Introduction to EVA

A Complete Orientation to Features and Functions

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Introduction

- EVA (short for Evaluation) is a program designed to provide the customer a quick and easy way to process data.

- Primary functions include:
  - Determining peak locations and FWHM.
  - Comparing scans against a database (Db) of known compounds and determining the phases which are present.
  - Making a scan with respect to a known standard, typically the ICDD Db file, to determine the lattice parameters and phase composition.
Introduction to EVA 10/21/2007

Layout of EVA (upper portion)

- Toolbox
- Search/Match

- Magnified view of the cursor location

- Set the Y scale to Counts or Counts per Second

- This window shows the entire scan
Layout of EVA
(lower portion)

- Main editing window
- Worksheet tabs
- Position of the cursor (coordinates)
Importing a Scan

1. Select **New Worksheet**
2. Select **Import a scan (.raw file) button**
3. Select a scan with a mouse-click. To import multiple scans, press the [Ctrl] key while clicking
4. Select **Open**

You can also open an existing EVA document
Zooming on a Scan Range

- To un-zoom, double click in this window

- To adjust the maximum intensity for the zoomed range, double click in this window

- To zoom-in on a peak, use the mouse to draw a box over the area of interest
**Stripping $K_{\alpha 2}$**

(Applicable to machines that do not have a monochromator)

1. Select **Toolbox**

2. Highlight the scan

3. Select **Strip KA2**

4. Use the slider to set the correct ratio of $K_{\alpha 2}$ to $K_{\alpha 1}$ (0.5 is the default ratio)

5. Select **Append**

**Append** creates a new scan with the background subtracted

**Replace** applies the background subtraction to the current scan
Determining the FWHM and Position of Peaks Using the Area Function

1. Zoom in on a peak
2. Select the Area tab in the Toolbox
3. Select Multi-Scans
4. Select Create
5. Using the mouse, drag a region over the peak

If you are interested in a single scan, highlight the scan of interest in the Scan tab, then select Area, and then select Create
Determining the FWHM and Position of Peaks Using the Area Function (continued)

6. Lines have been added to the window

7. Use the scrollbar to scroll to the right to view these additional fields:

- **FWHM** - Full Width of the peak at Half Maximum
- **Observed Maximum** - Point with maximum intensity
- **Chord Middle** - Middle of the cord used to determine the FWHM
- **Gravity Center** - Weights the determination of the peak center using the intensity
- **Net Area** – The area under the peak with background subtraction taken into account. Used for IQOQ

Note that **Gravity Center**, **Chord Mid** and **FWHM** are only valid for isolated peaks!
Subtracting the Background
In preparation for doing a Search / Match

1. Highlight the red scan
2. Set the threshold to 0 and move the slider until the red background line fits the background of the data
3. Select **Append**
4. Repeat steps 1-5 with the black scan
Cleaning Up the Worksheet

1. Hide the “non background subtracted” scans by double clicking the checkbox.

2. Highlight the pre-$K_{\alpha 2}$ stripping scan.

3. Set Max to $\frac{1}{4}$ the intensity of the highest peak and Min to 0. Then using the slide translate the scan vertically.

3. Select Y-Scale

4. Check the Add circle

6. Select Replace
Smoothing the Scan
If the scan has an unacceptable amount of noise

1. Highlight the Scan with $K_{\alpha 2}$ subtracted
2. Select Fourier (You could also try Smooth but we have gotten better results with Fourier)
3. Use the slider to set the red line on the right side of the bend
4. Select Replace
Additional Toolbox Functions

- Delete the highlighted scan
- Move the scan up or down in the list
- Various properties of the scan
- Change the color of the scan
- Select which columns to display/hide
Peak Search

1. Ensure that the background subtracted Kα₂ stripped scan is highlighted

2. Select Peak Search

3. Adjust the Threshold and Width until the peak locations are satisfactory

4. Select Make DIF or Append to List

Make a DIF is used to create a list of angles and intensities

Append to List is used to label the peaks in a scan
Peak Search - Exporting the DIF
(Used to create custom patterns in a PDF Db)

1. Ensure the DIF is highlighted in the Toolbox: Pattern window

2. Select File > Export > Current DIF Pattern
Peak Search - Append to List

Append to List prints the peak positions on the Graph.

The default setup is to label the peaks with d-spacings.
Changing the Default Peak Label

To change the default labels to **Angle, Intensity**:

1. Select **View > Settings**, then the **Sizes Tab**

2. Change the text box in the Peaks category from `d=%%2` to `%%1, %%3`
Changing the Default Peak Label

3. Highlight the old peaks and select X to delete them.

4. Redo the peak search on the scan tab and select Append to List.
Changing Individual Peak Properties

1. Highlight the peak
2. Select **Properties**
Setting the Database Location

1. Open the **Settings** Palette: Select **View > Settings**…

2. Select the **Database** tab

3. Type a title for the **Master Database** and navigate to the PDF Db (Usually located in C:\ PDF or C:\DPRD)

4. Repeat if the user has a custom user Db
Opening the Search/Match Windows

1. Open the Search/Match window
2. Open the Search Results window
Search/Match Window

- **Criterion:**
  - Favor Simple Patterns - Patterns with the least matching peaks
  - Neutral - Usual Setting; no preference
  - Favor Complex Patterns - Patterns with the most matching peaks

- **Subfiles:** Which subdatabases should be included

- **Quality Marks**
  - Yellow are the most reliable
  - Red indicates the pattern is missing some information
  - Grey are not reliable

- **Experimental/Structural**
  - Experimental: ICDD patterns
  - Structure: Patterns calculated from the structure Db

- **Skip Non Ambient** - Skip patterns where the measurement was not carried out at room temperature / pressure
Search/ Match Window (continued)

- **Chemical Filter** - Click the element to change its color
  - Red = not present
  - Grey = might be present
  - Green = must be present
  - Toggle all will change all of the elements’ colors

- **Scan**
  - The scan which will be searched

- **Eliminate Duplicates**
  - If 2 patterns had the exact same name and line positions, it will eliminate them from the results
Performing a Search/Match

1. Highlight the last scan on the list. This scan had the background subtracted, $K_{\alpha 2}$ stripped, and Fourier smoothing applied.

2. Input the appropriate settings.

3. If a user database is present, check this box.

4. Select Search.
Search / Match Results

- Results are displayed in the **Search Results** window and the **Toolbox: Pattern** window.

- The **Figure of Merit** (FOM) column gives a rough idea of how well the pattern matches. The lower the number, the better the match.

- Highlighting a pattern shows the lines in the scan window.
Displaying the PDF for a Pattern

Select the PDF Database button to view the PDF
Refining Lattice Parameters

1. Navigate to the **Toolbox: Scan** window
2. Check the box next to the original scan so it is not hidden
3. Return to the **Toolbox: Pattern** window
4. Highlight the pattern that fits the scan the best
5. Select the **Properties** button and check the **FPM boxes**
Lattice Parameter Refinement (continued)

6. Select **FPM Model** *(FPM Model is refining a single phase, and FPM Eval. is for quantitatively refining a mixture)*

7. Select the original scan file

8. Select **Fit Param**, and the **Model Parameters** dialog will pop-up

9. In **Model Parameters** make sure none of the **Fixed** boxes are checked and select **OK**
Lattice Parameter Refinement Result

- R/R0 is a measure of the fit, 1 is a perfect R/R0
- Approximate crystal (grain) size
- Refined lattice parameters