JADE Workshop 2025



Exercise Booklet

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Note on the Exercises

These exercises are meant to be complementary (homework).

They may not cover all topics that were covered in the workshop or in our InSession video recordings.

They are listed in no particular order and intentionally not categorized as S/M exercises, WPF exercises etc., because all JADE functions work together organically and JADE power users would not make such a distinction.

The MDI Toolkit is only used sparingly, since JADE's core functions cover most of the tools that one normally needs.

Vimeo Video Showcase

Showcase URL: https://vimeo.com/showcase/11952354
Login Password: **JADEanswers**

Use the provided Vimeo access password to log into the showcase once.
After that, the video links embedded here should take you directly to the individual exercise videos.

JADE Documentation

In addition to JADE's integrated helpfile (F1-key), there is an Adobe PDF version of it located in the JADE folder. It can also be launched by pressing the CtrlKey when selecting the menu "Help: Help Topics".

How to use this booklet

Of course, we would like you to try the instructions first and then watch the exercise video, but it may be more efficient to watch the video right away and then go over the instructions, in order to see what you have retained.

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Abbreviations

BC	-	Background Curve (BG=background)
CA	-	Cluster Analysis
CSD	-	Custom Structure Database
CIF, CSF	-	Crystal Structure Files (CIF=IUCR, CSF=MDI)
DB	-	Database
DD, DDM	-	Direct Derivation Method (Quantitative Analysis in IPF, WPF)
ESD	-	Estimated Standard Deviation (usually in parentheses)
FWHM	-	Full Width at Half-Maximum (peak width)
IPC	-	Instrument Profile Curve
IPF	-	Individual Profile Fitting
IS	-	Internal Standard
OCA	-	One-Click Analysis (Qual+Quant)
POC	-	Preferred Orientation Correction (March function, SH)
PSF	-	Profile Shape Function (Pseudo-Voigt, Pearson 7)
PXRD	-	Powder Xray Diffraction
RIR	-	Reference Intensity Ratio (e.g.: I/Ic for Corundum)
RIR Method	-	Semi-Quantitative Analysis
SH	-	Spherical Harmonics (POC for phase with several stronger peaks)
SI	-	Similarity Index
S/M	-	Search/Match (Phase ID, Qualitative Analysis)
SRM	-	Standard Reference Material (Quartz, LaB_6 etc.)
WPF	-	Whole Pattern Fitting (Quantitative Analysis)
WPF/R	-	Whole Pattern Fitting/Rietveld (Quantitative Analysis/Structure Refinement)
XRD	-	Xray Diffraction
XS	-	Crystallite Size
XSS	-	Crystallite Size & Strain

Useful Key Shortcuts

SPACE	-	Unzoom and Zoom Up (may not work in Chrome)
Ctrl-X	-	Erase All / Clear Plot
F8	-	Roll JADE Window Up/Down
F9	-	Toggle Tab Pane
F10	-	Toggle Side Panes
F11	-	Toggle All Panes
F12	-	Maximize JADE window

Mouse Conventions

Wheel	-	Used frequently for changing parameter values on toolbars & lists
Ctrl+Click	-	Reset non-default values to default values
RightClick	-	Many buttons have separate function (indicated by vertical bar in tooltips!)

Context Menus

While all lists have context menus, some lists have several context menus depending on which column one RightClicks. When a menu item shows a (numerical value) in parentheses, one can usually change it with the MouseWheel.

Dialog Window Types

A Modal Window is for exclusive interaction. It needs to be closed first, in order to do something outside of it. They are marked by a reddish bottom edge (e.g.: PDF Retrieval, PTE).

A Non-Modal Window does not need to be closed (e.g.: Pattern Indexing, Structure Viewer). Some of them are dockable (e.g.: 3D/2D Pattern Viewer).

JADE Exercises

Exercise 1

Convert a powder pattern to a denoised Kα1 pattern *

XRD File

- DEMO08.MDI

Suggested Steps

- Denoise the pattern with a suitable option from the [Derive]-menu
- Fit a suitable background curve (BC)
- Remove BC and Kα2 contribution

Tips

- ** This is just an exercise (one may never need to do this)*
- Use Kα-cursor to verify presence of Kα2 (synchrotron data don't have Kα2)
- Consult difference plot when choosing a denoising method

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105867

Exercise 2

Stitch up pattern ranges to get a full pattern for further processing

XRD File

- Quartz-500.raw

Suggested Steps

- Check if intensity scaling treatment is required
- Locate “Merge Scans”-context menu (Scan-tab, Preview pane)
- Save full pattern as DIF file

Tips

- Pay attention to the measurement time of each range
- It may be necessary to use CPS scaling (counts per second)
- An “Auto-stitch” option is available for when stitching is required often

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105887

Exercise 3

Save a background curve for reuse

XRD File

- DEMO14.MDI

Suggested Steps

- Adjust spline anchor point frequency
- Manually edit anchor points till BC is acceptable
- Save the BC as a private BG-Curve for future reloading

Tips

- Anchor points can be fine-tuned with the MouseWheel
- The BC button shows a green light when a saved BC is available

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105899

Exercise 4

Import XRD data from unknown text file format

XRD File

- unknown_format_1.pxs

Suggested Steps

- Assign proper column headers in the ASCII importer
- Verify wavelength!
- Decide if X- or Y-scaling factors need to be applied
- Test the created importer template on other *.psx files

Tips

- If intensities are too low, the use of an I-Multiplier is recommended
- We usually aim to see a pattern intensity maximum of >1000,
  so that routines that rely on sigma thresholds works reliably
- For plotting non-XRD data (e.g.: RAMAN spectra) an X-Multiplier is recommended

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105918

Exercise **5**

Remove a phase from a powder pattern (using IPF) *

XRD File

- DEMO06.MDI

Suggested Steps

- Perform S/M to identify all 3 phases
- Modify background curve (BC) if necessary
- Perform IPF using Line-Markers for profile initialization
- Click (h k l)-column header for assigning phases to the profiles
- Remove all Anatase peak profiles

Tips

- * *This is just an exercise (one may never need to do this)*
- One can use multi-select (CtrlKey) to strip all selected profiles at once
- We just added a context menu function for “Strip Profiles”, making this very easy

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105932

Exercise **6**

Remove a phase from a powder pattern (using WPF) *

XRD File

- DEMO06.MDI

Suggested Steps

- Perform S/M to identify all 3 phases
- Perform WPF
- Overlay individual scans of fitted phases (from WPF Save menu)
- Select Scan-tab
- Delete all but one of those overlays
- Perform pattern arithmetic to subtract phase from original pattern
- Add subtraction pattern as overlay

Tips

- * *This is just an exercise (one may never need to do this)*
- Make the overlay the primary pattern, so that subtraction pattern is positive
- The easy way would be to use “Miscellaneous: Strip This Phase” from the phase list context menu on the WPF panel 😊
- We also just added RightClick the [1]-button when performing WPF from the WPF toolbar instead of the WPF window or docked pane

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105944

Exercise 7

Correct the Zero offset of a pattern manually

XRD File

- DEMO08.MDI

Suggested Steps

- Select the Peaks-tab and activate the Corundum peak markers (Al2O3)
- Zoom in to main peak
- Scroll MouseWheel over the 2Theta label for manual adjustment
  (finer increments with Shift & Scroll)

Tips

- One could use CtrlKey+Click the 2theta label for an automatic correction using harmonic peak pairs, such as (012) & (024) etc.
- When an actual structure phase is overlaid (e.g.: MDI500 Corundum) the automatic correction with CtrlKey+Click would use the structure peaks
- When finding Corundum by S/M one can CtrlKey+Click the theta button on the secondary toolbar to shift the pattern

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105963

Exercise 8

Find the unit cell for a single phase powder pattern (Pattern Indexing)

