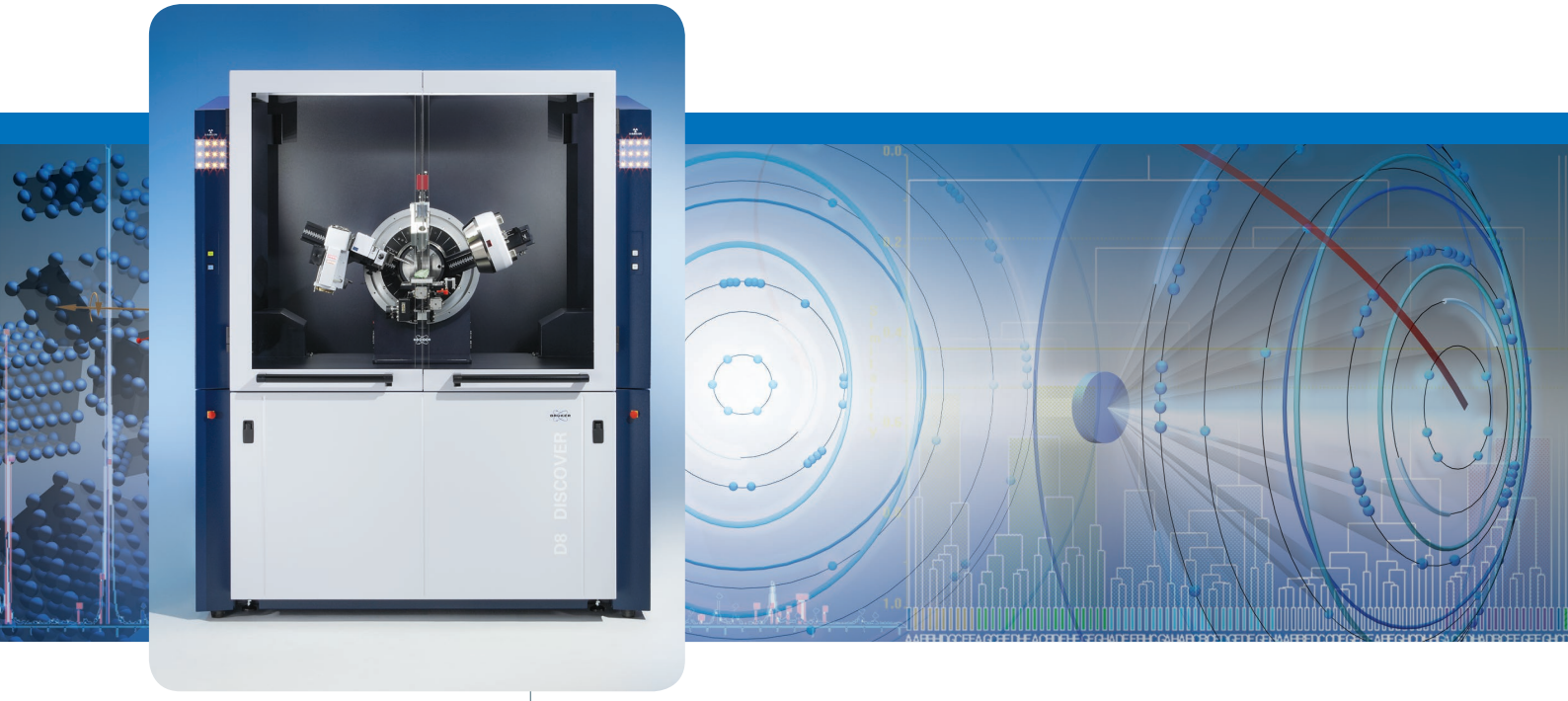
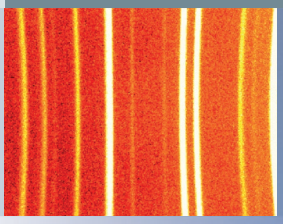
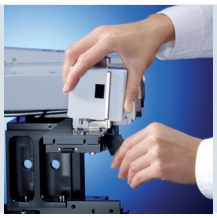
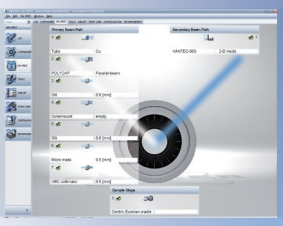
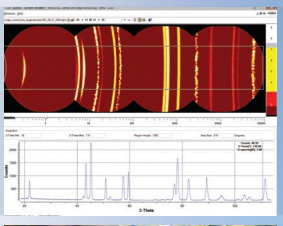
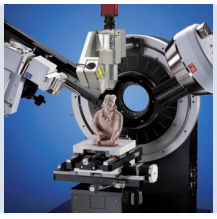
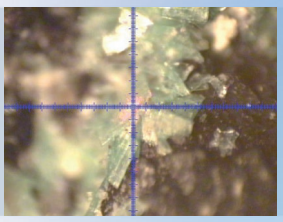
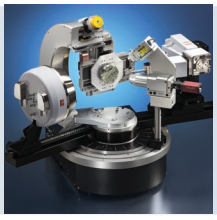
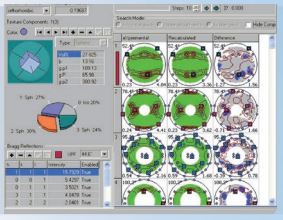
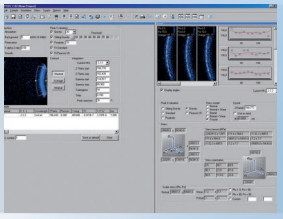
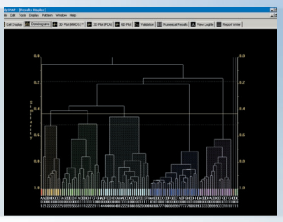
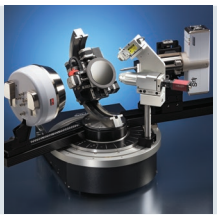
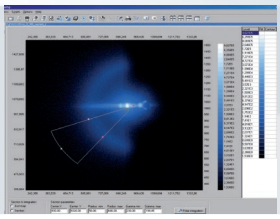


XRD²
Technology Guide

- D8 DISCOVER Diffraction Solutions

	Dedicated hardware components	Integrated software solutions
4 **XRD² –** True musts		
8 **DAVINCI design –** Fully loaded		
10 **Don't miss a single phase –** Phase ID & Quantification		
12 **Get right to the point –** Micro Diffraction		
14 **Focus on the relevant –** Texture		
16 **Under control –** Stress		
18 **Master the flood of samples –** High-Throughput Screening		
20 **Micro – Nano – Å –** Structure Analysis		

XRD² - discover the γ-information

XRD² – X-ray diffraction by means of a 2-dimensional detector – is the method of choice for examining any type of sample in a nondestructive way.

