MDI Jade (2010) Tutorial

Revised July 2013

Jade is a product of MDI
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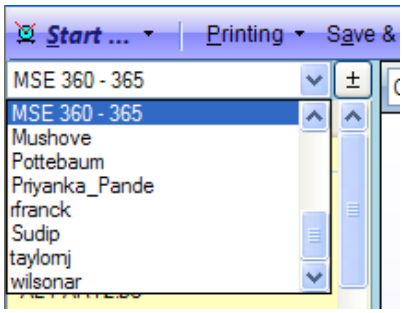
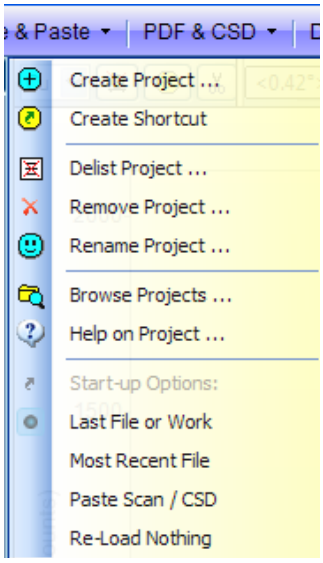
1) Open MDI Jade (2010) from the desktop 

2) The main Jade window will open. Make sure the correct project id is chosen from the drop down menu. For example, for the lab class it should be “MSE 360 – 365”.



3) For light Jade use, please use the “Default/General Project”. To create new project click the ± button and choose “Create a Project” from the menu.

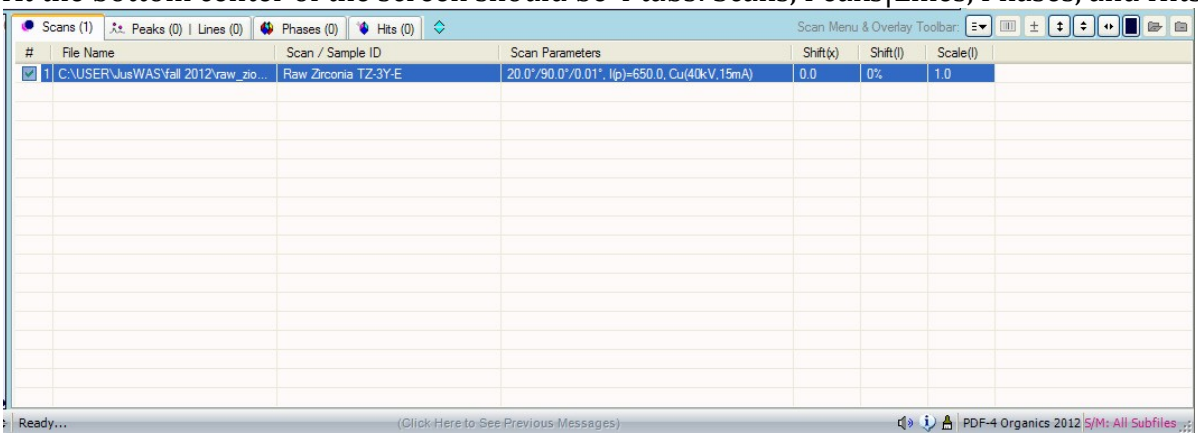


4) On the upper left panel click the small folder icon to choose the appropriate folder. 

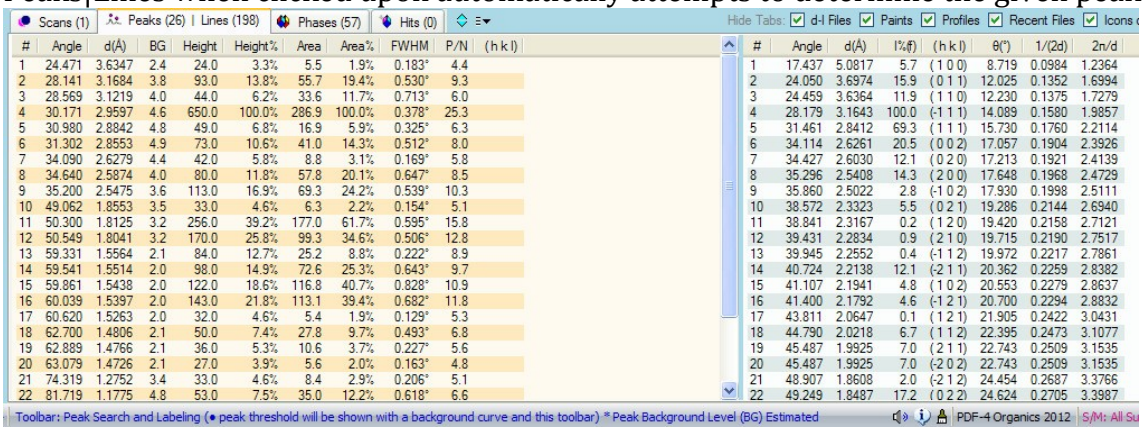
   a. If the desired folder is not found in the recent list click on the “Open Other Folder…”