XRD File

- DEMO08.MDI

Suggested Steps

- Select Peaks-tab and ensure suitable peak list
- Select “StartMenu:Pattern Indexing”
- Select crystal systems to search and run “Seek”
- Screen candidates and select a solution
- Switch the toolbar to “Refine” and perform a line-based cell refinement
- Perform a WPF cell refinement
- JADE would also accept fitted profiles (instead of peak search list) for indexing (one may get better peak positions if indexing fails otherwise)

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105979

Exercise **9**

Simulate a powder pattern from a structure

Database

- MDI-500

Suggested Steps

- Select any phase from the MDI-500
- From context menu select “View Structure”
- Select Parameters-tab in the structure viewer/editor window
- Verify settings (2Theta range, PSF, etc.)
- Click [Create]-button

Tips

- Add noise (~3 σ) for more realistic patterns
- Check the [F^2] option, so that simulated patterns can be used for creating mixture patterns with true wt% scaling (using pattern arithmetic on Scan-tab)
- One can also open CIF & CSF structure files (CIF, CSF) instead of using a DB
- The viewer also can be launched from “StartMenu: Calculate Pattern”
- JADE also accepts drag/drop of structure files

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105994

Exercise **10**

Switch between various trace fill styles & trace styles

XRD File

- demo3ds.bin (12 scans: 1+11 overlays)

Suggested Steps

- Offset the patterns using the context menu “Offset Scans” (from Preview pane, Scans list, Scan-tab toolbar) or by scrolling on left side of Y-axis
- From menu “Display: Fill Style & Dots” test all options
- Additionally you can test trace styles from “ScansListContexMenu: Trace Line Style”, which acts on the scan that is currently selected in the list

Tips

- When a menu item shows the (opacity%), one can change that value with the MouseWheel while hovering over that menu item

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106018

Exercise **11**

Change scan colors (edit palette)

XRD File

- demo3ds.bin (12 scans: 1+11 overlays)
- You can overlay the same file for a total of 24 scans (see all palette colors)

Suggested Steps

- Offset overlays for better visibility
- Select any scan from the Scan List and click color button on toolbar
- Change color in the “Scan Overlay Palette” dialog window
- Click the small blue arrow reset button to reset the whole palette

Tips

- JADE uses revolving 16-color palettes for the Scan Traces and the S/M Phases
- One can assign the color of a selected Scan List row to all scans by RightClicking the color button on the scans toolbar as indicated in its tooltip

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106035

Exercise **12**

Determine similarity among loaded patterns *

XRD Files

- DEMO09-12.MDI (1+3 overlays)

Suggested Steps

- Optionally offset the overlays for better visibility
- Select “ScanListContextMenu: Calculate SI% (0.75)”
- A new “SI(%)” column will appear
- Optionally change the Spearman-Pearson mixing factor with MouseWheel
- Try to maximize the similarity by shifting one overlay at a time left/right

Tips

- ** This is just an exercise (one may never need to do this)*
- The mixing factor is taken from and transferred to the Cluster Analysis; The higher the value the more emphasis on the peaks in the SI%
- One can automatically shift an overlay to the maximum similarity by Ctrl+Click the shift button on the toolbar

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106044

Exercise **13**

Create a User Structure Database from CIF files

XRD Files

- ..\Exercise 13*.*

Suggested Steps

- Select “Create User SD” from the [Database]-menu
- Click “New CSD” and provide a name for it
- Enter a starting number that does not overlap with other CSDs
- Add structure files from a folder with CIF/CSF files
- Click “Yes” when asked to create a d-I list subfile for S/M
- The new CSD is then available for S/M from all subfile selectors

Tips

- You can also click “No” for the d-I list and inspect the imported structures for accuracy first, before selecting “Menu: Calculate d-I% List”
- The numbers ‘starting number+sequence number’ are converted to 9-digit PDF numbers starting with set number “98” to indicate calculated patterns

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106062

Exercise **14**

Create a chemistry filter for Li-Battery materials and save it

XRD File

- SKCM005.RAW

Suggested Steps

- Select Phase-tab and open PTE for setting up a chemistry filter (click “Chem…”)
- Select Li as a required element and all others as allowed/possible elements
- Select the “Battery Materials” subclass on the “Unit Cell”-tab
- Require atom structures by checking “[x] Has Coordinates”
- Click diskette-button on “Chemistry”-tab to save filter for reuse

Tips

- RightClick the diskette button to retrieve previously saved filters
- You can use the same procedure in the PDF Retrieval window for importing matching phases and creating a custom hit-list (see next exercise)

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106087

Exercise **15**

Create a custom hitlist for Li-Battery materials

XRD File

- SKCM005.RAW

Suggested Steps

- Select “Retrievals” from the [Database]-menu (modal window)
- Set up a Li-Battery filter as in the previous exercise or just reload that filter
- From the drop-down selector next to the diskette button select “All Subfiles in This List” and wait for table to be populated
- Click the “Add”-button to send retrievals to JADE’s hit-list
- Close the modal window and from the hitlists toolbar save a custom hitlist, which will then appear on the right-side pane

Tips

- If your hit-list already contained some entries you can RightClick the “Add”-button first to clear the hitlist, before adding the retrieved phases
- Any structure list on the right side can be searched directly with the magnifying glass button on its toolbar, instead of searching the selected subfile

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106109

Exercise **16**

S/M a polymer in the default way with subfiles & filter

XRD File

- Z02129.RAW

Suggested Steps

- On Peaks-tab, manually insert missing crystalline peaks
- Select the RDB-Organics subfile for S/M
- Switch to Phases-tab and launch chemistry filter window (“Chem…”)
- On its “Unit Cell”-tab select subclass “Polymers”
- On S/M toolbar activate 1% solid solution search (S^3)
- Perform phase id and screen candidates for α-Polypropylene

Tips

- Without the 1% S^3 the α-PP would have been hidden among the γ-IPP tally
- Here some peak can’t be detected by Jade, because it lacks a peak shoulder

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106117

Exercise 17

S/M a polymer by matching analog PDF patterns (PD3 files)

XRD File

- Z02129.RAW

Suggested Steps

- Select the RDB-Organics subfile for S/M
- Switch to Phases-tab and launch chemistry filter window (“Chem…”)
- On its “Unit Cell”-tab select subclass “Polymers”
- Click button “S/M PD3 Phases (Patterns)…”
- Screen candidates for α-Polypropylene (around #10)

Tips

- From the PhaseListContextMenu one can then overlay the PD3 pattern
- It may be a Co-Kα pattern, which we would need to convert to Cu-Kα and rescale its intensity on the Scans-tab so that we can visually compare the two scans

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106133

Exercise **18**

Fit profiles for a polymer & determine crystallinity%

XRD File

- Z02129.RAW

Suggested Steps

- Use peak editing cursor to add missing crystalline peaks OR
- Use the profile editing cursor to add those peaks
- Insert suitable amorphous peaks (AP)

Tips

- Use Shift+Click for inserting amorphous peaks (solid dot in the AP column)
- The number of used crystalline peaks will affect the calculated area ratio
  crystallinity% = (sum of crystalline peak areas) / (total fitted area) x 100%
- Compare with α-Polypropylene peaks

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106148

Exercise **19**

Determine Purity% using IPF (by hijacking Crystallinity% function)

XRD File

- Sim-Impurity-IPF.dif
  (simulated pattern where corundum peaks stand in for 'impurity' peaks)

Suggested Steps

- Create a snuggly fitting background curve (~25 anchor points)
- Select Peaks-tab and verify that all 18 peaks have been found
- Perform S/M on 'Mineral Subfiles' to find & check main phase (Quartz)
- The leftover peaks will be considered as belonging to an impurity
- Select Profiles-tab and set options: 'Fixed-BG', 'Pseudo-Voigt'
- Click the "Init" drop-down arrow and set "Current Peaks > Initial Profiles"
- Click "Init" (for full zoom range) and then "Fit" all 18 profiles
- Turn on filmstrip for easy identification of "impurity peaks"
- Multi-select all 5 profiles not belonging to Quartz (with CtrlKey) #2,4,6,10,13
- RightClick one of the selected rows in the "AP" column (!) and check "Amorphous"
- This will convert the impurity peaks to "amorphous" peaks and the calculated Crystallinity% will represent Purity%