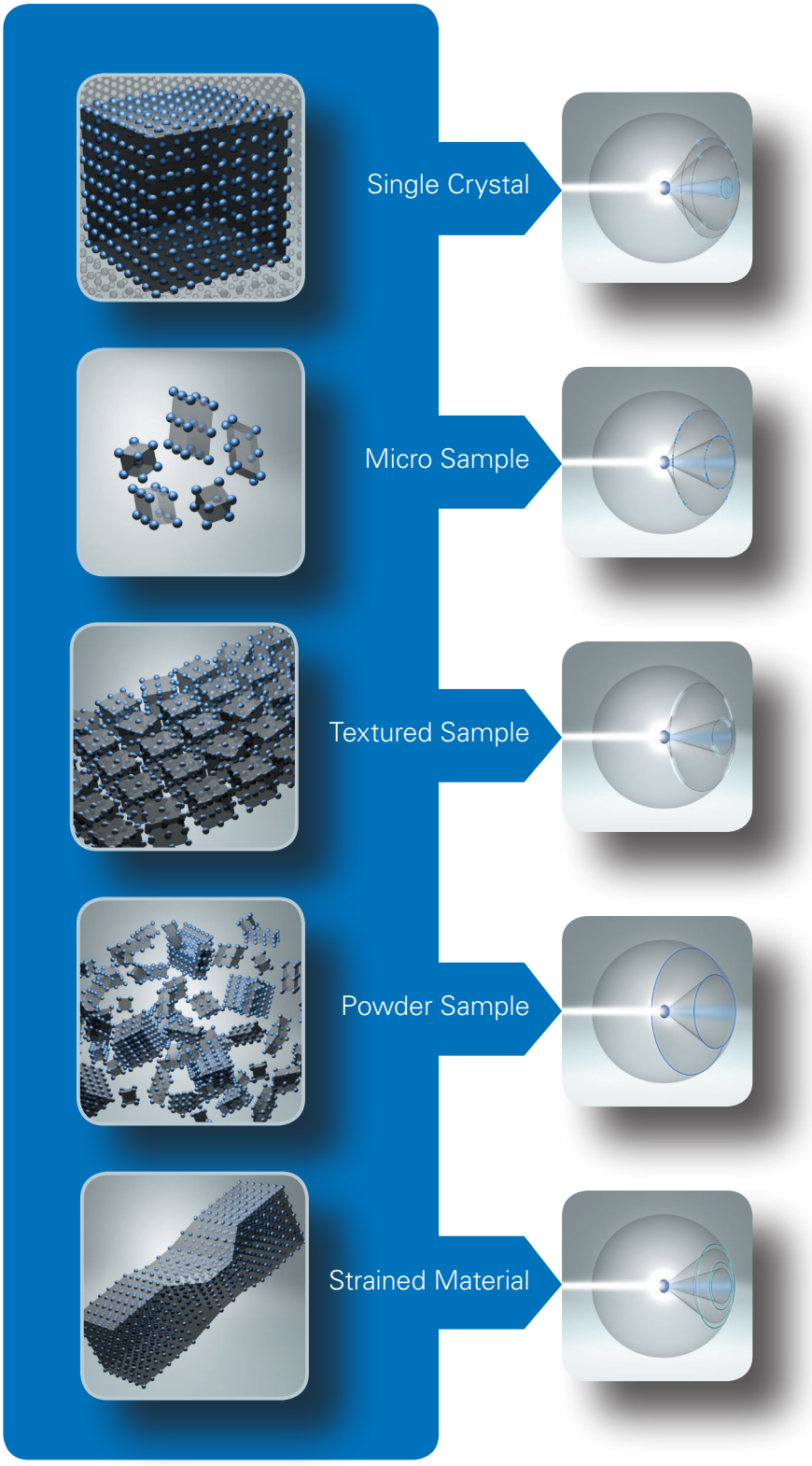
An XRD² pattern covers a large solid angle containing several complete or large portions of Debye rings that describe the diffracted intensity distribution in both 2θ and γ directions. An XRD² pattern therefore contains abundant information about the properties of a crystalline material. Extracting this information is straightforward using our comprehensive XRD² algorithms. Here's how it works:

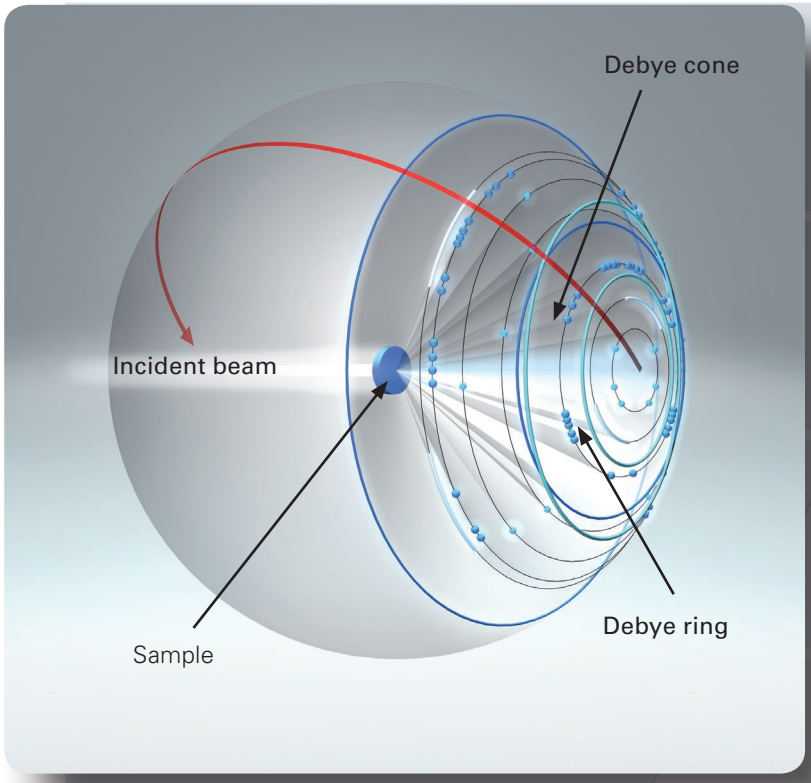
- The sample structure is determined from the position and intensity of the reflections.
- By comparing the pattern with a database of known patterns, the crystalline phases are identified.
- In addition, the respective quantities of those phases are determined.
- Measured intensities are also used to quantify the orientation distribution of the crystallites.
- Last but not least, residual stress and external stresses are determined from shifts in the XRD² pattern.

A major advantage of the XRD² method is its incredible speed. Data collection time can be very short since the simple integration along the Debye cones results in conventional diffractograms with superb statistics. In addition, samples can be measured as they are, avoiding time-consuming sample preparation.

