

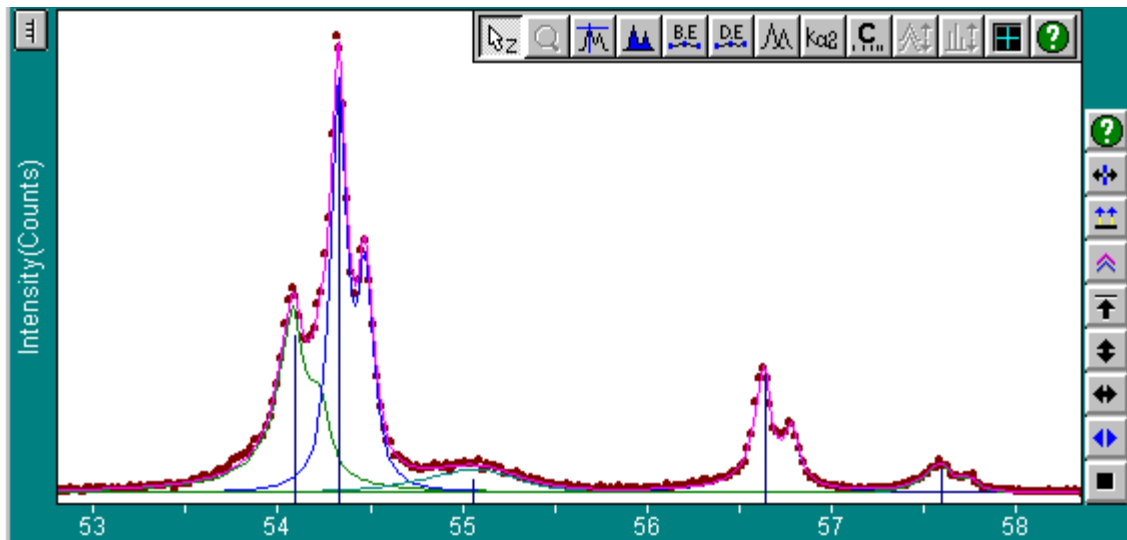
Zoom Window Data & Display

Jade utilizes the zoom window data & display for a number of analysis tasks besides printing. The following 'View | Zoom Window' menu is provided so that you have greater control over some of the display properties in the zoom window:

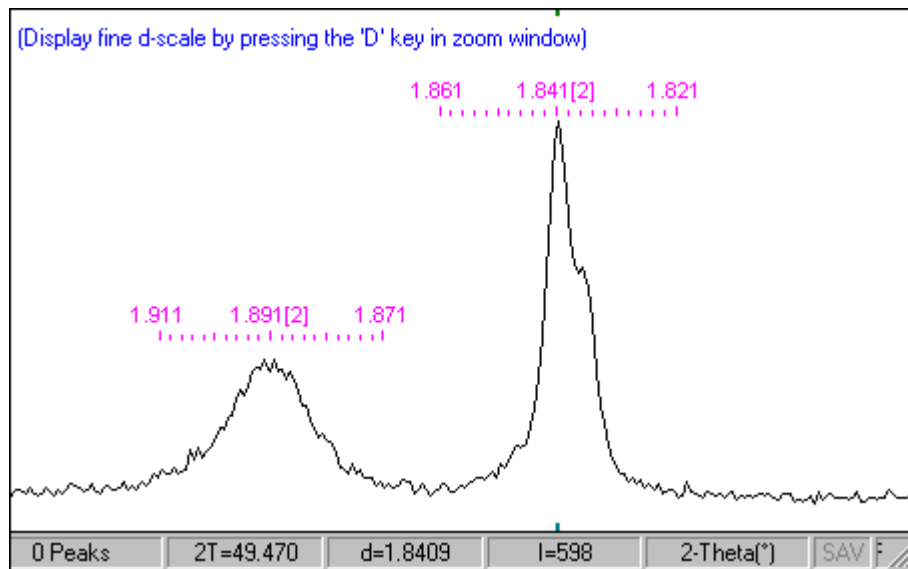
<u>A</u> uto Scale	Ctrl+End
<u>F</u> ull Range	Ctrl+Home
<u>D</u> isplay Range...	Ctrl+D
Paint Peaks (Auto)	Ctrl+;
<u>P</u> aint Peaks (Full)	Ctrl+'
✓ Paint Info- <u>B</u> ox(s)	Ctrl+H
✓ <u>R</u> eflection Plot	Ctrl+?
<u>O</u> verlay Profiles	
✓ Data Points OFF	Ctrl+.
Data Points ON	
Data Points Only	
✓ Grid OFF	Ctrl+,
Grid ON (X)	
Grid ON (Y)	
Grid ON (X+Y)	
✓ <u>V</u> ertical Marker	

