DIFFRAC.EVA - What's new in version 4?

Cluster analysis fully integrated into DIFFRAC. EVA brings our basic data evaluation program to the next level and provides deeper understanding and intuitive presentations of large amounts of X-ray data. But not only this is new. Working with EVA is now faster, more flexible and as easy and self-explaining as it has never been before. All users benefit from the new look-and-feel, icons, toolbars and big number of data tree operations through our courtesy and bug-fix upgrade.

User friendliness with a new look and feel

A clean and fresh new appearance of the user interface has been achieved by a new set of larger icons. Additional icons now cover the majority of all commands in EVA. This makes working with EVA more direct and reduces the number of steps through several sub-menus. Sets of icons are color coded and grouped into toolbars, depending on their purpose. There are prefigured toolbars available for all operations related to 1D views, Search/Match, Patterns, Peaks and Areas, Scans, and the create view commands. Furthermore, users may configure customized toolbars that contain just the set of their preferred tools.

Innovation with Integrity

Individual screen layouts and program settings can now directly be saved and loaded. New commands were added to the tools menu for starting the utility programs AbsorbDX, FileExchange and the DSRD database compiler.

New in Search/Match

Element and database filters may be predefined or loaded in the Settings node of the data tree. To make Search/Match more powerful a number of pre-defined element filters is delivered with version 4. Pre-compiled filters may be saved to the computer hard disk. This makes search faster. A "Search by name" command was added to the scan objects. Selected candidates now show a colored background in the Search/Match dialog. Patterns that are displayed while the Search/Match dialog is open have a new "Minimum auto-scale value". This helps visualizing minor and trace phases in the process of matching potential search results in case a semi-quantitative phase analysis is not required.

Other new features that assist in Search/Match include to grey out all but the current scan or pattern, and the direct graphical representation of pattern related peak positions on the x-axis. Another new functionality is to color the scan regions in red that are not explained by the Search/Math results.

Enhanced data-tree functionality

Improved productivity and added flexibility has been introduced by new data tree functionality. Tree items such as entire lists or individual list-items for scans, patterns or peaks can be moved, copied and pasted. If one wants, for instance, to quickly compare the phase content between two measurements, simply copy the Search/Match result (a pattern list) to the new measurement. Moving items via mouse drag-and-drop allows changing the order of scans in the graphical view and simultaneously in the related 1D-view legend and tables.

Furthermore the order of list items may not only be rearranged manually but also be sorted by various criteria. Those criteria depend on the data type. Scans can be sorted by their import order, name, database or sample ID, scan type, external variables like temperature or humidity, time of creation and others. Pattern lists can be arranged by the order in which the phases were identified, compound names, pattern numbers, concentration or even membership to majors, minors and traces. The threshold values for these categories are user defined. Lists containing areas or peaks may be sorted by diffraction angle, d-spacing, or intensity, just to name a few. Finally, the visibility of data tree items such as e.g. scans or patterns is easily controlled by the new check boxes in front of the data tree items.
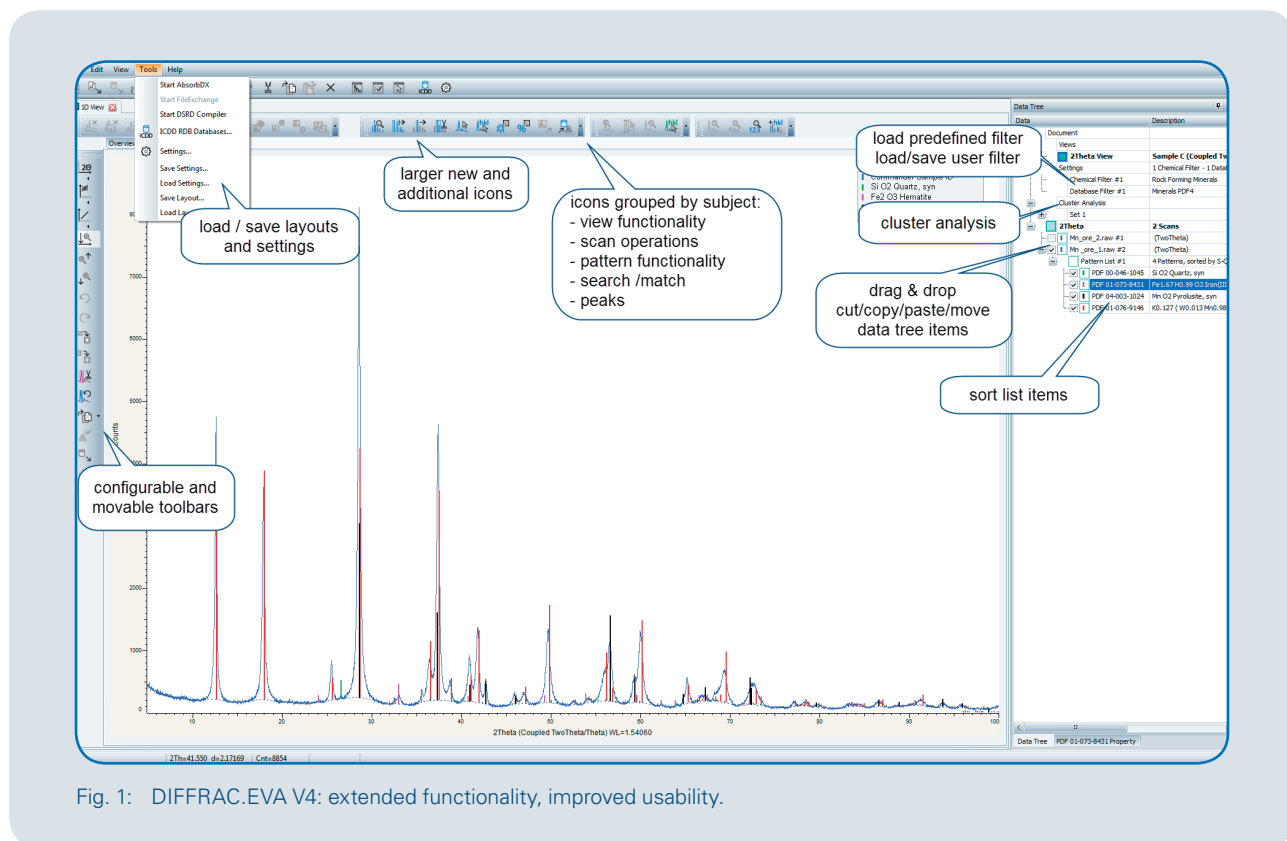