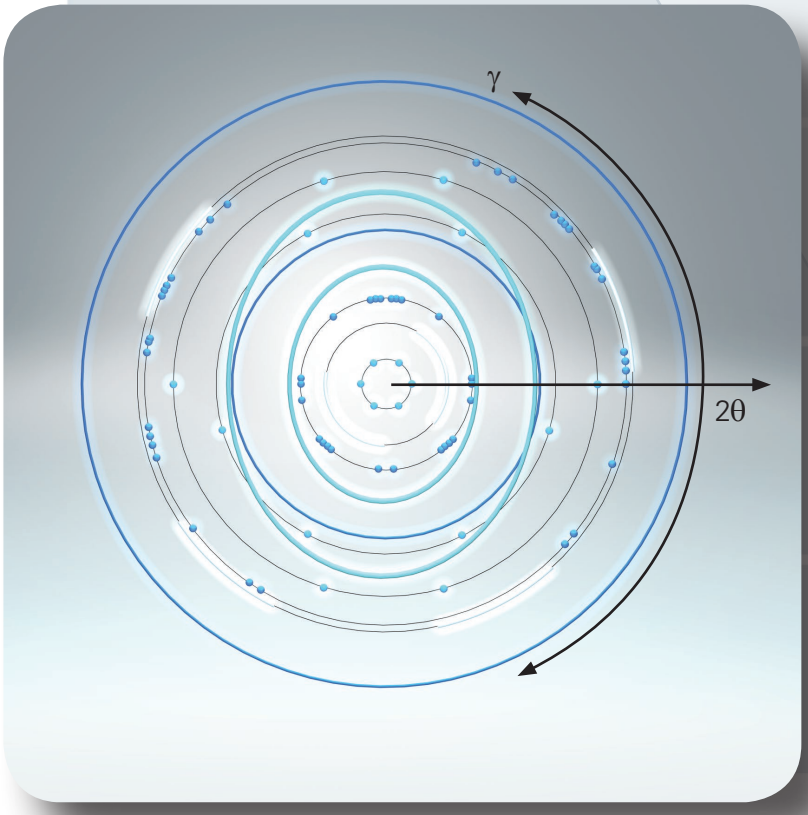
The successful application of the XRD² method requires an intelligent and integrated approach, both on the hardware and software level. The DAVINCI design is the synthesis of all of our know-how and excels with distinctive key features that put it at the top of the class.

