X-RAY DIFFRACTION

DIFFRAC.TEXTURE V4

All-around Texture Analysis Meets Ease-of-Use

Material and component properties are significantly influenced by an inherent or applied preferred orientation, commonly referred to as texture, which can be non-destructively investigated by X-ray diffraction.

DIFFRAC.TEXTURE is a powerful and easy-to-use software suite designed to analyze texture measurements. By utilizing a systematic flow-chart approach, DIFFRAC.TEXTURE delivers comprehensive texture information with just a few clicks of the mouse.

DIFFRAC.TEXTURE features two well established and complementary techniques to provide accurate and reliable results: the model independent Spherical Harmonics Method and the model dependent Component Method.

The Component Method allows direct modelling of a samples unique texture with support for all crystal systems as well as both component and process symmetry.

Main features

- Straightforward creation of pole figures from 0D, 1D and 2D measurements with automatic indexing.
- Spherical Harmonics method for direct computation of the Orientation Distribution Function (ODF).
- Component method for quantitative model-based texture analysis.
- Comprehensive, extensible Material Database
- Powerful texture representation with extensive report generation capability.

DIFFRAC.TEXTURE workflow

DIFFRAC.TEXTURE is a comprehensive software suite for texture analysis of XRD data designed to support the user through the entire workflow. From data processing to texture evaluation and result reporting – DIFFRAC.TEXTURE provides better results in shorter time.

1. Data import and pole figure generation

The generation of pole figures from measured data has never been easier.
DIFFRAC.TEXTURE can import 0D, 1D or 2D data and instantly create pole figures with single click operation either from selected angular regions or directly from 2D frames.

2. Linking texture model and pole figures

DIFFRAC.TEXTURE comes with a comprehensive crystal structure database that allows linking of pole figures to the corresponding hkl reflections with the least little effort. Overlapping signals from different phases can be easily assigned to facilitate data analysis.

3. Pole figure analysis

DIFFRAC.TEXTURE features two complementary and powerful analysis methods that deliver accurate and reliable results:

- The model-independent Spherical Harmonics method directly calculates the Orientation Distribution Function (ODF) from pole figures with a single mouse-click.

- The Component method is a model-based approach that fits a set of texture components to the pole figures using fast and robust least-squares optimization.

With the ODF at hand and the ability to model the process symmetry of texture components, DIFFRAC.TEXTURE provides a self-consistent and comprehensive picture of the texture.

4. Texture representation

DIFFRAC.TEXTURE includes powerful tools and options for a more detailed analysis of the obtained textures:

- ODFs represented in 3D or as a set of 2D sections.

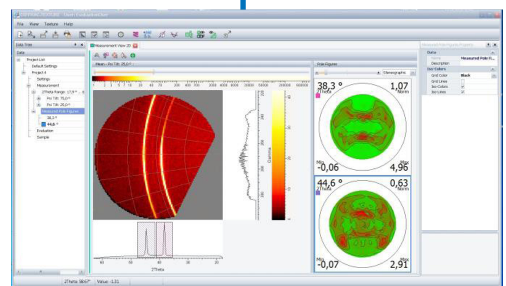
- Calculated pole figures allow visualization of the complete pole figure to better understand the sample's texture.

- Inverse pole figures along the surface normal, in-plane rolling and transverse directions give clues to the origin of a components texture.

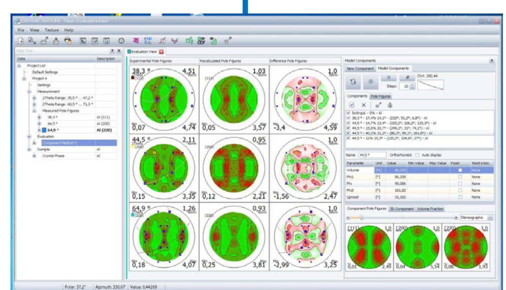
- 3D visualization of the individual texture components to support a better understanding of their orientation.

- Pie-chart representation of the components' volume fractions, including the isotropic content.