You can also bring up this menu by right-clicking in the right side of the zoom window. The 'Auto Scale' and 'Full Range' menu items reset the display range in the zoom window and their functions are readily duplicated on [zoom & pan toolbar](#). The 'Paint Peaks (Auto/Full)' menu items paint and integrate peaks in the zoom window. See [paint & integrate peaks](#) for more information. The 'Reflection Plot' menu item hides or shows the reflection plots which are generated in the zoom window from analyses such as FWHM curve plot, theta calibration, cell refinement, and pattern indexing.

You can display a background grid in the zoom window to simulate strip charts, and put little dots or circles on individual data points in the observed pattern. Jade won't display these dots when there are more than 1001 points in the zoom window. You can choose small (1-pixel) or large (2-pixel) dot size on the Display tab of [user preferences](#) dialog. An example of a dot view is given below:



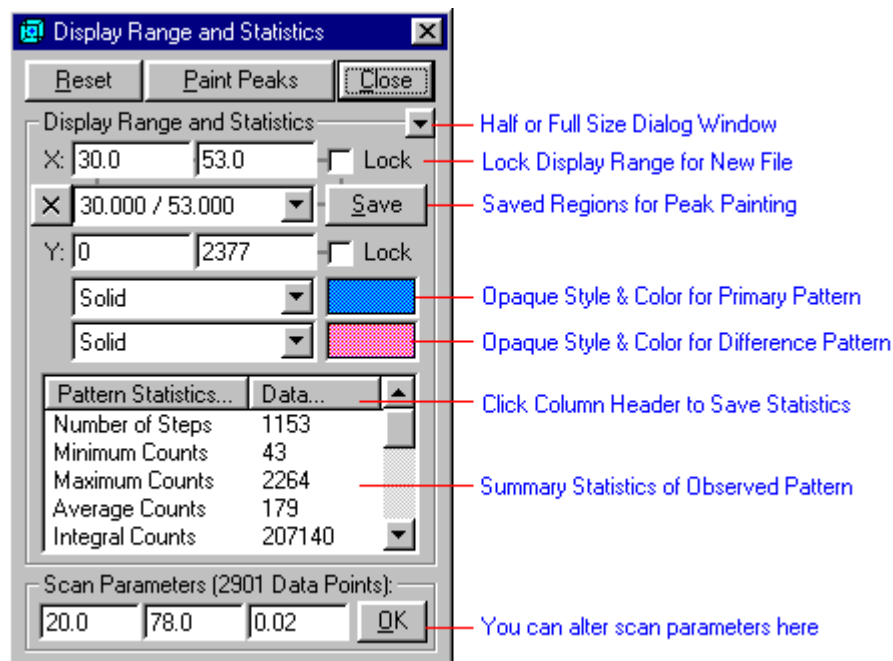
When the zoom window has the keyboard focus and 2θ range is less than 20 degrees, you can also print a fine d-scale where the mouse points at by pressing the 'D' key, for example,



Jade prints 10 scale ticks on either side of mouse pointer with dynamic scaling and intelligent digits, and the number in square brackets gives the d-spacing increment between the tick marks which are not equally spaced in 2 θ axis. While these d-scale prints are not permanent in the zoom window, you can print them in the [print preview](#) window as well by pressing the 'D' key and produce a hardcopy.

