Malvern Panalytical
a spectris company

New advanced 2D analysis tools in the XRD2DScan software

Crystallite size determination, orientation analysis and much more...

XRD2DScan

2D X-ray diffraction is one of the most appealing techniques for users who are interested in extracting every bit of information about their samples such as anisotropic features in polymers or crystallite size of polycrystalline samples. The software XRD2DScan[1] from Malvern Panalytical is the most comprehensive solution in the market for displaying, processing and analysis of 2D X-ray diffraction data. This software can be easily and intuitively handled by novice and more advanced users, alike.

2D Data visualization

In addition to data collected with 2D detectors it is possible open and visualize other data types, such as 2-axis measurements, reciprocal space maps, repeated and wobbled scans, frame-based 1D measurements, X-Y maps and CT slices etc. Also, users can easily compare two 2D data files measured in the same conditions.

2D Data processing

The processing of 2D data and the integration to 1D scans are important steps for accurate and reliable results. Flat field correction, masking, background subtraction are examples of 2D data processing. They can also be saved in a project file for later use.

Three different modes are available for integration of 2D data into 1D data:

- 2Theta scan
- Gamma scan
- Line scan

2D Data processing analysis

- New functionality in version 7.0.
- Crystallite size analysis
- Orientation analysis
- Automatic data processing using scripts
- Export and further analysis of the 1D data

Applications of the XRD2DScan software:

Crystallite size analysis

A spotty diffraction pattern can be used to analyze the average crystallite size of a polycrystalline sample. The crystallite size tool can be used in two different ways to extract crystallite size information of a sample:

(1) If samples with the same composition and known crystallite sizes (standards) are available, a calibration method can be used.

(2) If no standards are available, the crystallite size can be estimated based on the geometrical parameters of the experiment, such as beam size and divergence.

- User friendly tool.
- Possible to directly correlate crystallite size with different parameters such as number of spots, spot intensity etc.
- Suitable for crystallite sizes in the range 5-100 microns.

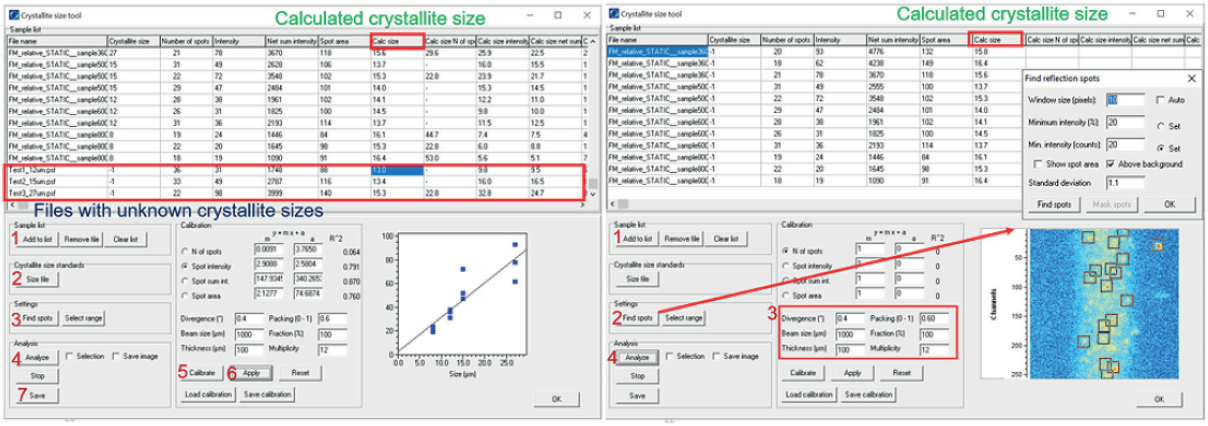

Figure 1. Windows of the Crystallite size tool with the various steps to calculate crystallite sizes using a calibration method (left) or using geometrical parameters (right).

1 This software is developed in cooperation with Prof. Alejandro Rodriguez Navarro, Universidad de Granada, Spain.

Orientation analysis

Information about the orientation of molecular chains in polymers, fibers or liquid crystals can be extracted from the intensity variation in Gamma direction of the diffraction rings in 2D WAXS (wide angle X-ray scattering) data.

- The state of order is easy to calculate and compare for different samples
- Three order parameters (Herman's order parameter S, Orientation index fc and Oriented fraction Rho) are calculated simultaneously from the same 2D dataset.