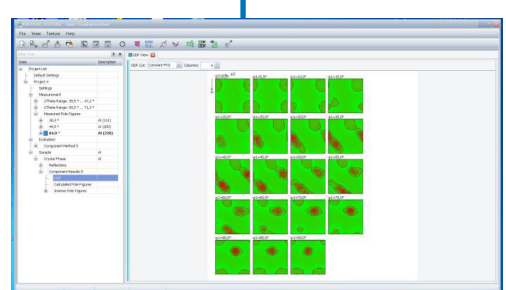
Data import and pole figure generation



Texture analysis of pole figures

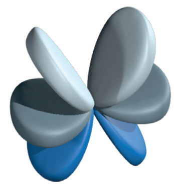


Texture representation via ODF



Reporting

Simple or detailed analysis – DIFFRAC.TEXTURE has the solution



Spherical Harmonics method

The Spherical Harmonics method is a model-free approach and the method of choice if the orientation distribution function is of primary interest. The ODF is directly calculated from a series expansion of the measured pole figures using a set of special functions defined on the surface of a sphere – the generalized spherical harmonics.

The advantage of the method is that it provides texture results in the form of the ODF in a fast and simple way without requiring prior sample knowledge.

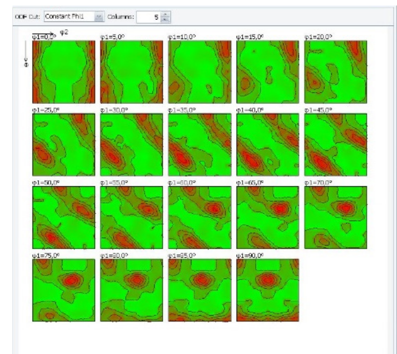
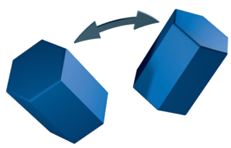


Fig. 1 2D representation of the Orientation Distribution Function obtained with the Spherical Harmonics method.



Component method

The Component method is a model-based approach: The texture is modelled by a set of components that describe the orientation, crystal and process symmetry of a part of the sample [1]. From these texture components the corresponding pole figures are calculated. The parameters of the components are then refined by fitting the simulated pole figures against the measured ones using robust least-squares optimization. Unlike the Spherical Harmonics method which uses mathematical functions to model the texture, the Component method provides a direct connection to the material's physical structure providing a deeper insight into the process symmetry of the sample. Texture components provide a direct link between the manufacturing and processing of the sample and the measured pole figures and overall ODF.

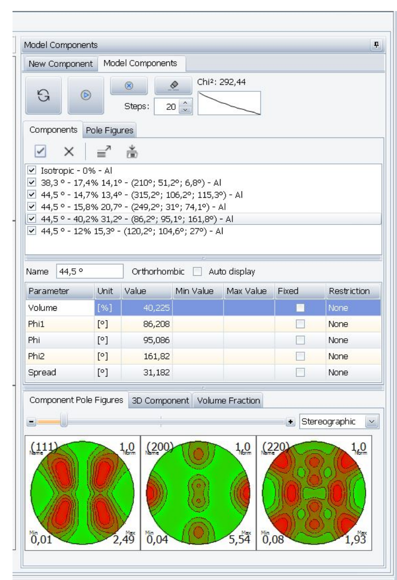


Fig. 2 Texture analysis using the Component method.

No reason to choose, both methods are only a few clicks away!

A typical analysis may begin with a quick fit with Spherical Harmonics to provide insights into the texture. Armed with this information, further fittng using the Component Method yields quantitative results directly connected to the physical structure of the material.

In the case of materials which exhibit broad textures, such as rolled metal sheets, Spherical Harmonics followed by inspection of the inverse pole figures is all that is needed. On the other hand for samples with strong preferred orientations, a full description of the texture can be achieved by using very few texture components. One important field is thin film research where pronounced textures occur. Here the Component method is the preferred analysis technique as it provides the quantitative direction and degree of orientaiton of both

[1] Helming, K. und T. Eschner: A new approach to texture analysis of multiphase materials using a texture component model. Cryst. Res. Technol. 25 (1990), K203-K208.