D8 DISCOVER - over 30 years of continued excellence in XRD²

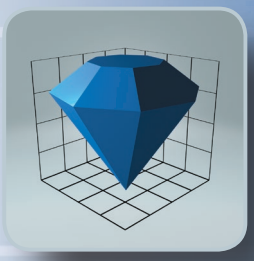




XRD² pattern



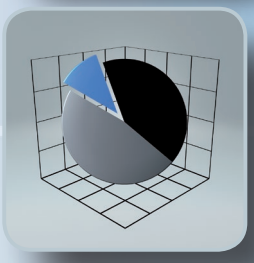
Structural Information



Phase Identification



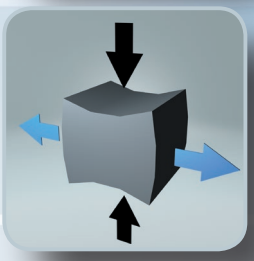
Orientation Quantification



Phase Quantification



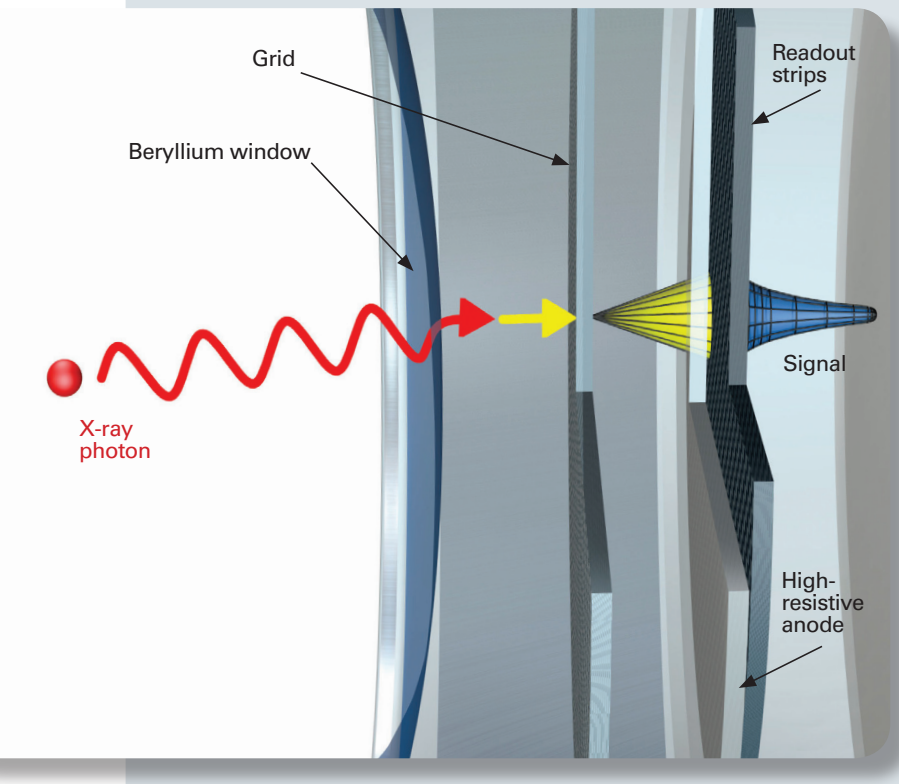
Residual Stress




X-RAYS ON
BRUKER
D8 DISCOVER

The true musts of XRD² – VÅNTEC-500





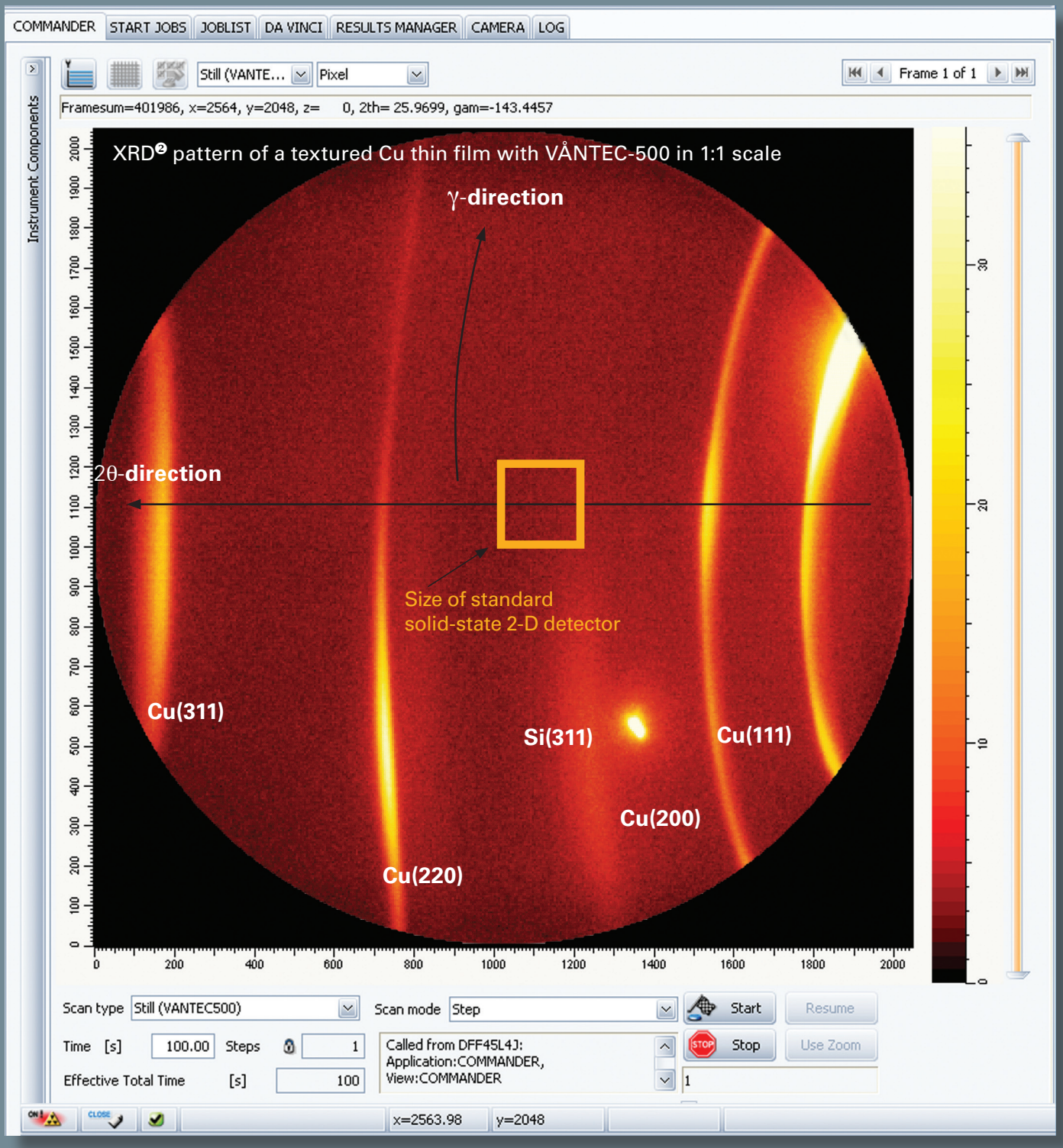
To really benefit from the extra dimension of XRD², you must have the best photon counting 2-D detector. No compromises!

For a 2-D detector, size is the most important feature. A large detector window not only enables increased data collection speed, it also provides information that is simply not accessible with 0-D, 1-D or smaller 2-D detectors. The VÅNTEC-500 detector features a huge 140-mm-diameter window, covering up to about 80° (2θ) and a large γ-range.

This allows you to:

- Simultaneously measure several pole figures with background correction
- Cover broad diffraction peaks of a stressed sample in a single shot
- Enhance the statistics on a spotty diffraction pattern of a micro sample

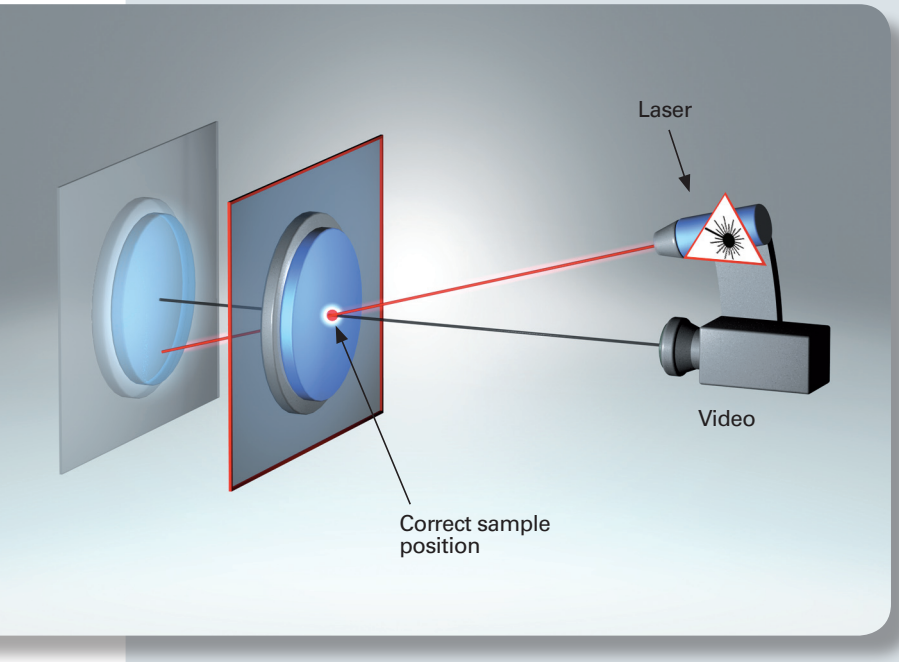
Thanks to Bruker AXS' proprietary MIKROGAP™ technology, the VÅNTEC-500 is capable of collecting 2-D images with both high count rate and excellent resolution. Since it operates virtually noise-free, the detector is highly sensitive to very weak diffraction signals. Its flexible positioning along the track allows for a wide range of sample-to-detector distances to optimize angular coverage and resolution for various applications. The actual distance is actively recognized and used to automatically pick up the required detector settings. The combination of all these technical features already qualifies the VÅNTEC-500 as the best detector for any type of XRD² application. On top of these advantages, like all detectors manufactured by Bruker AXS, you get our unique detector guarantee – no defective detector areas.



- Huge detection area covering more than 15,000 mm²
- Variable detector positioning with real-time distance recognition
- Maintenance-free design
- Guaranteed to have no dead or defective areas

The true musts of XRD² – sources, optics, sampling handling





Before you can start collecting XRD² data from your sample, you need to position the sample and define the region of interest.

With our patented Laser-Video microscope, any type of sample can be accurately aligned and positioned in a simple way without touching its surface. Just zoom in on the region of interest and move your sample to the desired XY-position; control sample height by monitoring the relative positions of the laser spot and microscope crosshair and start your measurement. It is as simple as that.

Our market-leading goniometer guarantees fast and extremely accurate positioning and is combined with our unique Universal Motion Concept (UMC) stages or Eulerian cradles for flexible sample handling. Even big and heavy samples can be accurately positioned and mapped with micrometer precision over a large range.

Various fully integrated and state-of-the-art X-ray sources are available for generating X-rays. We offer our unique TWIST-TUBE for easy switching from line to spot focus, our high-brilliance microfocus X-ray source (IμS™) or our TURBO X-RAY SOURCE for ultimate speed and power.