b. For the lab class go to "C:\Users\MSE 360\2012\<Day of lab>\<Group#>"
c. Click a file to open the folder in side panel. Double click file you wish to analyze.
d. For analysis please use the .raw files inside of Jade.

5) At the bottom center of the screen should be 4 tabs: Scans, Peaks|Lines, Phases, and Hits



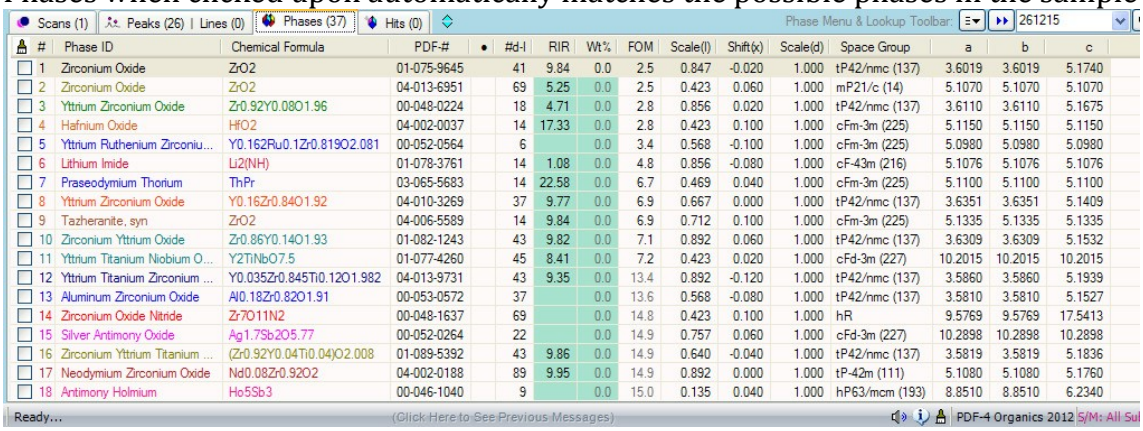
6) Peaks|Lines when clicked upon automatically attempts to determine the given peaks in the file



a. Manual adjustments to the default parameters can be adjusted at the top of the screen

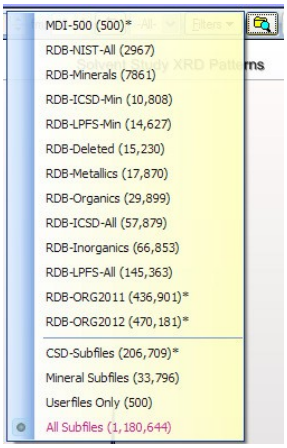
b. Or peaks can be added manually by left clicking inside the pattern itself and subtracted by right clicking on top of a peak.

7) Phases when clicked upon automatically matches the possible phases in the sample