Tips

- Make sure that a peak area ratio approach is suitable for the type of material you are analyzing, especially when phases have very different RIR values / scattering power. That goes for both the crystallinity% and purity%.
- WPF can also be used for purity%, as long as one has a phase for the impurity

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106159

Exercise **20**

Create an instrument profile curve (IPC)

XRD File

- CPD-Y2O3.RD

Suggested Steps

- Select Peaks-tab and verify that all peaks are found
- Select Profiles-tab and set options: 'Linear-BG', 'Pseudo-Voigt'
- Press CtrlKey and click "Fit"-button
- This will segment the pattern and fit all peak profiles
- On the toolbar LeftClick the "IPC" to view the curve FWHM(uvw)
- RightClick "IPC" to name, save and set it as the current IPC

Tips

- An IPC is a prerequisite to performing any XSS
- Use an SRM that has enough peaks to cover most of the 2Theta range that you wish to analyze
- One can usually uncheck "Unify Skew" in IPF since SRM patterns rarely have any peak overlap
- If one does not know which PSF to choose, try both the PV and P7 and use the one that gives the lower R-factor (shown on statusbar)

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106173

Exercise **21**

Size & Strain Analysis using WPF (direct fitting)

XRD File

- CPD-3.RD

Suggested Steps

- In instrument setup select the IPC(Y2O3)
- Perform S/M on “Mineral Subfiles” to find the 3 phases
- Click “WPF”-button to open WPF window or docked WPF pane
- Increase starting angle to 24°, so that we don’t have to deal with the hump
- Select “Crystallite Size & Strain” on the WPF’s Phase-tab
- Check box “XS” and optionally “ST”
- Run refinement and view “FW-Curve” plot for results

Tips

- Make sure a suitable IPC for the same instrument is selected
  (not always the case in our demos)
- This refinement mode (instead of “Individual FWHM Curve”) can also lead to a more stable refinement for complex patterns with many phases and it enables fitting of “Anisotropic Broadening”

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106191

Exercise **22**

Size & Strain Analysis using IPF (Williamson-Hall plot)

XRD File

- DEMO06.MDI

Suggested Steps

- In instrument setup select the IPC(Y2O3) even though not from same instrument
- Perform S/M on “Mineral Subfiles” to find the 3 phases (Rutile, Hematite, Anatase)
- Zoom out to full 2theta range; proceed like for the IPC creation
- Select Profiles-tab and set options: ‘Linear-BG’, ’Pseudo-Voigt’, but ‘Unify Skew’
- Click the “Init” drop-down arrow and set “Line Markers > Initial Profiles”
- Press CtrlKey and click “Fit” to fit all ~16 peaks in pattern segments
- On the toolbar click “XSS” to open the Williamson-Hall plot window
- In W-H select “Fit Size & Strain” for a linear fit
- In W-H select individual phases from the top right phase selector and see results

Tips

- In a single phase pattern we do not need to use the phase selector in W-H, since all fitted peaks are assigned to only one phase
- One could use a smaller 2theta range with a fixed or polynomial BG
- At least 2 peaks per phase need to be fitted for W-H XSS
- Different 2theta ranges may give different XS, ST values because of the different number of peaks used per phase
- Note that the W-H XSS is affected by some instrument options (integral breadth vs FWHM, deconvolution parameter, crystallite shape factor)

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106213

Exercise **23**

Batch profile fitting (IPF)

XRD File

- demo3ds.bin (contains 12 scans)

Suggested Steps

- Offset the scans (MouseDrag or MouseWheel in left plot margin)
- Reverse the order of the scans, so that the primary scan has the most peaks
- Select Profiles-tab and set options: 'Linear-BG', 'Pseudo-Voigt', 'Unify Skew'
- Click "Init" to initialize the found crystalline peaks
- Click under 36° peak to insert missing crystalline peak
- Press Shift and click ~24° to insert an amorphous peak (AP)
- *(Optionally click "Fit" to test fitting the primary scan)*
- Click "Run" to open menu and select "Create One Listing File for All Scans"
- Provide output file name and proceed; then review output file

Tips

- The scan order can be reversed by clicking the "#"-column header in the scans list or by RightClicking the filename label in top left plot corner
- To remove all fitted profiles for all scans, press CtrlKey when selecting "Fitted Profiles" from the Erase-menu

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106232

Exercise **24**

Create IPC & analyze XSS for CeO_2 (IPF)

XRD Files

- lebailsh.xy (sharp; for IPC creation)
- lebailbr.xy (broadened; for XSS)

Suggested Steps

- Make sure the XY files are imported correctly with Cu-Kα
- Load 'lebailsh.xy' and create an IPC as in Exercise 20
- Save IPC with the suggested name "Le Bail - sharp - Cu Kalpha"
- Load 'lebailbr.xy' and perform S/M on "Mineral Subfiles" to find Cerianite CeO_2
- Proceed with W-H XSS as in Exercise 22, but with this new IPC and phase

Tips

- These data files were used in a round-robin competition
- You can save the imported XY files as DIF if you prefer that format for future use

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106248

Exercise **25**

Simulate a pattern using crystallite size profile (XS PSF)

XRD File

- lebailbr.xy

Suggested Steps

- Make sure the XY file is imported correctly with Cu-Kα
- We don't want to analyze this pattern but use it for a visual comparison
- Perform S/M on "Mineral Subfiles" to find a Cerianite phase with structure data
- RightClick cerianite in the phase list and select "View Structure"
- Select the Parameters-tab in the structure editor window
- The IPC "Le Bail - sharp - Cu Kalpha" should be selected below the "Create" button
- Expand the 2theta range to 150° by editing the end angle box
- Press CtrlKey and click the "Create" button to overlay the simulated pattern
- Modify XS value (+slider) to ~200 and the Gamma Distribution Variance (+slider) to ~10, so that the simulated pattern approaches the loaded scan trace
- This would represent a visual crystallite size analysis

Tips

- The choice of using neutral atoms vs ionized atoms may affect the match due to the different scattering factors used

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133106266

Exercise **26**

Quantitative Analysis using the RIR Method (IPF)

XRD File

- DEMO06.MDI

Suggested Steps

- Perform S/M on “Mineral Subfiles” to identify all 3 phases
- Select a zoom range with strong peaks (e.g.: 23°-51° or 23°-34°)
- Select Profiles-tab and set options: ‘4th-Order’, ’Pseudo-Voigt’
- Perform IPF using Line-Markers for profile initialization
- LeftClick the “RIR | DDM”-button to open RIR method window
- Select “Wt% Chart”-tab therein to see the pie chart
- A “Wt%” column is also being added to the main phase list

Tips

- At least 1 peak per phase is needed (ideally select the strongest peaks)
- RIR values must be reliable for the used phases !
- Compare your RIR wt% with WPF wt% by RightClicking the “WPF”-button to run WPF from the toolbar

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105691

Exercise **27**

Quantitative Analysis using the DD Method (IPF)

XRD File

- DEMO06.MDI

Suggested Steps

- Perform S/M on “Mineral Subfiles” to identify all 3 phases
- Select Profiles-tab and set options: ‘Linear’, ’Pseudo-Voigt’, ‘Line Markers > Initial Profiles’
- Press CtrlKey and click “Fit”-button (as in IPC creation exercises)
- RightClick the “RIR | DDM”-button to see the DDM pie chart
- A “DD%” column is also being added to the main phase list