Display Range & Statistics:

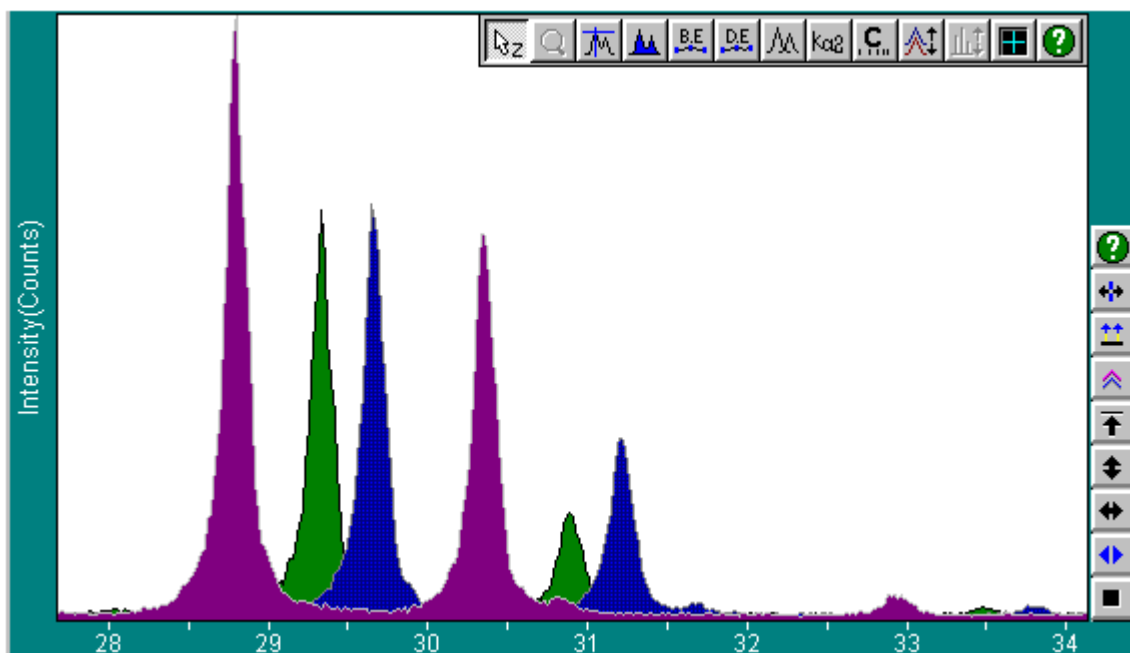
The 'Display Range...' menu item brings up the following dialog:



The precise display ranges can be specified on this dialog if consistent and comparable views or prints are desired. You may even enter a display range that's wider than the scan range of your data. Jade accepts display ranges of ± 360 degrees but will not calculate d-spacing when the cursor is below 0.001 or above 180 degrees.

If you check the X and/or Y Locks, the current display range is locked only for reading a new pattern file. The locks do not prevent you from scrolling the current zoom window. When the range is unlocked, Jade always displays a new pattern file in its full range. The Reset button on this dialog lets you toggle the zoom window display between full range and the last few zooms. You can also save and restore a list of display ranges for purposes such as painting peaks. See [paint & integrate peaks](#) for more information.

You can select the fill styles to view the primary & difference patterns in opaque mode on the above dialog. If you have the derived pattern (such as the smoothed or simulated pattern), Jade paints it instead of the primary pattern. You can set the opaque colors independent of the trace colors by clicking the color rectangles. Refer to [scan overlay list](#) dialog for how to set opaque properties of scan overlays. An example of an opaque view with two pattern overlays is given below:



Note: opaque visualization is limited to <4002 data points per pattern in the zoom window, and to <8002 points on the printout.

Summary Statistics of the Observed Pattern:

Summary statistics of the observed pattern in the *current display range* are also shown on this dialog. These statistics may be useful in pattern characterization and comparison. If there is a background curve in the zoom window, the 'Areas above BG' will be calculated as percentage of total (integral) counts for the data in the zoom window as well. If there are peaks located in the zoom window, you can produce a report file (*.sta) of more complete pattern statistics by clicking the column headers, and browse it from the 'View | Reports & Files | Browse Report File...' menu, for example:

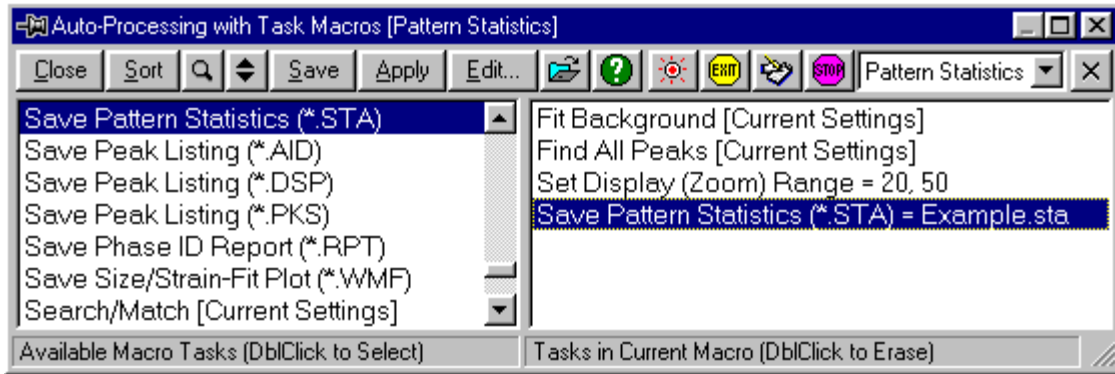
```
c:\program files\mdi jade 6.0\demofile\DEMO06.sta [1KB]
Close Print 2 3 4 5
JADE: Pattern Range & Statistics
DATE: Friday, Feb 16, 2001 05:19p
FILE: [DEMO06 MDI] Red Paint Pigment Mixture
SCAN: 20.0/78.0/0.02/4(sec), Cu, I(max)=5188, 01/01/99 12:00
STAT: 2-Theta Range = 30.0 - 53.0

Number of Steps = 1153
Minimum Counts = 43 @50.72
Maximum Counts = 2264 @36.1
Average Counts = 179
Integral Counts = 207140

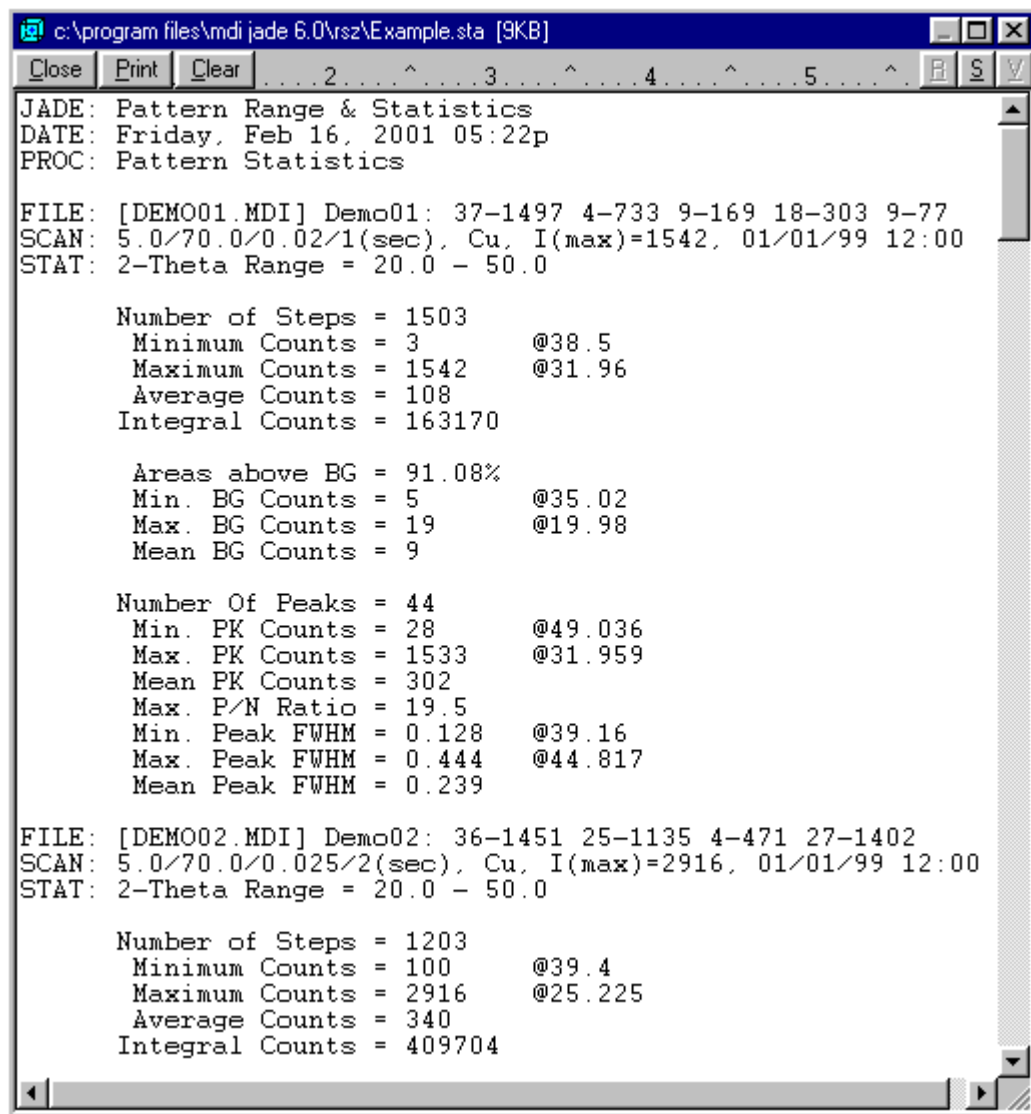
Areas above BG = 49.06%
Min. BG Counts = 53 @49.4
Max. BG Counts = 172 @29.98
Mean BG Counts = 91

Number Of Peaks = 12
Min. PK Counts = 49 @43.564
Max. PK Counts = 2143 @36.103
Mean PK Counts = 732
Max. P/N Ratio = 22.5
Min. Peak FWHM = 0.169 @36.103
Max. Peak FWHM = 0.482 @48.06
Mean Peak FWHM = 0.286
```