Fig. 1: DIFFRAC.EVA V4: extended functionality, improved usability.

Cluster analysis

High power X-ray sources, fast detectors, automated sample changer, and non-ambient chambers generate more and more data in shorter time in modern powder diffraction. To keep the overview over all those data and to quickly identify the essentials, cluster analysis has been added to EVA. It provides chemometrics, statistics and graphics tools to

- Group and visualize large amounts of data
- Identify phases
- Perform similarity analysis, polymorph and salt screening
- Identify most and least representative members of clusters
- Assist in crystallization experiments
- Look for amorphous phases
- Compare scans to a set of references for phase ID and quantification purposes
- Quality control and pass/fail analysis

The cluster analysis tool in EVA is an adaption of the well-known POLYSNAP software, developed at Glasgow University, with significant upgrades including the use of multiple CPU cores. A nearly unlimited number of patterns (> 10000) can be pre-screened, and the clustering algorithm allows for datasets of up to 2000 patterns with four different data sets to then be analyzed in a single run. The cluster analysis provides highly flexible graphical output to summarize and visualize the results. This highlights any unusual data, and means that time is not

Why is pattern matching useful?

- Identification of known and unknown samples
- Have I seen this sample before?
- Is this sample new or a mixture
- Quantitative analysis – What is in my mixture?
- Quality control – Am I making what I think I'm making?

wasted looking at the many patterns that behave exactly as expected. It can work with or without the provision of reference patterns. Data may be loaded from the file system or the internal experiment database.

In cluster analysis a full pattern matching is performed, that is based on a statistical comparison of each measured data point in each scan. This approach takes full advantage of all scan information including the presence or absence of peaks, peak shoulders, background regions and more. Consequently, it provides for the most reliable and accurate results possible, even for poor data quality, as it minimizes effects due to e.g. preferred orientation or crystallite statistics. Cluster analysis is used in the pharmaceutical, cement, minerals and semiconductor industries for research, development and production control.
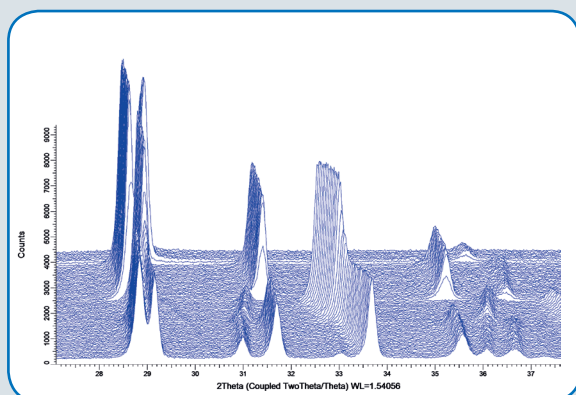
Example views