Tips

- DDM (Direct Derivation Method) requires a large 2Theta range, so that the fitted peak area sum for each phase approaches its total scattering intensity! (this is almost opposite to the RIR method, where one peak per phase may suffice)
- Accurate & parsable chemical formulas required !
- One can also enable a DD% column for the phase list on the WPF pane. The XRD(wt%) and DD(wt%) should be comparable. A discrepancy may indicate a problem with the phase selection.
- In the absence of structure data and RIR values, the DDM is the only option left for a quantitative analysis

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105705

Exercise **28**

Advanced chemistry filter for OCA *

XRD File

- Yttrium Silicate.raw

Suggested Steps

- We need to find 5 phases with these elements: Y, Si, O, Mo
- Select Scans-tab (don't go to Phase-tab for manual S/M)
- Select "All Subfiles" from S/M subfile selector at bottom right corner
- RightClick "One-Click Analysis"-button to set up a chemistry filter
- Clear any existing filter by DoubleClicking tab-stubs if they show a fat dot
- Select Si, O as allowed/possible elements (blue)
- Select Y, Mo as required elements (golden)
- Uncheck "Require All" (so that only Y or Mo must be present in formula!)
- Run OCA

Tips

- ** This is just an exercise (one may not know what elements are present & required)*
- Take advantage of available XRF data for setting up a chemistry filter, in order to narrow down the search results and avoid many false hits

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105729

Exercise **29**

Amorphous content from modeling hump (WPF)

XRD File

- CPD-3.RD

Suggested Steps

- Perform S/M on “Mineral Subfiles” to find all 3 phases
- Click “WPF”-button and select the “Global”-tab
- Set starting angle to 12°, select “Refinable Polynomial-BG” with a low order polynomial (Parabolic or 3rd-Order)
- Check “Amorphous Humps”-box (this may reset the starting angle in older JADE)
- If needed modify initial values in hump setup fields
- Run refinement; amorphous wt% should be ~29%

Tips

- A valid pseudo-RIR value is required (nominal density)
- The default value 2.5 is an empirical value for SiO_2
- CPD Quantitative Phase Analysis Round Robin - Weighed and Measured Values of Distributed Samples and Data

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105753

Exercise **30**

Amorphous content from internal standard IS (WPF)

XRD File

- CPD-3.RD

Suggested Steps

- Perform S/M on “Mineral Subfiles” to find all 3 phases
- Click “WPF”-button and select the “Global”-tab
- Set starting angle to 24°, select ‘Refinable Polynomial-BG’, ‘3rd-Order’ with ‘C-3’ and ‘C-1’ checked for the low-angle rise of the BC
- Select Corundum in the phase list (we’ll pretend that this is the IS)
- On the “Wt%+XRF”-tab check “Internal Wt% Standard” and uncheck “Before Mix”
- Enter a value of 32% for the “known” IS wt% and Run refinement

  One could have run the fit first and then set the IS and IS wt%, since that just involves rescaling the pie chart; One could also leave a fitted hump in as in previous exercise. That would just simplify the BG modeling for a lower starting angle of ~12°. The hump would then not be used for the wt%.

Tips

- Using an internal standard (IS) is the most accurate way for performing a quantitative analysis including for the determination of amorphous content
- The IS should be chosen such that its peaks don’t overlap with the peaks of the other phases of interest
- Amorphous+Missing Phases wt%=100%-Sum(wt%)
- Make sure you know if the entered IS wt% is from before the mix (Sum>100%) or after the mix (Sum=100%) and check the box ”Before Mix” if needed
- The pie chart will not show the IS slice when ”Before Mix” was selected and the remaining wt% will be rescaled to Sum=100%

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105768

Exercise **31**

Batch processing in WPF

XRD File

- Step 1: DEMO09.MDI (for WPF control file creation)
- Step 2: DEMO09-12.MDI (1+3 overlays)

Suggested Steps

Step 1

- Perform S/M on “Mineral Subfiles” to find all 4 phases (Quartz,Corundum,Calcite,Dolomite)
- Click “WPF”-button, set all parameter choices and Run refinement
- Calcite and Dolomite will need a POC (SH, March; to decide, examine the number of peaks present)
- Refine again and save WPF control file from WPF menu [Save][Save Control File]

Step 2

- Close WPF and Erase All (Ctrl-X)
- Load all 4 patterns and click “WPF”-button to proceed directly to WPF
- Select the created control file from control file selector and open [Run]-menu
- Check options and click “Start WPF to All Scan Overlays”

Tips

- Make sure you modify the filename when saving the control file, e.g.: by adding a prefix “WPF “, “Batch “. Otherwise you may be creating a private control file in the pattern folder instead of a common control file for batch processing in the project folder!
- Always enable the “BR%” column (Bragg-R value), so that you spot outlier phases and understand why JADE appends “(?)” to some phases.

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105778

Exercise **32**

Solve structure of Sodium Oxalate - $Na_2C_2O_4$ (WPF/R)

XRD File

- Powbase_9.dif

Suggested Steps

- Select Peaks-tab and make sure all peaks are found and marked
- Select menu “Start: Pattern Indexing”-tab and accept offset correction if offered
- Choose crystal systems to index and click “Seek” to run the cell search
- One should find a monoclinic cell in space group ‘$P2_1/c$ (14)’
  (Usually one would have to test several space group candidates, but $P2_1/c$ is very common; also solvable in $P2_1/n$)
- From the WPF toolbar select “Save: Run Structure Solver”
- Enter filename and for the formula enter “**2 Na2 C2 O4**” (Z=2; formula units)
- Run charge flipping in the toolkit window and click ‘Yes’ when asked “Copy structure to JADE?”
- One can also use menu “Structure: Find Polyhedra” and the structure model should be ok if polyhedra (octahedra) are displayed
- Minimize or close charge flipper window;
- The structure viewer should be visible in JADE; Click its WPF button to add the structure to the WPF phase list; Delete or uncheck the previous structureless phase
- Uncheck “TF” on the Phase-tab and select “C” and “B” on the Atomic-tab
- Run Rietveld refinement (try to get R<10%; e.g.: BG, POC, FWHM options)

Tips

- Don’t expect this to be very easy (in the past one could do a whole PhD about solving a single structure)

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105809

Exercise **33**

Solve structure of Cimetidine in Structure Solver Toolkit (not in JADE)

XRD File

- cime.dif

Suggested Steps

- Open file and select menu "Start: MDI Toolkit: Solve Structure"
- Use the top flowbar to go from "Background" to "Peaks" to "Indexing"
- Find a cell candidate for space group $P2_1/a$ or $P2_1/c$
- Go to "WPF" and click "Start WPF"-button (this fit is a required step for intensity extraction)
- Go to "Structure" and enter "**4 C 10 H 16 N 6 S 1**" in the formula field (with Spaces!)
- Click "CF"-button to run charge flipping without a GUI; wait for model to appear
- Go to "Refinement" on flowbar and click "Start Refinement" (includes xyz, Biso)
- Go to "Finish" to see HTML report and structure files
- Use menu "File: Save Structure" to choose specific format and filename

Tips

- This is a quick exercise without being thorough, e.g.: no element swapping performed, which can be done in charge flipper GUI ("Flipper"-button)
- The Rietveld refinement in this toolkit is pretty basic and not as powerful as the one in JADE; there are no geometry constraints etc.
- One can also copy this model to JADE and do the WPF/R there like in the previous exercise using menu "File: Copy Structure" (JADE must still be running to receive paste command)
- One could also download the free SUPERFLIP for an alternative flipper algorithm; It should be placed in the folder "C:\Program Files (x86)\MDI JADE\Tools\Taos\"

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105828

Exercise **34**

Analyze unknown rock sample

XRD File

- E5.xrdml

Suggested Steps

- Perform S/M on “Mineral Subfiles” and try to find reasonable matches
- There seems to be a zero-offset present (try S/M again after correction)
- There could be 6-8 phases present