You can also create and browse the above report file simply by selecting the 'View | Reports & Files | Pattern Statistics...' menu. You can produce a summary report of pattern statistics from multiple data files, using the following [task macro](#), for example,



When this macro is run with multiple data files on [read pattern file](#) dialog, it will generate a report file that looks like this:



```

Number Of Peaks = 44
Min. PK Counts = 28      @49.036
Max. PK Counts = 1533   @31.959
Mean PK Counts = 302
Max. P/N Ratio = 19.5
Min. Peak FWHM = 0.128  @39.16
Max. Peak FWHM = 0.444  @44.817
Mean Peak FWHM = 0.239

FILE: [DEMO02.MDI] Demo02: 36-1451 25-1135 4-471 27-1402
SCAN: 5.0/70.0/0.025/2(sec), Cu, I(max)=2916, 01/01/99 12:00
STAT: 2-Theta Range = 20.0 - 50.0

Number of Steps = 1203
Minimum Counts = 100     @39.4
Maximum Counts = 2916   @25.225
Average Counts = 340
Integral Counts = 409704

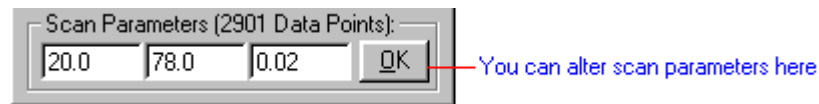
```

Refer to [task macro](#) topic for how to concatenate results in a report file like the *.sta in this example.

If there is a derived pattern being overlayed in the zoom window, an agreement R-value between it and the primary pattern will be calculated using the following formula: $R\% = 100 * \text{Sqrt}(\sum((I(r)-I(d))^2/I(r)) / \sum(I(r)))$, where the sum is over the data points in the current zoom window. A similar R% value is also calculated using *all* data points in the patterns, and displayed in the main status bar. You can clone the derived pattern as a pattern overlay by selecting the 'Filters | Clone Derived Pattern' menu.

Alter or Correct Scan Parameters:

While Jade does its best to read all types of pattern files created by other vendors, there may be occasions when you need to alter or correct the scan parameters (i.e., starting, ending, and stepping angles) of the pattern being displayed.



In case the parameters were read incorrectly, you should try other file types first or review the [Ascii import filter](#) carefully before altering the parameters from the above dialog. Jade will maintain the same number of data points in the pattern when you alter the scan parameters. But you will be prevented from doing so (i.e., the bottom frame of the above dialog will be hidden) when derived data such as peak listings are present in the zoom window.