Fig. 2: Waterfall plot of ammonium nitrate showing peak shift and splitting related to a series of temperature induced phase transformations (data courtesy Fraunhofer Institute Pfinztal, Germany).
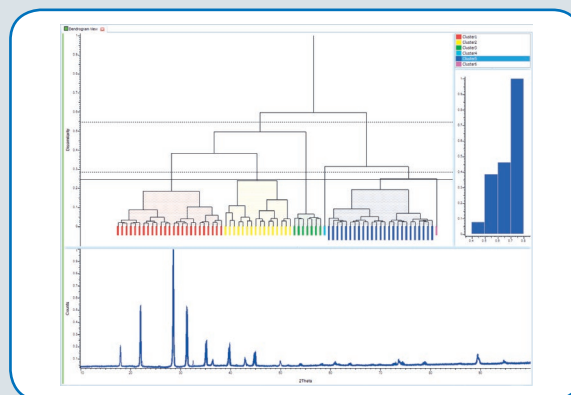

Fig. 3: A typical dendrogram view of the data shown in Fig. 2, also showing the silhouette view of a selected cluster and a scan graphics showing all selected scans.
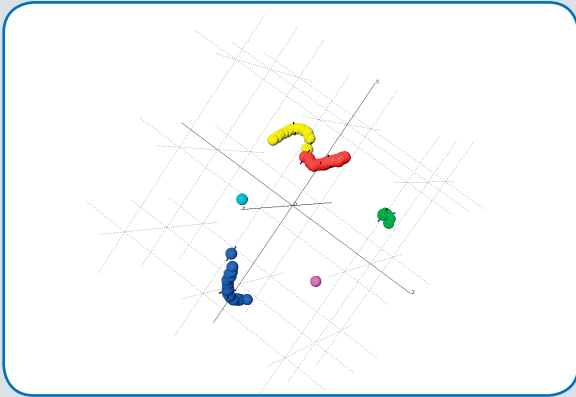
Fig. 4: MMDS (metric multi-dimensional scaling) chart, showing a 3-dimensional representation of the data from Fig. 2. Each dot represents one measurement, colors correspond to the clusters, determined in the Dendrogram (Fig. 3).

Fig. 5: Cell view, presenting the different phases identified during the clustering process and samples showing coexisting phases.
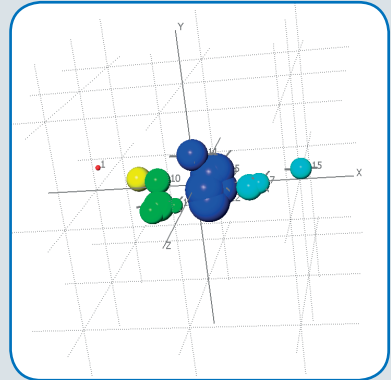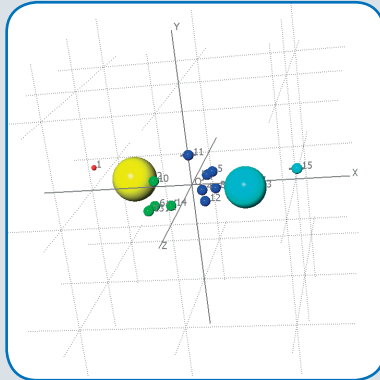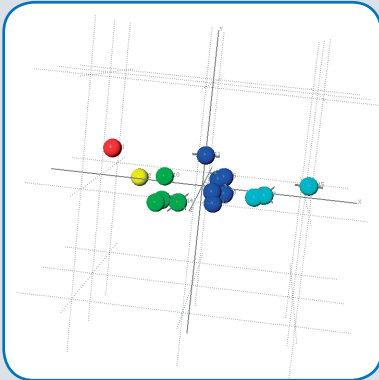

Fig. 6: Panel (a) shows the 3-dimensional MMDS view of some iron ore samples from Brazil. Up to 6 dimensions may be visualized with the 6D view. It may be used to visualize additional information, e.g. low concentrations of Ca (b) but high concentrations of Ti (c) in the blue cluster.

For a full feature list please refer to www.bruker.com/eva-features.

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