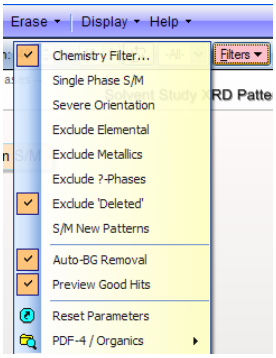


#	Phase ID	Chemical Formula	PDF-#	•	#d-I	RIR	Wt%	FOM	Scale(I)	Shift(x)	Scale(d)	Space Group	a	b	c
1	Zirconium Oxide	ZrO2	01-075-9645		41	9.84	0.0	2.5	0.847	-0.020	1.000	tP42/nmc (137)	3.6019	3.6019	5.1740
2	Zirconium Oxide	ZrO2	04-013-6951		69	5.25	0.0	2.5	0.423	0.060	1.000	mP21/c (14)	5.1070	5.1070	5.1070
3	Yttrium Zirconium Oxide	Zr0.92Y0.08O1.96	00-048-0224		18	4.71	0.0	2.8	0.856	0.020	1.000	tP42/nmc (137)	3.6110	3.6110	5.1675
4	Hafnium Oxide	HfO2	04-002-0037		14	17.33	0.0	2.8	0.423	0.100	1.000	cFm-3m (225)	5.1150	5.1150	5.1150
5	Yttrium Ruthenium Zirconiu...	Y0.162Ru0.1Zr0.819O2.081	00-052-0564		6		0.0	3.4	0.568	-0.100	1.000	cFm-3m (225)	5.0980	5.0980	5.0980
6	Lithium Imide	Li2(NH)	01-078-3761		14	1.08	0.0	4.8	0.856	-0.080	1.000	cF-43m (216)	5.1076	5.1076	5.1076
7	Praseodymium Thorium	ThPr	03-065-5683		14	22.58	0.0	6.7	0.469	0.040	1.000	cFm-3m (225)	5.1100	5.1100	5.1100
8	Yttrium Zirconium Oxide	Y0.16Zr0.84O1.92	04-010-3269		37	9.77	0.0	6.9	0.667	0.000	1.000	tP42/nmc (137)	3.6351	3.6351	5.1409
9	Tazheranite, syn	ZrO2	04-006-5589		14	9.84	0.0	6.9	0.712	0.100	1.000	cFm-3m (225)	5.1335	5.1335	5.1335
10	Zirconium Yttrium Oxide	Zr0.86Y0.14O1.93	01-082-1243		43	9.82	0.0	7.1	0.892	0.060	1.000	tP42/nmc (137)	3.6309	3.6309	5.1532
11	Yttrium Titanium Niobium O...	Y2TiNbO7.5	01-077-4260		45	8.41	0.0	7.2	0.423	0.020	1.000	cFd-3m (227)	10.2015	10.2015	10.2015
12	Yttrium Titanium Zirconium ...	Y0.035Zr0.845Ti0.12O1.982	04-013-9731		43	9.35	0.0	13.4	0.892	-0.120	1.000	tP42/nmc (137)	3.5860	3.5860	5.1939
13	Aluminum Zirconium Oxide	Al0.18Zr0.82O1.91	00-053-0572		37		0.0	13.6	0.568	-0.080	1.000	tP42/nmc (137)	3.5810	3.5810	5.1527
14	Zirconium Oxide Nitride	Zr7O11N2	00-048-1637		69		0.0	14.8	0.423	0.100	1.000	hR	9.5769	9.5769	17.5413
15	Silver Antimony Oxide	Ag1.7Sb2O5.77	00-052-0264		22		0.0	14.9	0.757	0.060	1.000	cFd-3m (227)	10.2898	10.2898	10.2898
16	Zirconium Yttrium Titanium ...	(Zr0.92Y0.04Ti0.04)O2.008	01-089-5392		43	9.86	0.0	14.9	0.640	-0.040	1.000	tP42/nmc (137)	3.5819	3.5819	5.1836
17	Neodymium Zirconium Oxide	Nd0.08Zr0.92O2	04-002-0188		89	9.95	0.0	14.9	0.892	0.000	1.000	tP-42m (111)	5.1080	5.1080	5.1760
18	Antimony Holmium	Ho5Sb3	00-046-1040		9		0.0	15.0	0.135	0.040	1.000	hP63/mcm (193)	8.8510	8.8510	6.2340

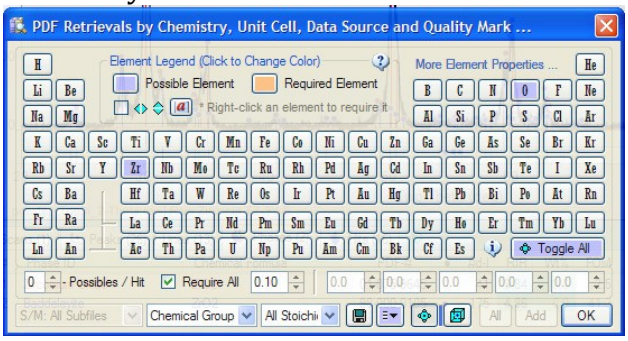
a. To overlay the pdf files, check the box in the left column.
b. For the lab class please make sure to have the entire powder diffraction file database available



