to the current data to correct for angular errors in your data. (Rt. click brings up theta calibration dialog).
    - Carries out profile fitting using current parameters (Rt. click brings up profile fitting dialog).



- **Identify Phases and Access the PDF**. BG removes background (Rt. click for dialog); S/M does Search/Match with default parameters (Rt. click for dialog); CD-ROM graphic loads dialog to access the online PDF2 Database (Rt. click for Chemistry retreival). The PDF= box lets you enter mineral names, PDF card numbers (i.e., 33-1145), chemical formula, or to add cards to the retrievals list in the zoom window. Jade will remember the last 99 entries typed in this list.
- The anode box shows the anode used to collect the data. This may be changed to redisplay the data as it would be if collected with another wavelength of x-rays.



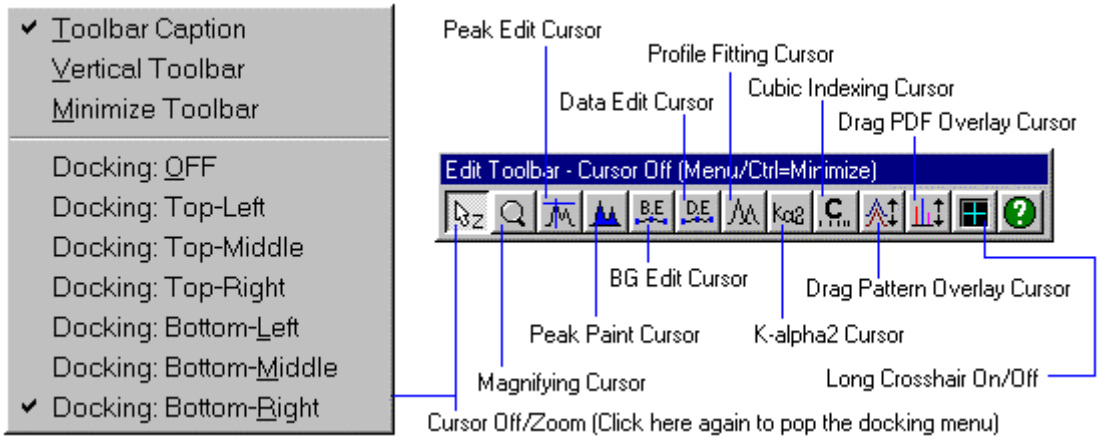
- The Macro Processing. Accesses task macro from list; Rt. click accesses the new macro dialog. Routine tasks in Jade may be automated with macros.



- **Most Recently Used (MRU) file list** is a pull-down selectable list of the most recently used files. Selecting will replace the current file; Ctrl-Select will overlay the selected file.
- **Editing & Cursor Toolbox**, shown below, provides access to a number of powerful data manipulation tools accessed through a variety specialized of "cursors". It is important to understand that modifications made with these tools do not change your original data, although the modified files may (in many cases) be saved as new files.

  It is important to know that with most of the data manipulation cursors, you can display the coordinate values at the crosshair position on a floating label if you hold down the Ctrl key and move the crosshair cursor, and if you press the Alt key at two different spots in the zoom window while holding down the Ctrl key, Jade will calculate the $\Delta 2\theta$ values between the two spots and display it in the message area of the main toolbar. This can be very handy in manual determination of peak parameters.

Notes on some of the tools are found following the graphic.



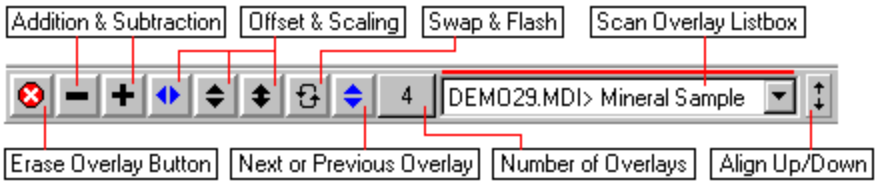
- **Cursor Off/Zoom:** This is the default state in which the zoom window can be "zoomed" by dragging a box around a region of interest, and the right-mouse accesses

zoom window menus. By default, the toolbar "floats"; double-clicking pops of the docking menu for the toolbar (as shown).