The IμS with integrated MONTEL optics is particularly suited for boosting intensity on small spots. Because it consumes very little power and uses integrated air-cooling, this unique X-ray source is a real “green” solution compared to other types of high-performance X-ray sources.



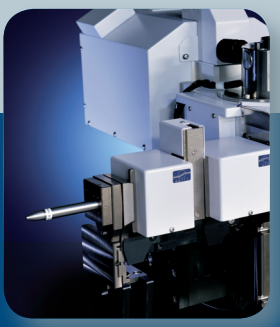
TWIST-TUBE

- Fast and easy switching between line and spot focus
- Compatible with standard sealed tube dimensions
- Patented design
- Automatic focus orientation detection
- No realignment, no need to disconnect cables and hoses
- For Cr, Co and Cu radiation



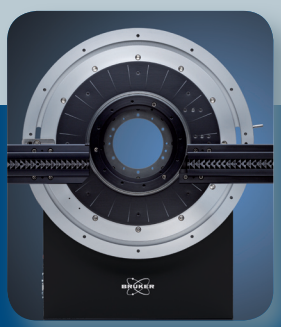
IμS™

- Microfocus X-ray source
- Fully integrated into the D8 platform
- With integrated parallel-beam MONTEL mirror
- Air-cooled
- Maintenance-free
- 3-year warranty
- For Cu radiation, others on request



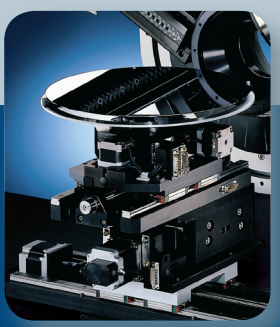
TURBO X-RAY SOURCE

- Rotating anode generator
- From 1.2 to 18 kW, depending on focus size and anode type
- Fully integrated into the D8 platform
- Spot, line and micro focus
- Variable source-to-sample distance
- Unique source alignment with 5 degrees of freedom
- Cr, Co and Cu anodes



High-Precision Goniometer

- Solid, maintenance-free design
- Vertical or horizontal goniometer, Theta/Theta or Theta/2Theta geometry
- Stepper motors with optical encoders
- Fast and reliable positioning
- Dovetail tracks for flexible positioning of components



Flexible Sample Handling

- XYZ stages for large and heavy samples
- Eulerian cradles
- Tilt stages
- Vacuum chucks
- Sample spinners for capillaries and flat powder samples
- Dome-type, non-ambient chambers



Cutting-Edge X-ray Optics

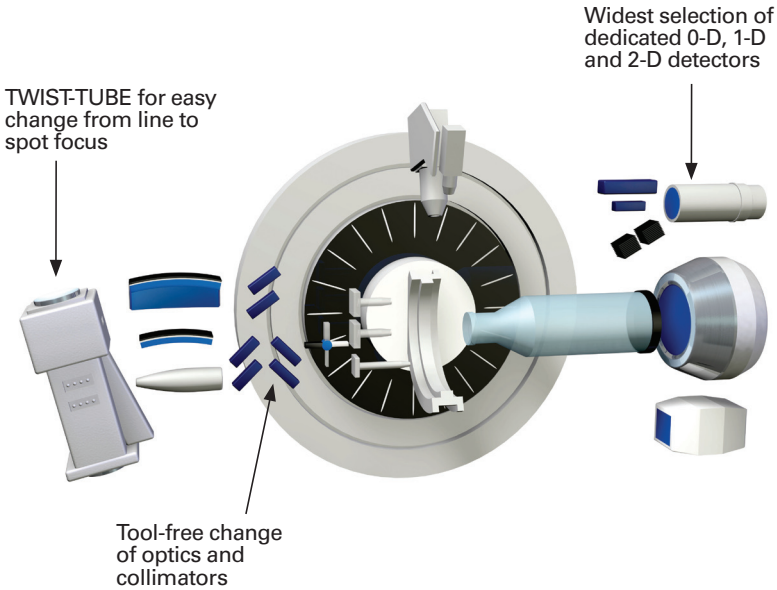
- Göbel mirrors
- MONTEL mirrors
- POLYCAP lenses
- Graphite monochromator
- 2-bounce and 4-bounce channel-cut monochromators
- Universal Beam Concept (UBC) collimators

DAVINCI – XRD² with infinite flexibility



The D8 DISCOVER is a uniquely modular diffractometer, incorporating all parts of the beam path. Easily select the tube focus direction with our patented TWIST-TUBE X-ray source. Snap in the desired X-ray optics to optimize the X-ray beam properties. Mount add-ons like vacuum chucks, sample spinners, capillary spinners or dome heating and cooling stages onto the Eulerian cradle or UMC stage to accommodate any type of sample. Put the VÅNTEC-500 at the required distance, then start measuring.

Need to switch configurations to 0-D or 1-D detectors combined with dedicated secondary optics? No problem. The diffractometer detects the new setup and reconfigures itself. The DAVINCI design eliminates the problems of awkward configuration and adjustments once and for all. It becomes trivial to exchange all components and geometries. This unparalleled adaptability enables the D8 DISCOVER with DAVINCI design to deal with any conceivable application in X-ray diffraction.



Rely on the "Da Vinci trio"!

DAVINCI.MODE
– real-time component recognition

DAVINCI.SNAP-LOCK
– changing components without tools or alignment

DIFFRAC.DAVINCI
– the virtual goniometer

DAVINCI.MODE – real-time component recognition

- Instant component registration with all specific properties
- Fail-safe component positioning
- True plug'n'play
- Automatic detector distance recognition

DAVINCI.SNAP-LOCK – changing components without tools

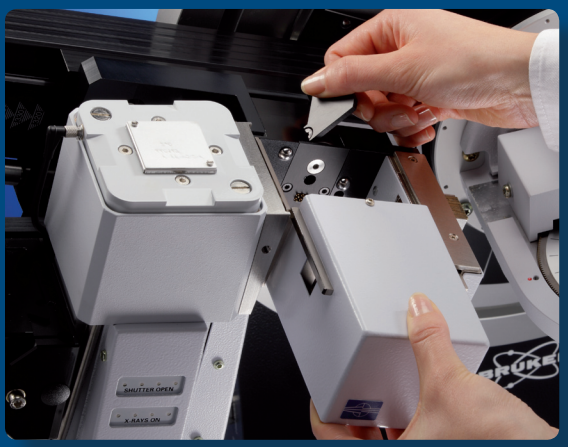
- Fast and easy
- Alignment-free: optics retain their alignment
- Variable positioning on the track

DIFFRAC.DAVINCI – the virtual goniometer

- Real-time component recognition and status display
- Push-button switch between high-resolution and high-flux beam path
- Detection of missing, misplaced or unsuitable components
- Choice between all components configured for the present system
- Parameterization of all fixed and motorized components