Tips

- Nothing is known about this sample other than that it is supposed to be from a rock
- No XRF data that would help in setting up a chemistry filter
- No optical microscopy image that would help consider preferred orientations
- Try your best; We don’t know for sure either

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105838

Exercise **35**

Digitize an XRD plot image in the Digitizer Toolkit

XRD File

- DEMO08.MDI

Suggested Steps

- Go to PrintPreview and click “Copy”-button (puts image on clipboard)
  (of course one could paste any other image or load an image file in the Digitizer instead)
- Select menu “Start: MDI Toolkit: XRD Digitizer”
- The Digitizer window should launch with the image pasted
- Set the 4 axis marker points (easier with zoom navigator) and enter axis values
- Verify wavelength and plot scaling
- Click “Digitize”-button
- Select menu “Digitizer: Save Pattern” to save it as a DIF file for JADE

Tips

- This digitizer is more powerful than the online JADE Digitizer app on the ICDD website: JADE Pattern Digitizer; e.g.: the eraser tool helps remove image artifacts, such as grid lines and text.
- A rainfall tracing algorithm is used, which means that the area above the pattern should be clear (i.e.: area between BG curve and maximum intensity)

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133105850

Exercise **36**

Amorphous WPF with Zincite IS

XRD File

- InternalStandard_ZnO.rasx

Suggested Steps

- Perform S/M on “Mineral Subfiles” and find Zincite
- Apply 2theta correction for Zincite (CtrlKey+theta button on toolbar)
- Run S/M again and find Quartz, Calcite, Akermanite
- Click “WPF”-button to open WPF window or docked WPF pane
- Set starting angle to 15°, select ‘Refinable Polynomial-BG’, ‘4rd-Order’
- Activate amorphous hump model at ~30°
- Select Zincite in the phase list
- On the “Wt%+XRF”-tab check “Internal Wt% Standard” and check “Before Mix”
- Enter a value of 10% for the “known” IS wt% and Run refinement

Tips

- See Exercise30

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133877656

Exercise **37**

WPF with anisotropic peak broadening

XRD File

- DEMO14.MDI

Suggested Steps

- Ensure a good BG curve (if the manual background saved in a previous exercise is not available)
- Perform S/M on “Mineral Subfiles” and find Corundum, Hydroxylapatite
- Click “WPF”-button to open WPF window or docked WPF pane
- Set starting angle to 17°, select ‘Current BG-Curve Fixed’
- Select Phase-tab and choose “Crystallite Size & Strain” fitting mode
- Select Hydroxylapatite in the phase list
- Check “Anisotropic Broadening” on the Phase-tab
- Run Refinement

Do the following if you want amorphous content:

- Select Corundum in the phase list
- On the “Wt%+XRF”-tab check “Internal Wt% Standard” and check “Before Mix”
- Enter a value of 10% for the “known” IS wt% and Run refinement
  (the correct IS wt% is not known to us)

Tips

- This pattern has a low count rate and is very noisy; One can improve the fitting by measuring for a longer time to reduce the noise

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133878074

Exercise **38**

SAXS pattern background fitting (IPF)

XRD File

- SAXS Demo.dif

Suggested Steps

- Select Peaks-tab and insert two missing peaks at ~3.3° and 7.8°
- Select Profiles-tab
- Set options 'Linear-BG' with 'c-1', 'c-3', 'Pseudo-Voigt', 'Unify Skew'
- Click "Init"-button and then the "Fit"-button
- Uncheck 'Unify Skew' and click "Fit" again (R-factor on statusbar may be ~0.7%)

Tips

- For inserting a peak exactly at the cursor position press CtrlKey
- In IPF try clicking "Fit" repeatedly, in order to see if improvement is still made

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133878101

Exercise **39**

Simulate a mixture pattern from structure data

XRD File

- MDI500 list and saved patterns

Suggested Steps

- Click “StartMenu: Calculate Pattern” to open the structure viewer/editor
- Select the Parameters-tab with the simulation setup (add noise, XS etc.)
- Select a phase from the MDI500 on the right-side pane
- Click “Create”-button to create a simulated pattern in the plot window and save it from menu “Save & Paste: Save Pattern Data”
- Select another phase from the MDI500 and do the same
- Load both saved patterns in JADE and use pattern arithmetic on the Scans-tab toolbar to create a summation pattern
- Change the individual intensity scaling factors before the pattern summation to get mixtures other than 50/50 mixtures

Tips

- CtrlKey+Click “Create”-button will overlay a simulation instead of replacing the main pattern;
  It can then be added to the scans list from menu “Derive: Save Pattern Data”
- One can also create mixture patterns from WPF, by manually editing the individual scale factors “SF” for the listed phases

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133878121

Exercise **40**

Predict the crystal morphology of a structure phase

XRD File

- DEMO20.MDI

Suggested Steps

- Perform S/M on “Mineral Subfiles” and find 4 phases
- Select a phase in the phaselist
- Click “StartMenu: MDI Toolkit: BFDH Morphology” (BFDH=Bravais-Friedel-Donnay-Harker)
- If all phases are checked, only the first one is used
- If all phases are unchecked, the highlighted one is transferred to the toolkit

Tips

- Uncheck all phases in the phase list, so that JADE forwards only the highlighted phase to the BFDH toolkit
- One can apply XRD Multipliers to create more realistic shapes sometimes
- The true BFDH only uses growth rates from d-spacings (1/d) and extinction rules
- One can print papermodels with glue tabs of the crystal shapes for folding
- When having fitted profiles, a Scherrer shape can be calculated from the different XS(hkl) values. However, since some peaks may be missing in the presence of PO, this may not turn out to be useful
- RightClick the “Create”-button to activate Auto-Run when selecting other options, otherwise one has to click the Create button again

Video Link with Solution

https://vimeo.com/showcase/11952354?video=1133878149

Exercise **41**

WPF batch processing of a temperature series - CeO_2

XRD File

- ..\TemperatureSeries*.xrdml

Suggested Steps

- Load all scans in that folder and optionally sort them by temperature (50C-1000C)
- Perform S/M on “Mineral Subfiles” to find Cerianite
- Click “WPF”-button to open WPF window or docked WPF pane
- Set suitable parameters and optionally Run Refinement for first pattern, in order to verify the setup
- Save a common control file from WPF’s Save-menu
- Review options in Run-menu that deal with treating peak migrations
- Click “Start WPF to All Scan Overlays” from the Run-menu
- When finished, review the ASCII report files and lattice parameter plot