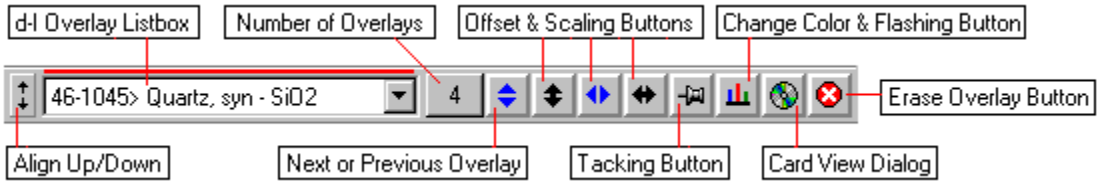
- **Magnifying Cursor** allows selection and expansion of a selected portion of the zoom window in a new popup window which can be resized or scrolled.
- **Peak Edit Cursor** enables moving, editing and erasing of peak markers. This is particularly useful if the automatic peak search produces too many or to few peaks.
- **Peak Paint Cursor** enables manual graphical marking of areas under peaks by selection of areas along the baseline. By using the Ctrl-key with the Paint cursor, you can also do automatic marking of peak areas (see Jade help for details).
- **BG Edit Cursor** enables you to insert, move, and erase the tie points (dots) that control the shape of the fitted background curve. The BG curve is created with the BG dialog accessed on the main toolbar.
- **Data Edit Cursor** lets you manipulate displayed data manually. This does not modify the original datafile, and is useful for aberrant spikes or other artifacts in your data file. See Jade help for details of how this cursor is used.
- **Profile Fitting Cursor:** With this cursor, you can insert and edit initial profiles or remove them graphically. Generally the best approach with a complex pattern is to use the Profile Fitting tool on the main menu initially, then modify the profiles with the profile fitting cursor before further refining the pattern. See the Jade help topic on "Profile Fitting and Peak Decomposition" for a thorough discussion of this process.
- **K-α_2 Cursor:** When you move the mouse into the zoom window with this cursor, you should be able to see the Kα_2 and Kβ lines of the active anode. You can also display the tungsten L-lines to check for filament contamination from an aging anode if you click the same button once more.
- **Cubic Indexing Cursor** creates stick patterns from your choice four cubic Bravais lattice that are dragged and resized as you drag them over your data in the zoom window. A good match will yield the unit cell length which can be used as input to a more precise indexing of your data (See "Unknown Pattern Indexing" in Jade help).
- **Drag Pattern Overlay Cursor** lets you separate overlaid patterns vertically for visual comparison.
- **Drag PDF Overlay Cursor** lets you move PDF card overlays up or down in the window. For both of these "drag" cursors, it is important that unique colors are assigned to each overlay since Jade uses the colors do distinguish the overlay patterns moved.
- **Long Crosshair On/Off** changes the small cursor to a large, full-window vertical-horizontal crosshair.

- **The Overlay Palette** provides direct access to colors of traces and overlays. Colors may also be changed from a variety of dialogs. All colors may be changed from the View – Custom Colors on the main menu.

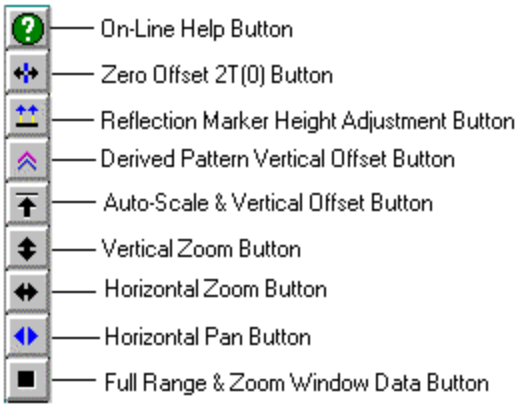
- **Scan (Pattern) Overlay Toolbar** is accessible when there is at least one overlaid pattern in the zoom window, and gives you individual control over the overlays displayed in the window. What each button does is labeled below. Consult the Jade help for different ways of adding and configuring overlays.



- **PDF (d-I) Overlay Toolbar** is accessible after any d-I list operations add PDF card data to the list for the pattern in the zoom window. These can come from a number of operations, most commonly Search/Match or PDF retrievals from the Main Toolbar dialogs. Most of the buttons are self explanatory. Of note are "Tacking" which is used to make a particular overlay permanent, "Erase Overlay" which permanently removes the selected overlay from the list, and the "Card View" which displays the PDF card data for the selected card.