TWIST-TUBE



SNAP-LOCK



VÅNTEC-500

XRD² – don't miss a single phase



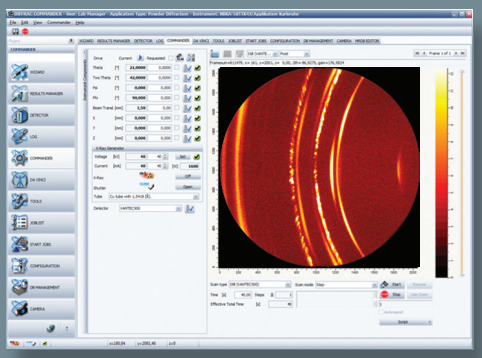


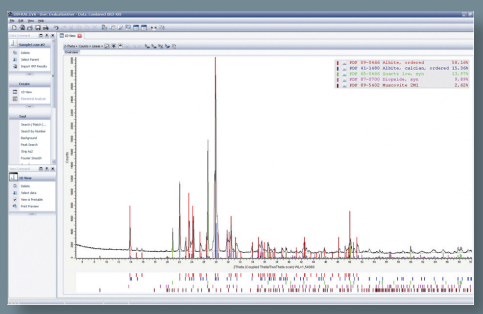
The D8 DISCOVER with XRD² each and every sample can be analyzed. The exceptional strength of XRD² excels at analyzing challenging samples with larger grains or textured materials. Samples like these can be analyzed in real time at dimensions unmatched by other diffractometers.

Preparation is quick and easy: place your sample, zoom in with the Laser-Video microscope and center your sample – nothing else required. Choose a start and end angle, measurement time, and resolution. Then go! The system starts collecting a series of XRD² patterns and displays them in a Debye view. The large size of the VÅNTEC-500 detector ensures that you get sufficient reflections.

Domed sample stages for controlled, non-ambient conditions take full advantage of the VÅNTEC-500 detector because intensities can be collected over a large solid angle. During phase transition studies, you will never miss a single phase.

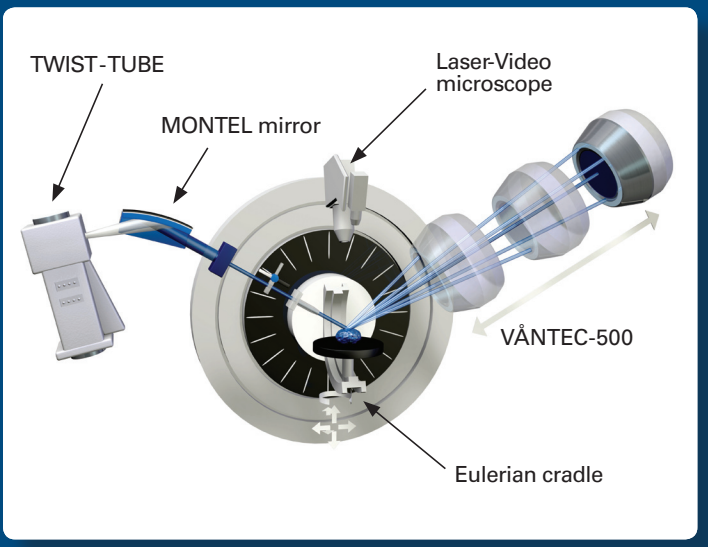
- Non-contact sample alignment with Laser-Video microscope patented
- Control terminal for intuitive sample positioning
- Adjustable detector distance with real-time distance recognition, for optimized angular resolution
- Eulerian cradles and Universal Motion Control (UMC) stages for easy and flexible sample handling
- Dome-type, non-ambient stages covering a temperature range from -180°C to +1400°C



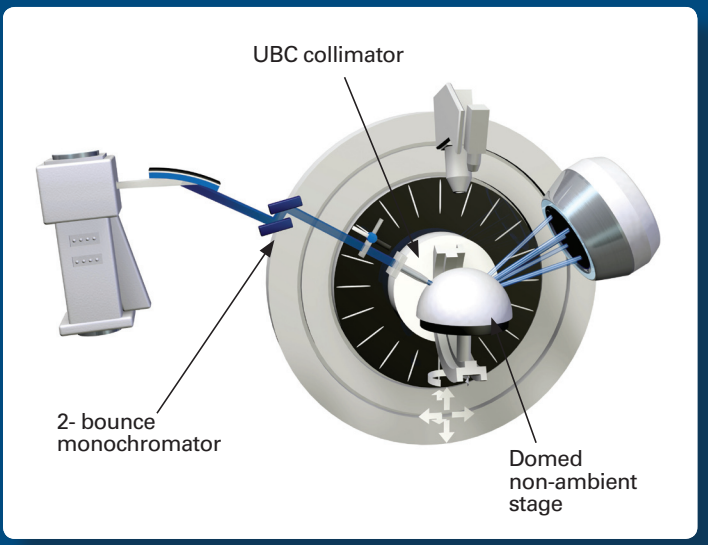


Our DIFFRAC.SUITE software provides the optimum measurement strategy. It proposes the best settings for optimized data collection in different geometries. The Debye view allows you to identify Debye rings with similar properties in terms of spottiness and texture, for example. Only the Debye rings with identical characteristics can belong to the same crystalline phase.

Use our unique SEARCH/MATCH function to identify the crystalline phases by matching the data to the ICDD, COD or your own database. The D8 DISCOVER with XRD² is the ideal choice for fast qualitative and quantitative phase analysis.



- Adjustable detector distance with real-time distance recognition, for optimized angular resolution.



- The high detection speed allows collection of SNAP-SHOTS and creation of full XRD² movies.

XRD² – get right to the point





Patterned wafers, forensic samples, inclusions in geological materials… These very diverse samples all have one thing in common: the area of interest is very tiny.

For these applications, our patented Laser-Video microscope and precise sample stages guarantee that you exactly measure the area of interest–regardless of sample size or shape.

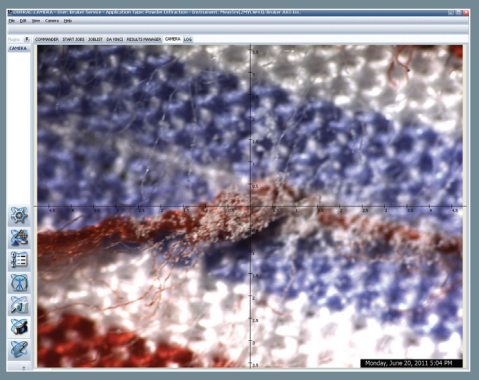
When an X-ray beam is collimated down to a micro-spot size, obviously only a few crystallites are hit by the incident beam and diffract the X-rays. This results in spotty diffraction patterns and in very weak diffraction signals.