Tips

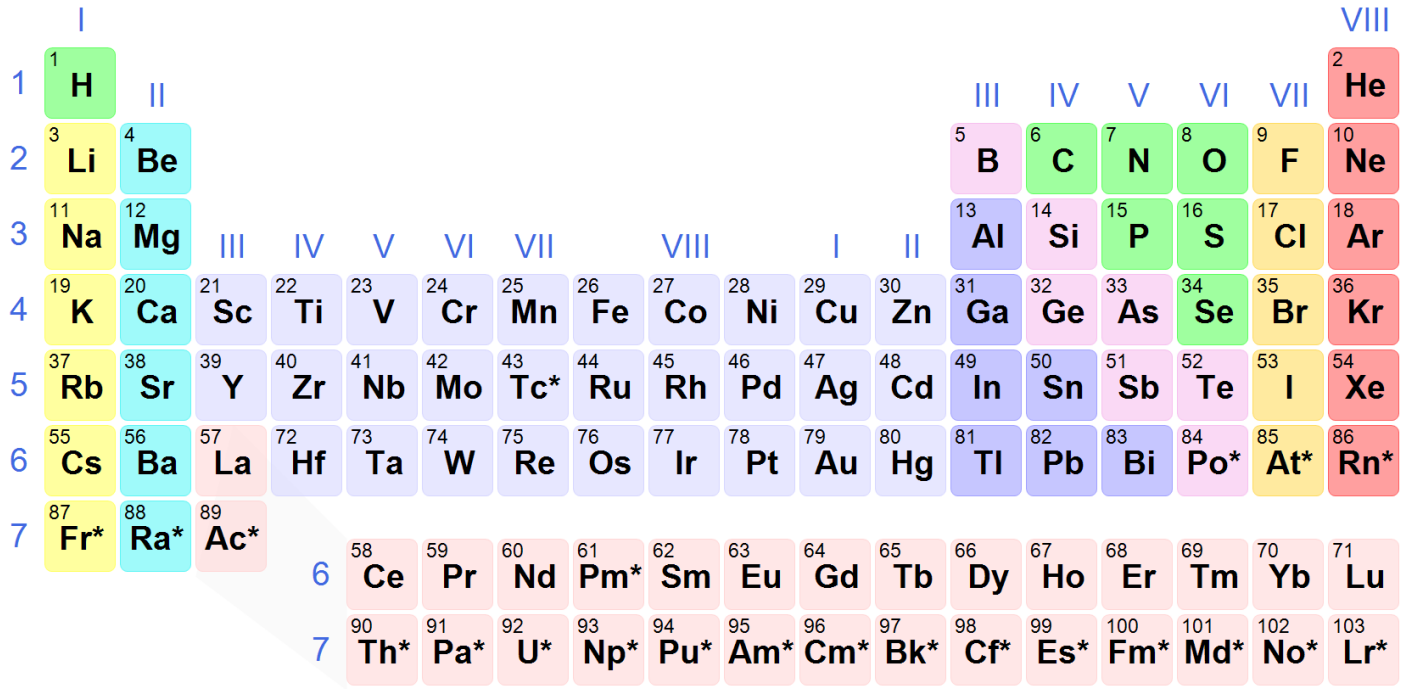
- The sorted scan list can be saved with Shift+”ScanListMenu: Copy Scan List”
- The saved *.lst file can then be reloaded from the XRD folder list on the left
- A common control file for batch processing must not start with the pattern file name

Video Link with Solution

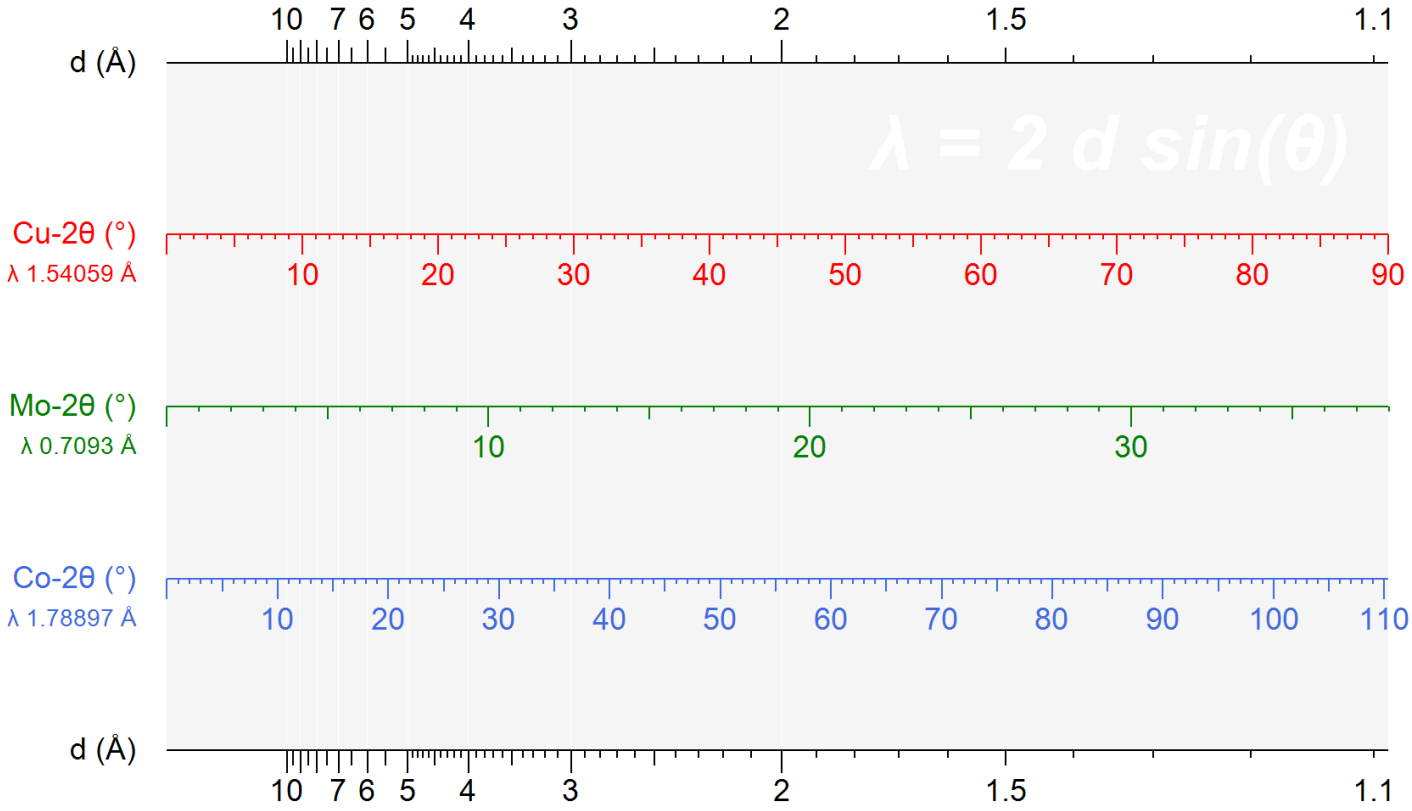
https://vimeo.com/showcase/11952354?video=1133878165

Appendix

Periodic Table



2Theta vs d-Spacing



Have some fun and create your own business cards. Select menu [Help][Business Card] in the RAMAN Mineral Toolkit, in order to design your front and back images. Then save them so that you can submit them to VistaPrint for printing. A PDF-5+ database is required to enable the structure rendering. The ICDD logo, if you include it, just indicates that the displayed structure comes from the PDF database.

The text fields can be moved around and the fontsize can be changed by mouse wheel. RightClick a text field to toggle bold vs regular. The structure can be manipulated in the RAMAN window while the business card wizard is open. Use the mouse wheel on the back design to scroll through all available design options.