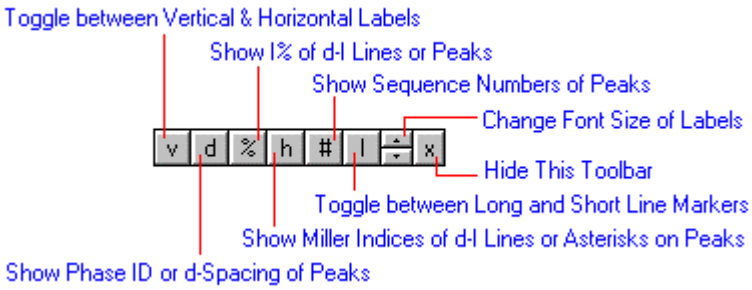
- **Zoom & Pan Toolbar** is shown at right. It allows you to modify the pattern displayed in the zoom window in a number of ways including:



  - **Zero Offset** is used to shift an entire pattern to correct for alignment or other errors in relation to a known standard.
  - **Reflection markers** are produced in pattern refinements; this allows you to adjust how they are displayed.
  - **Derived patterns** may be offset vertically for display purposes
  - **Auto-Scale and Offset** button toggles the vertical scale of the zoom window between the maximum peaks in the zoom window and the whole pattern.
  - **Vertical and Horizontal Zoom Buttons** zoom the pattern in or out vertically and horizontally.
  - **Horizontal Pan** pans the zoom window left and right.
  - **Full Range & Zoom** moves through the last few zoom window displays.

For more details about how to use the zoom and pan toolbar, consult the Jade help file.

- **Quick annotation Toolbar** (shown at right with explanatory labels indicating what each button does) is used to quickly modify how the pattern in the zoom window is labeled



A note on Modal vs. Modeless Operations: Dialog windows in Jade fall into two general groups with regard to their behavior: (a) modal dialog windows, and (b) modeless dialog windows. A modal dialog window requires you to close it down in order to interact with its parent window. When you click outside the frame of such a dialog window, you will hear a beep from the PC speaker telling you that the click is invalid and thus ignored. A modeless dialog window has no such restriction, behaves very much like a toolbar or toolbox, and usually has no OK and Cancel buttons to dismiss it. The word 'modeless' means that the program is not constrained into a particular mode of operation which it needs to be released from. Many of the large scale operations in Jade (Search/Match, Card retrieval, profile fitting) are modeless in that they can be left open (or minimized) to interact with Jade's main window.

Search Match Notes

By far the best way to learn how to use Jade's Search/Match is to study the sections on "Search Match for Phase ID" in the Jade online help. The approach is far more comprehensive than is possible here. The few suggestions below are from the author's experience with what tends to work best.

- The full pattern search/match is generally the best. For this to be effective it is important that background be removed and $K\alpha_2$ peaks stripped before the search. This can be done automatically (the program will offer to do it for you before the search) or manually using the background removal tool.
- Search/Match is very fast and can be done as many times as is necessary to produce good results. Start with the default settings, and vary them only as necessary to get good results.
- The following steps are suggested in Jade's documentation to produce good S/M results:
    1. Select the relevant PDF subfile(s).
    2. Start the initial search with the default parameters on the S/M setup dialog (right-click the Reset button).
    3. If no positive hit is found, increase the 2 q error window and do another search.
    4. If no positive hit is found, do a solid-solution search in the few % range.

5. If no positive hit is found, focus the search on a few of the strong peaks at low angle. If there is a cluster of peaks, zoom around them and do another search.
6. If no positive hit is found, check the 'Preferred Orientation S/M' box and do another search.
7. If no positive hit is found, check the 'Perform Single Phase S/M' box and do another search.