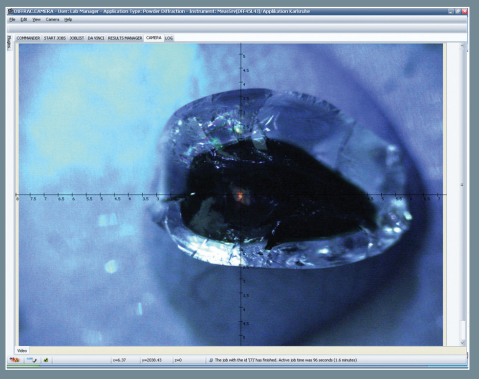
Our VÅNTEC-500 is the 2-D detector of choice to measure such poor-quality diffraction patterns. Its unparalleled signal-to-noise performance and extra-large active area enable detecting even the weakest diffraction signals. The simple integration of a diffraction pattern along the Debye cones converts the measurement into conventional diffractograms for further evaluation.

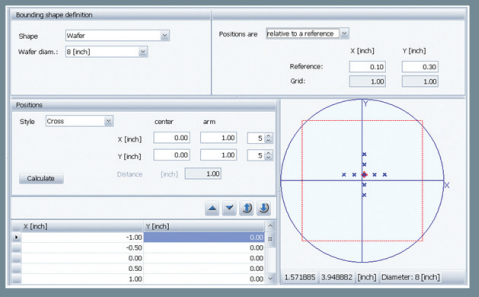
Our VÅNTEC-500 offers superior capabilities compared to conventional 0-D, 1-D and smaller 2-D detectors, while allowing you to perform any data treatment the way you are used to.

To even further boost primary beam intensity on a small area of interest, just use our high-brilliance IμS or TURBO X-RAY SOURCE in combination with dedicated MONTEL optics.

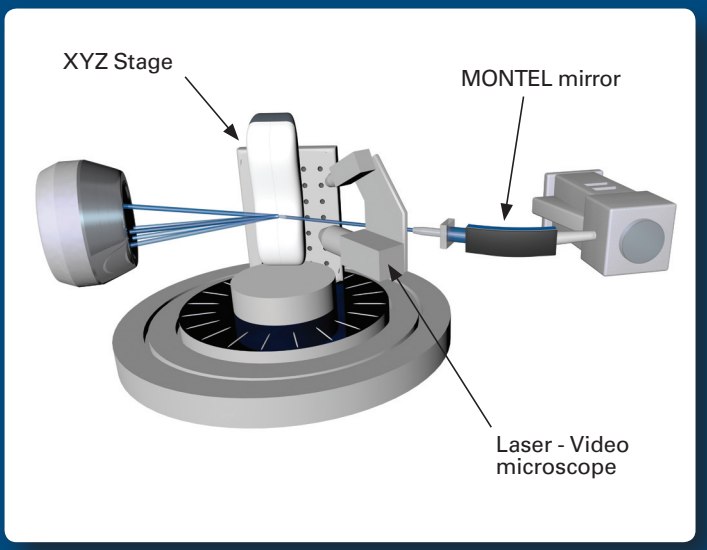
D8 DISCOVER with XRD²
– the only true Micro Diffraction!



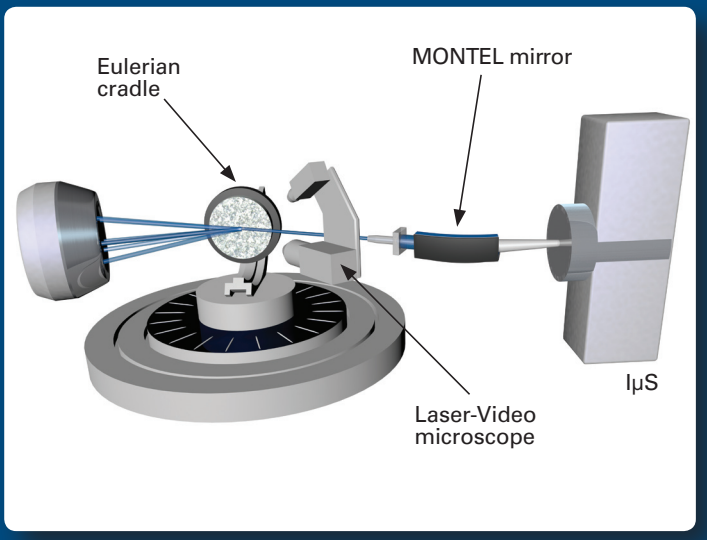




Thanks to the Laser-Video microscope, you can observe your sample right from your computer. Zoom in to define the measurement region. Simply select the spots of interest by clicking the mouse, launch the measurement, and document the measured spot with images.



- Patented Laser-Video microscope for exact sample positioning
- Sample stages with up to 300 mm mapping capability
- Non-destructive trace analysis, e.g. for forensic applications



- IμS X-ray source with MONTEL mirror for high flux on a small spot
- Tool-free, reproducible collimator exchange for ultra-fast beam size optimization

XRD² – focus on the relevant





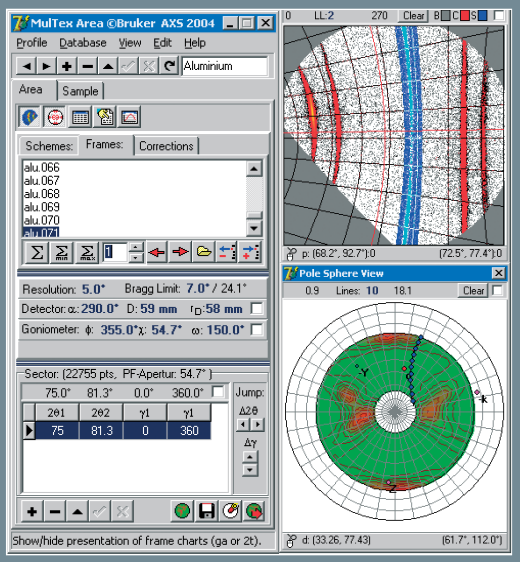
When you are working with metals, superconductors, coatings, fibers, polymers, nanomaterials, thin films, or wires, you know that the texture of your sample is a critical parameter.

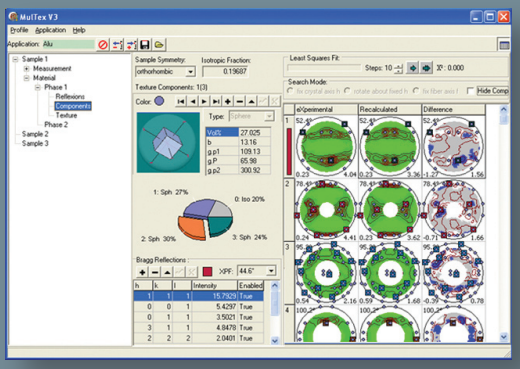
The D8 DISCOVER with XRD² puts you in the best position to solve the complete texture of your sample in a very fast and elegant way.

Our 2-D VÅNTEC-500 detector is the obvious choice for measuring textured samples. Its 140-mm-diameter detector window captures a huge area, covering wide sections of the Debye cones all at once. It can simultaneously collect multiple reflections and complete background, taking full advantage of the XRD² technology. Being a true photon counter guarantees an excellent signal-to-noise ratio due to the virtually absent intrinsic noise.