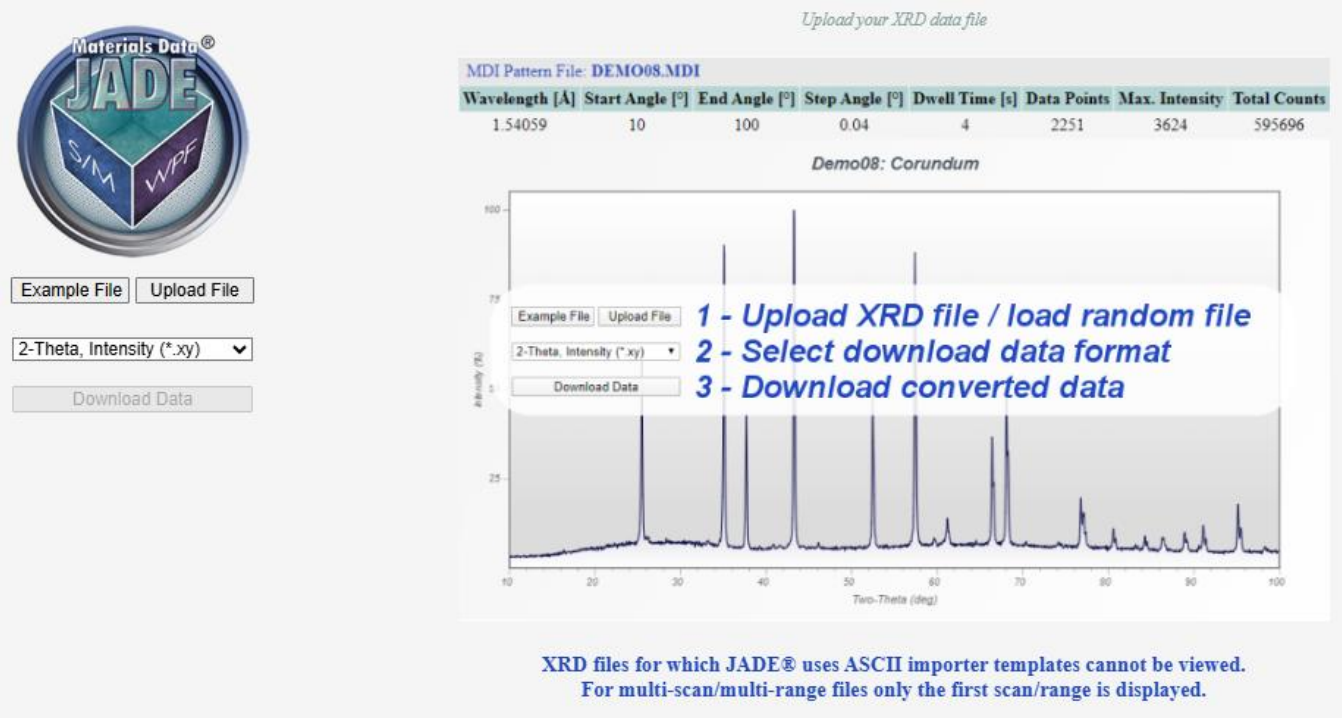


To include your own logo, select menu [Front Design][Logo Image][None], which will leave a blank space where you can later paste your logo into the saved image using an image editor of your choice.

Online Resources

JADE Pattern Converter

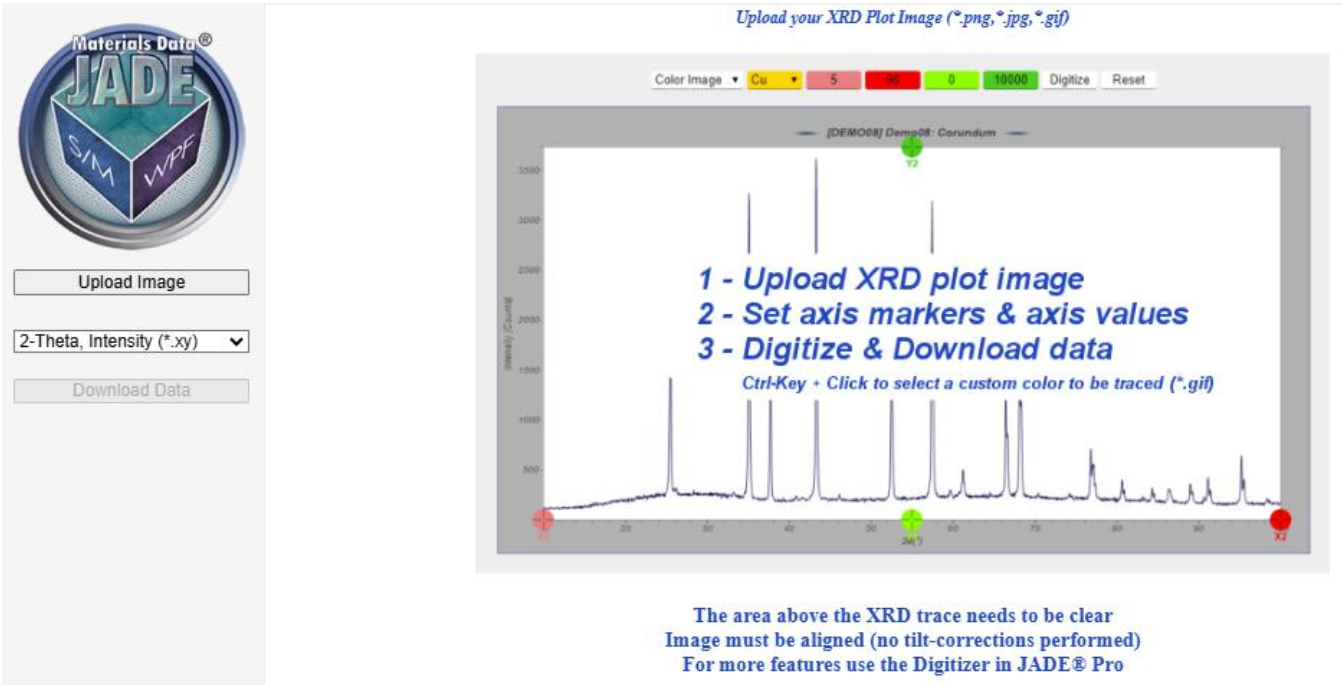
Home Page & FullScreen Version



XRD files for which JADE® uses ASCII importer templates cannot be viewed.
For multi-scan/multi-range files only the first scan/range is displayed.

JADE Pattern Digitizer

Home Page & FullScreen Version & Tutorial Videos



The area above the XRD trace needs to be clear
Image must be aligned (no tilt-corrections performed)
For more features use the Digitizer in JADE® Pro

InSession Chapter Links

A separate Vimeo password is required to access these previously recorded InSession JADE webinars.
Obtain the current month's password by email from mdi@materialsdata.com

Navigating JADE

03:08	**Graphical User Interface (GUI)**	https://vimeo.com/showcase/9227425/video/517143444#t=3m8s
17:32	**Feature Overview**	https://vimeo.com/showcase/9227425/video/517143444#t=17m32s
31:59	**Feature Demos**	https://vimeo.com/showcase/9227425/video/517143444#t=31m59s
40:46	**Utilities**	https://vimeo.com/showcase/9227425/video/517143444#t=40m46s

Introduction to JADE

01:23	**1 - GUI Layout & Customization**	https://vimeo.com/showcase/9227425/video/1080315856#t=1m23s
08:11	**2 - Pattern Processing Options**	https://vimeo.com/showcase/9227425/video/1080315856#t=8m11s
16:12	**3 - Database Options**	https://vimeo.com/showcase/9227425/video/1080315856#t=16m12s
21:47	**4 - Structure Handling**	https://vimeo.com/showcase/9227425/video/1080315856#t=21m47s
26:59	**5 - Main Tasks in JADE**	https://vimeo.com/showcase/9227425/video/1080315856#t=26m59s
40:07	**6 - Main Toolkit Options**	https://vimeo.com/showcase/9227425/video/1080315856#t=40m7s

Get Things Done with JADE - Part 1

01:43	**User Interface Overview**	https://vimeo.com/showcase/9227425/video/822150353#t=1m43s
06:35	**Database Connection / Creation**	https://vimeo.com/showcase/9227425/video/822150353#t=6m35s
19:36	**Getting Data into JADE**	https://vimeo.com/showcase/9227425/video/822150353#t=19m36s
25:08	**Basic Pattern Processing**	https://vimeo.com/showcase/9227425/video/822150353#t=25m8s
46:17	**Individual Profile Fitting (IPF)**	https://vimeo.com/showcase/9227425/video/822150353#t=46m17s

Get Things Done with JADE - Part 2

01:06	**Phase ID by Search/Match (S/M)**	https://vimeo.com/showcase/9227425/video/832035237#t=1m6s
36:18	**Whole Pattern Fitting / Rietveld**	https://vimeo.com/showcase/9227425/video/832035237#t=36m18s
53:45	**Recall Your Work**	https://vimeo.com/showcase/9227425/video/832035237#t=53m45s

Get Things Done with JADE - Part 3

00:41	**Size & Strain Analysis (XSS)**	https://vimeo.com/showcase/9227425/video/840972852#t=0m41s
26:05	**Pattern Indexing & Cell Refinement**	https://vimeo.com/showcase/9227425/video/840972852#t=26m5s
37:33	**Cluster Analysis**	https://vimeo.com/showcase/9227425/video/840972852#t=37m33s
46:50	**Structure Editing / Viewing**	https://vimeo.com/showcase/9227425/video/840972852#t=46m50s