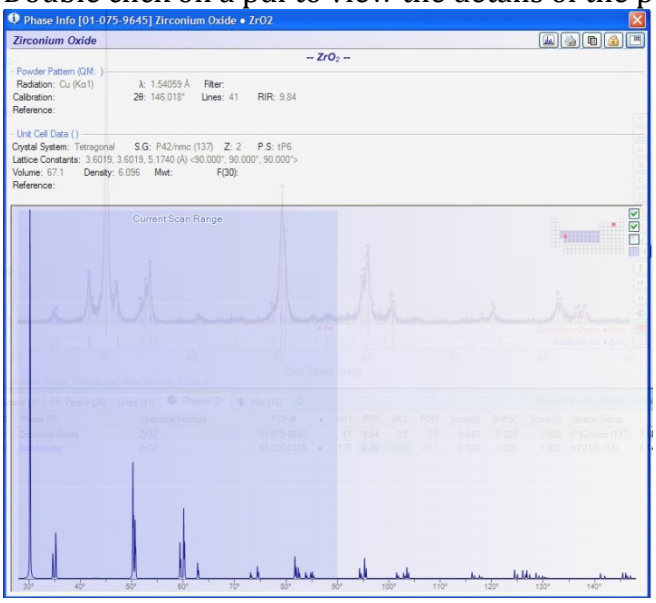
c. Filters can be used to put constraints on the results.



d. Chemistry filters are used to limit to certain elements, either possible or required.



8) Double click on a pdf to view the details of the pdf card



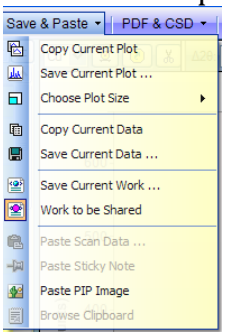
a. The icons in the top right corner can help you view the peak list, print, copy to clipboard, keep file, and add to attach to plot window
b. Copy to clipboard and paste into a text window

9) Hits is similar to Phases:

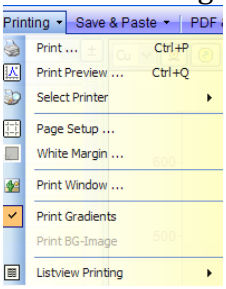
Note: phase identification (S/M) is enabled on both the Phase & Hit tab, but with two differences: (a) duplicate hits won't be allowed on the Phase tab in the S/M, and (b) S/M can be iterated on the remaining peaks automatically with the Phase tab. Also phase list on the Phase tab will be used for WPF-Refinement and RIR-Quant analysis (• indicates a phase with available crystal structure data), whereas only the current hit on the Hit tab will be used if the Phase tab is empty. Hit tab is also used to display all PDF retrieval results. You can perform S/M and clear existing phase or hit list by double-clicking its tab stub, and summon list menu by right-clicking the tab stub. Jade will do S/M on a new pattern file if this tab is selected and the phases are not kept.

10) Saving and Printing:

a. Use "Save & Paste" to "Copy Current Data" into notepad (save as a .txt file) or copy an image of the current plot display