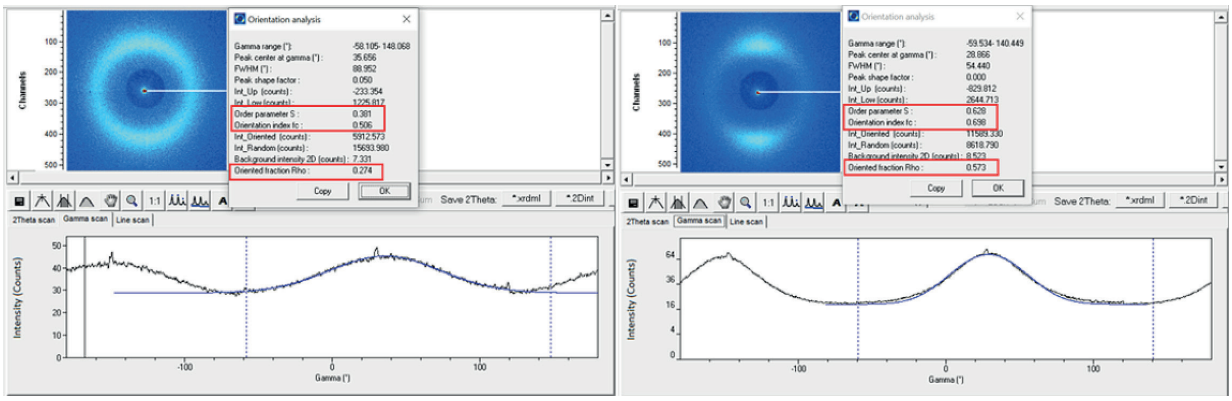

Figure 2 compares 2D WAXS measurements of an LCE (Liquid Crystal Elastomer) sample. In the image on the left, the LCE has lower degree of orientation (0.38), while the right one shows higher degree of orientation (0.63).

Automatic data processing using scripts

In version 7.0 of XRD2DScan it is possible to perform predefined data processing steps by using the new scripting capability.

- Easy and efficient automation of 2D data processing.
- The script can be executed on one data file or all open files

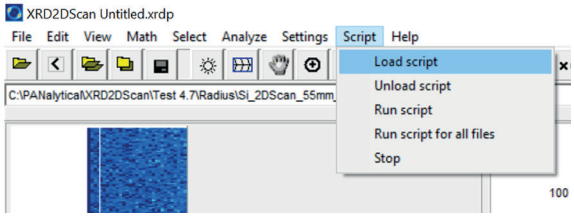

Figure 3. Automatic data processing using scripts.

A typical example of a script is shown below in Figure 4. The scripts consist of a series of commands that are executed sequentially when the script is started. A detailed explanation of the commands is available in the XRD2DSCan help file.

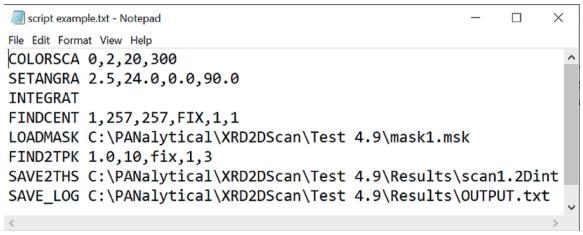

Figure 4. Example script in XRD2DScan.

Export and further analysis of the 1D data

When the processing of 2D data is finished, the extracted 1D scans can be saved or exported for further analysis:

- Save 1D data (*.xrdml, *.2Dint and *.dat) and analyze without user intervention by pressing 1D scan buttons. The same buttons can be configured to transfer the data and start analysis in other programs, like HighScore Plus from Malvern Panalytical.

Figure 5. Save the 1D data in three different formats

Malvern Panalytical
a spectris company

Why choose us?

When you make the invisible visible, the impossible is possible.

Our analytical systems and services help our customers to create a better world. Through chemical, physical and structural analysis of materials, they improve everything from the energies that power us and the materials we build with, to the medicines that cure us and the foods we enjoy.

We partner with many of the world's biggest companies, universities and research organizations. They value us not only for the power of our solutions, but also for the depth of our expertise, collaboration and integrity.

With over 2200 employees, we serve the world, and we are part of Spectris plc, the world-leading precision measurements group.

Malvern Panalytical. We're BIG on small™

Service & Support

Malvern Panalytical provides the global training, service and support you need to continuously drive your analytical processes at the highest level. We help you increase the return on your investment with us, and ensure that as your laboratory and analytical needs grow, we are there to support you.

Our worldwide team of specialists adds value to your business processes by ensuring applications expertise, rapid response and maximum instrument uptime.

- Local and remote support
- Full and flexible range of support agreements
- Compliance and validation support
- Onsite or classroom-based training courses
- e-Learning training courses and web seminars
- Sample and application consultancy

Malvern Panalytical

Grovewood Road, Malvern,
Worcestershire, WR14 1XZ,
United Kingdom

Tel. +44 1684 892456
Fax. +44 1684 892789

Lelyweg 1,
7602 EA Almelo,
The Netherlands

Tel. +31 546 534 444
Fax. +31 546 534 598

www.malvernpanalytical.com