DIFFRAC.TEXTURE – Anisotrophic Textures with the Ellipse

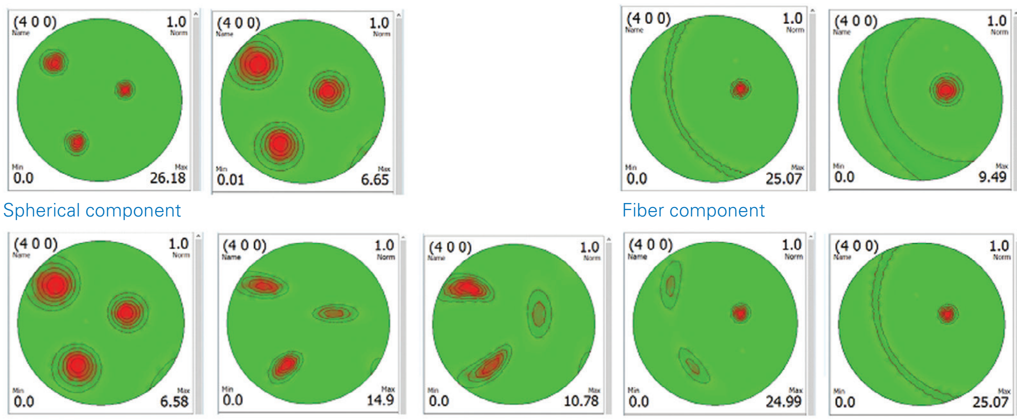


Fig. 3 Pole figures of the differents texture components: The Spherical component has an isotropic spread and the fiber texture allows only a sread of the fiber axis. The newly implmented Elipse component provides much more flexibility in the modelling of textures.

Ellipse component — Bridging the gap

The Ellipse component bridges the gap between the spherical component (isotropic orientaton spread) and the fiber component (fiber axis with orientation spread) .

The ellipse's additional degrees of freedom (shape & orientation) allow the description of anisotropic textures that have been difficult to model up to now.

Maximimun flexibility

An ellipse component is defined by:

- preferred Orientation of the component given by the Euler-Bunge Notation: (φ_1, Φ,ϕ_2)
- Orientation of the Ellipsoid relative to the preferred orientation
- Spread (Spread1, Spread 2, Spread 3) of the rotated ellipsoid

Highly anisotrophic textures and preferred orientations typically occur due to mechanical treatment. Ellipse componens not only simplify modelling of these samples by reducing the number of components, but also provide a more direct connection to the process!

Fig. 4 A single ellipse component is sufficient to model the rolling texture of an Aluminum sheet. The texture is highly anisotropic with spreads varying from 10° to 32° .

DIFFRAC.TEXTURE feature list

Data import and pole figure generation

- Import of 0D, 1D and 2D data files
- Pole figures are generated from 1D data or 2D data via a single cursor-selection operation
- Automated pole figure correction of background and defocussing
- Direct import of pole figures (.txt format)

Material database

- Support of amorphous and crystalline materials, including mixed crystals up to quaternary compounds.
- Comprehensive definition of crystal structures via all 230 space groups, lattice parameters and Wyckoff positions of individual atoms or ions.
- Transformation to higher or lower crystal symmetries.
- Calculation of X-ray properties like penetration and information depth, dispersion and absorption.
- Import and export of crystal structures in .cif and .str file format.
- Structure factor calculation for any wavelength.
- Operator Method: calculation of X-ray atomic scattering factors and Debye-Waller coefficients.
- Various tables for the calculation of X-ray scattering factors, e.g. Henke, Brennan Cowan, Sasaki, Cromer Mann.

Auto indexing

- Single-click assignment of pole figures to texture phases
- Coincidences between different phases can be defined to support the texture analysis

Spherical Harmonics method

- Approximation of the Orientation Distribution Function (ODF) by a series expansion of generalized harmonic functions
- ODF from incomplete pole figures
- Harmonics series expansion a maximum rank of 34.
- The actual possible rank depends on the crystal symmetry and number of pole figures to analyze
- Positivity refinement option in addition for determination of the odd C-coefficients (“ghost correction”)
- Available sample symmetries: orthorhombic, monoclinic, fiber and triclinic
- Crystal systems: cubic and hexagonal

Texture result presentation

- Recalculation of pole figures for arbitrary reflections.
- 3D display of the ODF 2D display of slices of the ODF with constant Phi1, Phi or Phi2
- Calculation and display the inverse poles figure along the surface normal, in-plane rolling and transverse directions
- Calculation of Kearns factors

Component Method

- Full support of all crystal systems
- Multiple-phase support combined with multiple components per phase enables flexible and comprehensive texture modelling of the sample
- Texture components can be of fiber, spherical or elliptical type.
- Available process symmetries: triclinic, monoclinic, orthorhombic, trigonal, tetragonal, hexagonal, axial, biaxial
- Definition of coincidences for assignment of pole figures to multi phases.
- Non-linear least-squares fitting of pole figures with refinement of all or individual parameters of the texture components
- Single-click assignment of additional components for further improvement of the texture model
- Refined texture components can be stored to a database for later reuse and are instantly accessible via a drop-down list
- Calculation of the ODF from the texture components
- 3D visualization of the orientation of the individual texture components to support a better understanding of their orientation
- Pie-chart representation of the component content in the pole figures, including the amorphous content

Data exchange and reporting options

- Creation of customizable, high quality analysis reports
- Data exchange options to and from any other Windows application: copy and paste, Windows bitmaps and metafiles.
- Export of pole figures and ODF in .txt format.