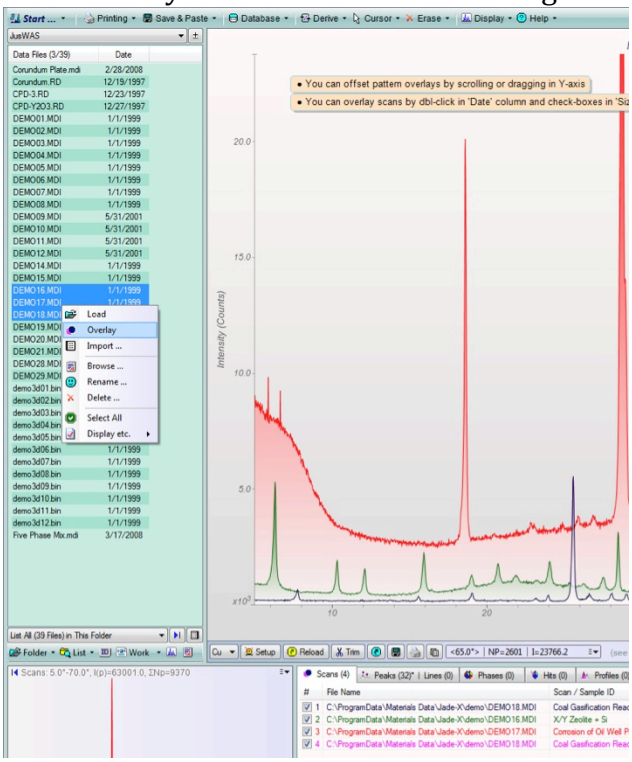


b. Use "Printing" to send a copy of the plot window to the printer or view a "Print Preview…" to save an image file in various formats

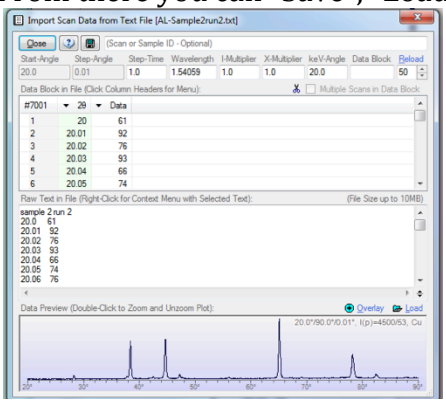


Jade (2010): Going beyond the basics

1.) Demonstration files can be found by clicking the Folder icon and then "Open Demo–File Folder"
2.) Overlaying multiple files:
   a. Hold Ctrl key and select desired files. Right click and select "overlay":

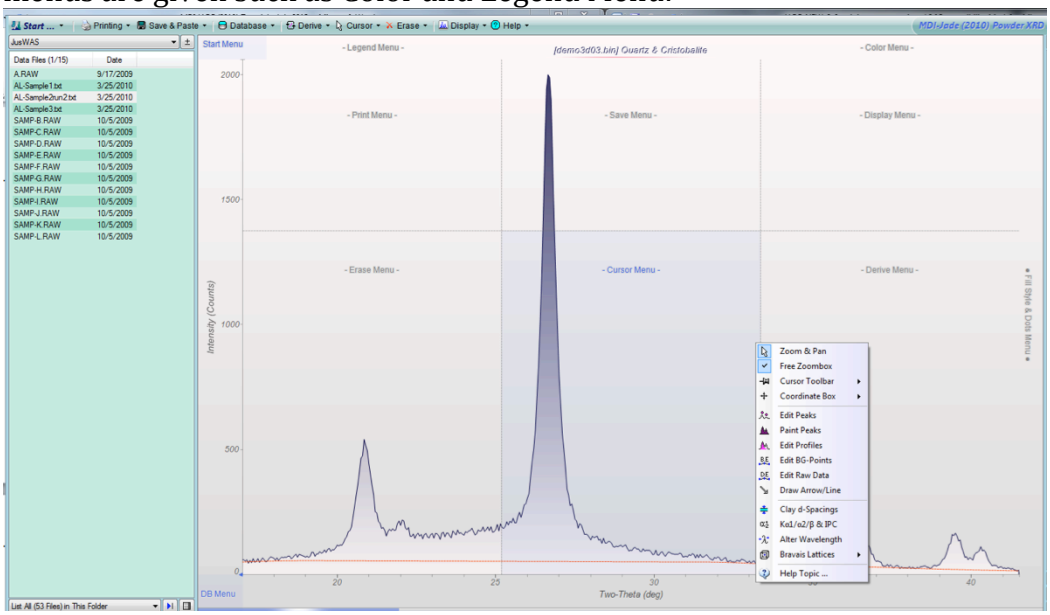


3.) If importing other X-ray diffraction files into Jade, right click on desired file and click "import". From there you can "Save", "Load" or "Overlay" a given file into jade



4.) Learning the menus:

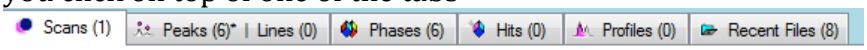
a. Menus are located along the top of the software “Start, Printing, Save & Paste, etc.”
b. Menus are also available by right clicking in the main window as seen below, additional menus are given such as Color and Legend Menu:



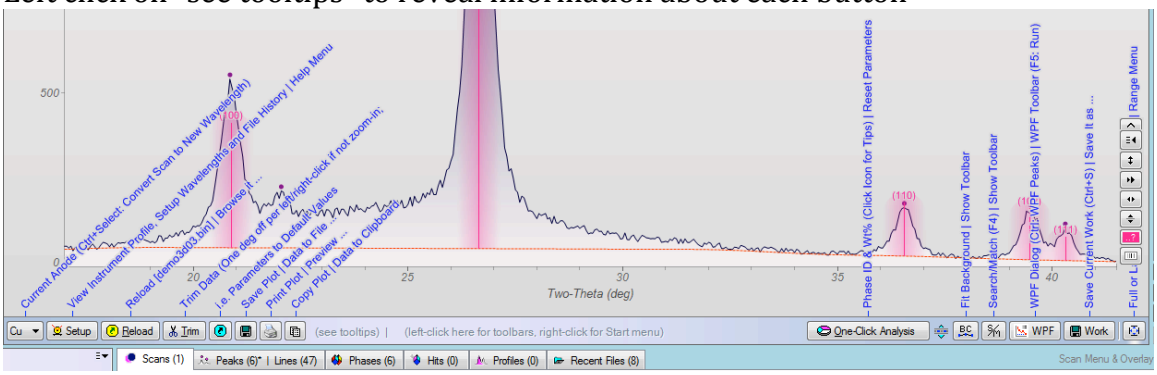
c. For additional information and methods to customize the appearance, see the Help Topics (F1) under “Jade’s User Interface>Customize Main Form”

5.) Learning the toolbars:

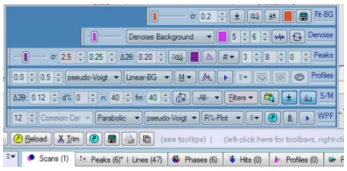
a. Toolbars change based upon the active tab, the software function automatically runs when you click on top of one of the tabs



b. Left click on “see tooltips” to reveal information about each button



c. “left-click here for toolbars…” to reveal advance settings and all available toolbars



d. For additional information and methods to customize the appearance, see the Help Topics (F1) under “Jade’s User Interface>Toolstrip and Toolbars”

6.) Applying a background (always in SQR scale):

a. Right click on “BC” to reveal background toolbar.

b. There are two reasons for applying a background: 1) to define where the peaks are for Search/Match; 2) to define where the noise is for profile fitting

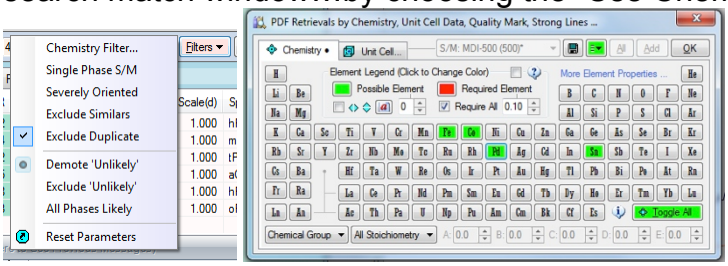
c. To edit a background point, left click on top of one of the red background points to move around, right click to delete point. Left click on an along red line to add a new point.

7.) Setting up Search/Match:

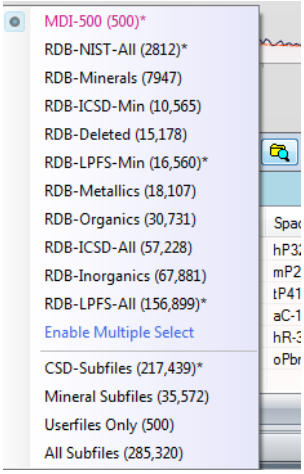
a. Choose "Phases" tab

b. The main areas to look at are the "Filters" drop down list and Database setup

c. Filters: If you know the specific elements present or have a good suspension you can improve the yield of returned matches by entering the chemistry information in the search match window…by choosing the "Use Chemistry filter option pictured below:



d. Make sure, if desired, that the appropriate database(s) are selected:



8.) PDF retrievals: similar to Chemistry filter in appearance and function. Found under "Database>Retrieve…" **ADD MORE TO THIS**