Using the JADE Toolkit

00:01:28	**Tk01 - MDI SizeStrain**	https://vimeo.com/showcase/9227425/video/670274029#t=1
00:07:20	**Tk02 - Area Detector**	https://vimeo.com/showcase/9227425/video/670274029#t=7
00:15:44	**Tk03 - XRD Digitizer**	https://vimeo.com/showcase/9227425/video/670274029#t=1
00:22:40	**Tk04 - Cluster Analysis**	https://vimeo.com/showcase/9227425/video/670274029#t=2
00:29:49	**Tk05 - Oriented Clays**	https://vimeo.com/showcase/9227425/video/670274029#t=2
00:41:45	**Tk06 - Full Pattern Matching**	https://vimeo.com/showcase/9227425/video/670274029#t=4
00:48:24	**Tk07 - MicroStructure**	https://vimeo.com/showcase/9227425/video/670274029#t=4
00:54:05	**Tk08 - Charge Flipper**	https://vimeo.com/showcase/9227425/video/670274029#t=5
01:00:48	**Tk09 - Solve Structure**	https://vimeo.com/showcase/9227425/video/670274029#t=1
01:06:56	**Tk10 - Structure, Laue-Simulations, ...**	https://vimeo.com/showcase/9227425/video/670274029#t=1
01:12:09	**Tk11 - Regression Analysis**	https://vimeo.com/showcase/9227425/video/670274029#t=1
01:19:34	**Tk12 - 3D Scatter Plot**	https://vimeo.com/showcase/9227425/video/670274029#t=1
01:25:38	**Tk13 - File Explorer Integration**	https://vimeo.com/showcase/9227425/video/670274029#t=1

Phase ID and JADE

03:11	**GUI Layout**	https://vimeo.com/showcase/9227425/video/704685518#t=3
05:07	**1 - Database Setup & Subfile Selection**	https://vimeo.com/showcase/9227425/video/704685518#t=5
12:20	**2 - Phase ID by One-Click Analysis (OCA)**	https://vimeo.com/showcase/9227425/video/704685518#t=1
17:01	**3 - Manual S/M for Major and Minor Phases**	https://vimeo.com/showcase/9227425/video/704685518#t=1
45:11	**4 - Single Peak S/M for missing Minor and Trace Phases**	https://vimeo.com/showcase/9227425/video/704685518#t=4
59:35	**5 - "Déjà-vu" Phase Search**	https://vimeo.com/showcase/9227425/video/704685518#t=5

Batch Processing Using JADE Pro

03:14	**1 - Profile Fitting Analysis**	https://vimeo.com/showcase/9227425/video/940935334#t=3
09:41	**2 - Whole Pattern Fitting (WPF)**	https://vimeo.com/showcase/9227425/video/940935334#t=9
25:32	**3 - One-Click Analysis (S/M + WPF)**	https://vimeo.com/showcase/9227425/video/940935334#t=2
28:52	**4 - Phase ID Only**	https://vimeo.com/showcase/9227425/video/940935334#t=2
30:51	**5 - Line-Based Cell Refinement**	https://vimeo.com/showcase/9227425/video/940935334#t=3
35:43	**6 - RIR Quantitative Analysis**	https://vimeo.com/showcase/9227425/video/940935334#t=3
38:41	**7 - Peak Search Analysis**	https://vimeo.com/showcase/9227425/video/940935334#t=3
39:51	**8 - Peak Painting Analysis**	https://vimeo.com/showcase/9227425/video/940935334#t=3
41:31	**9 - Command Line Runs**	https://vimeo.com/showcase/9227425/video/940935334#t=4
43:28	**10 - Pattern file format conversions**	https://vimeo.com/showcase/9227425/video/940935334#t=4
44:18	**11 - Convert scans to another wavelength**	https://vimeo.com/showcase/9227425/video/940935334#t=4
45:38	**12 - Powder Pattern Simulations**	https://vimeo.com/showcase/9227425/video/940935334#t=4
46:39	**13 - Strip background, Trim Range, Denoise**	https://vimeo.com/showcase/9227425/video/940935334#t=4
51:33	**14 - Area Detector Image Integration**	https://vimeo.com/showcase/9227425/video/940935334#t=5
52:01	**15 - Raman Mineral ID**	https://vimeo.com/showcase/9227425/video/940935334#t=5

RAMAN Search Match

04:17	**PDF-5+ Raman Search**	https://vimeo.com/showcase/9227425/video/1024061714#t=4m17s
06:50	**Introduction & Overview Slides**	https://vimeo.com/showcase/9227425/video/1024061714#t=6m50s
13:21	**Live Demo**	https://vimeo.com/showcase/9227425/video/1024061714#t=13m21s
22:48	**Cluster Analysis**	https://vimeo.com/showcase/9227425/video/1024061714#t=22m48s
26:37	**Importing other databases**	https://vimeo.com/showcase/9227425/video/1024061714#t=26m37s
34:58	**Batch Search**	https://vimeo.com/showcase/9227425/video/1024061714#t=34m58s

Phase Identification with JADE

03:24	**Database Setup**	https://vimeo.com/showcase/9227425/video/543288161#t=3m24s
10:36	**PDF Retrieval**	https://vimeo.com/showcase/9227425/video/543288161#t=10m36s
14:24	**Custom Database**	https://vimeo.com/showcase/9227425/video/543288161#t=14m24s
17:58	**Load XRD Data**	https://vimeo.com/showcase/9227425/video/543288161#t=17m58s
23:10	**Phase ID**	https://vimeo.com/showcase/9227425/video/543288161#t=23m10s
32:45	**Counting Statistics**	https://vimeo.com/showcase/9227425/video/543288161#t=32m45s
34:20	**Step Size Issue**	https://vimeo.com/showcase/9227425/video/543288161#t=34m20s
35:35	**Phases-Tab for S/M**	https://vimeo.com/showcase/9227425/video/543288161#t=35m35s
41:54	**Minor & Trace Phases**	https://vimeo.com/showcase/9227425/video/543288161#t=41m54s
48:16	**Oriented Pattern Issue**	https://vimeo.com/showcase/9227425/video/543288161#t=48m16s
50:19	**Solid Solution Search**	https://vimeo.com/showcase/9227425/video/543288161#t=50m19s
52:18	**One-Click Analysis**	https://vimeo.com/showcase/9227425/video/543288161#t=52m18s
56:13	**Q&A**	https://vimeo.com/showcase/9227425/video/543288161#t=56m13s

Quantitative Analysis with JADE

03:43	**Counting Statistics**	https://vimeo.com/showcase/9227425/video/613785191#t=3m43s
08:50	**S/M of 7-Phase Mixture**	https://vimeo.com/showcase/9227425/video/613785191#t=8m50s
10:33	**WPF of 7-Phase Mixture**	https://vimeo.com/showcase/9227425/video/613785191#t=10m33s
19:56	**Structureless Phases**	https://vimeo.com/showcase/9227425/video/613785191#t=19m56s
34:01	**Amorphous Hump Model**	https://vimeo.com/showcase/9227425/video/613785191#t=34m1s
36:44	**Internal Standard**	https://vimeo.com/showcase/9227425/video/613785191#t=36m44s
40:20	**Batch Refinement**	https://vimeo.com/showcase/9227425/video/613785191#t=40m20s
46:22	**Pattern Simulation**	https://vimeo.com/showcase/9227425/video/613785191#t=46m22s
49:10	**Mixture Simulation**	https://vimeo.com/showcase/9227425/video/613785191#t=49m10s
51:33	**Q&A**	https://vimeo.com/showcase/9227425/video/613785191#t=51m33s

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