- The line-based search/match is generally not as good at matching patterns exactly, but it does have a much higher tolerance for angular errors than the full pattern search. The line-based search dialog is accessed from the "Identify – Line-Based Search..." menu, and requires a peak ID before the search can proceed.
- Use the Search/Match setup rather than the defaults in your S/M to be assured that you are searching the correct data file(s). "Inorganics" includes only experimental patterns; to select the ICSD calculated patterns be included in the search, it must be selected in the subfile list.
- Specimens containing more than a single simple phase can produce a large number of false hits in some situations. If you know the chemical composition of your specimen, you can use the chemical information to limit the permissible matches and reduce the false hits.
- The S/M process can be set to automatically shift patterns in a search by as much as ±0.42° 2θ, but large the angular deviation will still reduce the chances of a successful match result. If your S/M is not yielding good results and it appears that you may have systematic 2θ error in your data, apply, if possible, a theta calibration. This is done from the Main Toolbar and requires a recent pattern of a known standard material acquired on the system. Ask your lab manager for a recent pattern that could be used for this purpose.
- Strong preferred orientation can severely alter peak intensities in your pattern. Jade's whole pattern S/M algorithms have trouble with strong preferred orientation. This can be alleviated somewhat by using the Preferred Orientation S/M checkbox in the search match setup.
- One of the best pattern matching tools is the human eye. Never accept a computer S/M result without making sure that it is a good match visually.
- Bulk analyses of complex multi-phase samples (a.k.a. rocks) will sometimes identify a few major phases with automated S/M, but will never get the minor ones. For rocks, use only the Minerals and ICSD Minerals subfiles. Know your samples. One of the best techniques for working with rocks is to create a set of likely phases in a special search set and limit your searches to that set. Another option is to create a d-I list for all of the possible phases in your sample and match the pattern visually, selecting the best matches from what you compare with your data.

Jade's documentation has tons of helpful hints and information. Make use of it and you will probably be pleased with the results.

Generalized Sequence of Data Analysis

How data is processed is totally dependent on the purpose of the analysis. You will generally start with the question you are trying to answer, devise your experiment to collect data to help you answer that question, collect your data, analyze your data, present your output in a form which transmits maximum information about what you have discovered and prepare a report of the results. Below is an example of one hypothetical project from received material to final report.

1. The client leaves a powdered sample for analysis. The material is a laboratory-produced powder that has certain known elements in it. The client is interested in what the major phase(s) are in the sample and if there are any leftover starting materials.
2. The powder is examined for uniformity. Since the work is qualitative in nature, no significant sample prep is required.
3. The specimen is side-drifted into a Plexiglas mount for analysis. It is run at 1°/min between 10° and 60° 2θ.
4. The resulting pattern is loaded in Jade and examined. Peaks generally sharp and well defined, but there are several smaller peaks that have a somewhat broader shape than the dominant peaks.
5. A peak search is done on the raw data pattern, and the printed and standard peak file list printed. This provides the raw data for the sample for the client.
6. A full pattern search/match is done on the pattern. Initial search with default parameters yields results not reasonable given the known chemistry. A repeat match with a slightly larger 2θ error window yields some phases which are good matches both visually and for the known chemistry. These phases are checked in the match results list to be saved.
7. The S/M results do not contain anything that matches the small peaks in the pattern. Repeat searches with larger error windows, and preferred orientation SM still yield nothing reasonable. The match results window is closed, returning to the zoom window interface.
8. It is decided to do a manual retrieval and compare the cards visually. Before doing this, the derived pattern with the background removed is erased leaving the raw data, and the Zoom window intensity rescaled to the full window. It is always a good idea to visually compare to the raw data because minor peaks that tend to be flattened into the background will be more visible to the human eye.
9. A PDF retrieval is selected using Chemistry. The five possible elements in the powder are selected and a list of all matches using the Inorganic and ICSD databases. This produces about 60 possible phases. Each of those phases is compared visually with the minor peaks in the pattern. A phase (identified as matching several calculated and experimental cards) is found that matches the minor peaks and also has minor peaks that match peaks hiding in the “noise” of the background. This phase is checked and added to the results, and the match results window closed.

10. In the main window, the PDF overlay tool is used to evaluate which of the selected cards best match the phases in the sample. The "Tack" button is used to select the best card matches, and the others are deleted with the Delete button.
11. Go to the Print – Setup window. The pattern can be displayed with the card file patterns overlaid on it, or in boxes adjacent to it. The latter is generally best to show matches of multiple phases. One of the output types is selected, and printed.
12. At the main menu, from the View – Reports menu, select and print the extended peak file report. This shows all of the peaks in the pattern and the peaks matches between the cards and the pattern.
13. From the PDF overlay tool, each matched phase is selected in succession and the PDF card for it is printed for the client.
14. The data as printed are assembled and a brief report of results prepared and delivered to the client.

This project can be described as a relatively simple qualitative search/match and report on results, but hopefully gives you an general idea about how data collection and reporting are approached.