Operating system

- Windows 10 (32-bit or 64-bit)

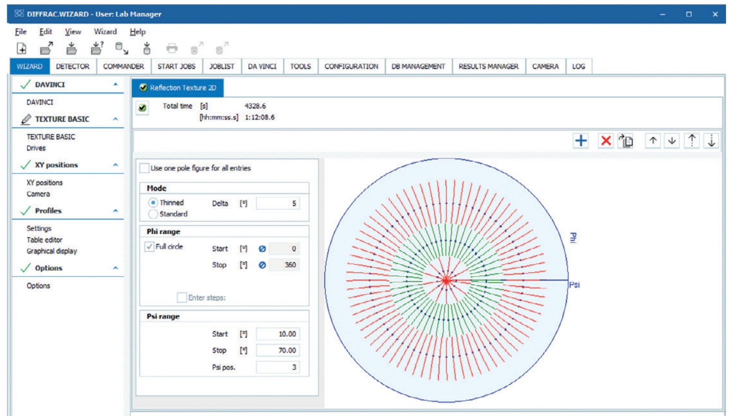
Language support

- English

DIFFRAC.SUITE Workflow for TEXTURE

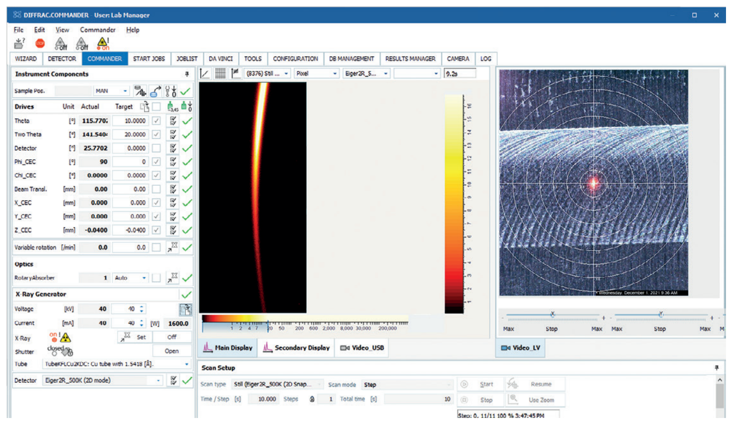
PLAN in DIFFRAC.WIZARD

- Plan pole figure measurements in 0D, 1D or 2D mode.
- Directly launch pre-measurements for measurment time optimization.
- Adjust gamma and phi coverage for minimum measuarement time and maximum efficiency.
- Thinned mode for an equidistant measurement grid on the polefigure.



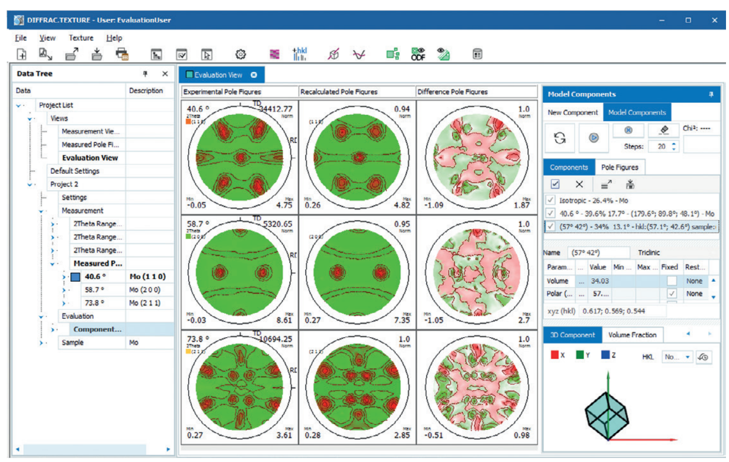
MEASURE in DIFFRAC.COMMANDER

- Direct measurement control or launch predefined experiment methods
- Laser-Video Microscope with Click‘n Go capability for easy sample positioning
- Direct position transfer to DIFFRAC.WIZARD
- Real time display of the current measurement (0D, 1D, 2D)



ANALYZE in DIFFRAC.TEXTURE

- Push-button pole figure generation from 0D, 1D or 2D data.
- Material database and auto indexing for easy and efficient analysis.
- Simple model-free analysis using the Spherical Harmonics Method
- Detailed texture analysis using the Component method to obtain quantitative and process related information.
- Clear, concise report generation



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