Our Eulerian cradles enable software-controlled positioning and mapping of large and heavy samples. You can boost the primary intensity, increase speed and statistics with our high-brilliance IμS or TURBO X-RAY SOURCE, combined with dedicated MONTEL optics.

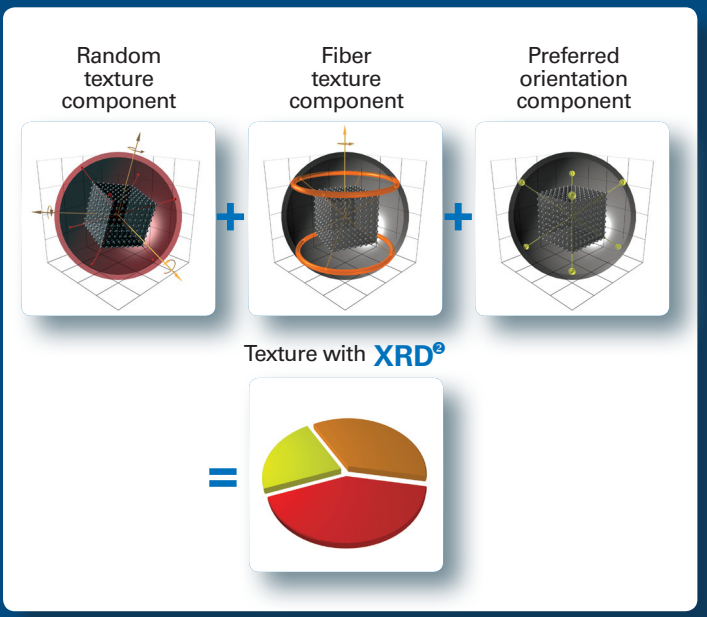
Looking for the right direction – XRD²!



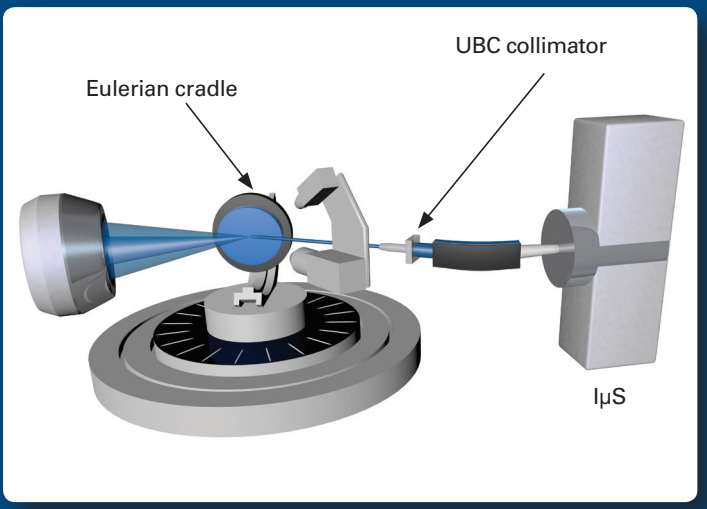


A single VÅNTEC-500 frame already contains plenty of qualitative texture information.

A comprehensive texture analysis can be done in a straightforward way with our unique DIFFRAC.MULTEX software, which supports you in all steps of texture analysis, from optimizing the data-collection strategy through interactive evaluation, to transparent results and the final reporting.

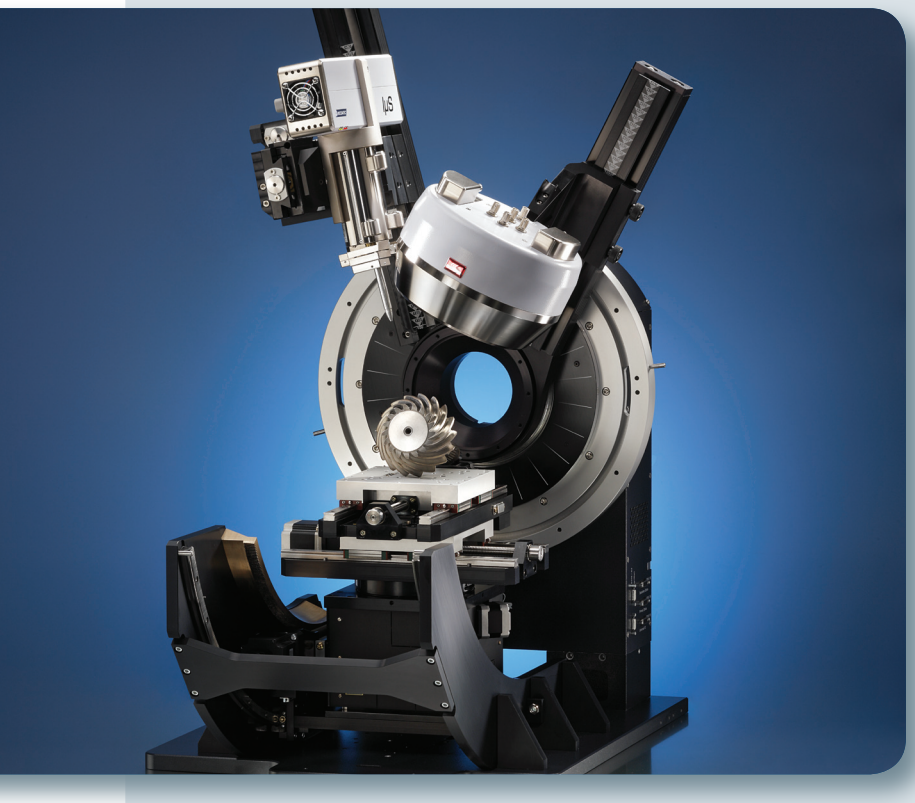


- POLYCAP™ for high-speed data collection, independent of the wavelength
- IμS X-ray source with MONTEL mirror for high flux on a small spot
- Heavy samples up to 3 kg, with full mapping functionality
- Several pole figures at once thanks to the large VÅNTEC-500
- Qualitative texture information from a single frame



XRD² – get stress under control





If residual stress or hardness is an important factor affecting the performance or lifetime of a component, the D8 DISCOVER with XRD² is the laboratory tool to get unambiguous stress analysis results.

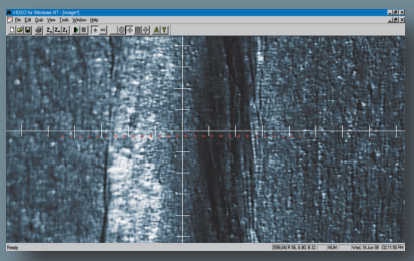
It is the only solution when you have to deal with complex geometries, heavy samples and textured and inhomogeneous materials. Precisely define your measurement location using the unique Laser-Video microscope.

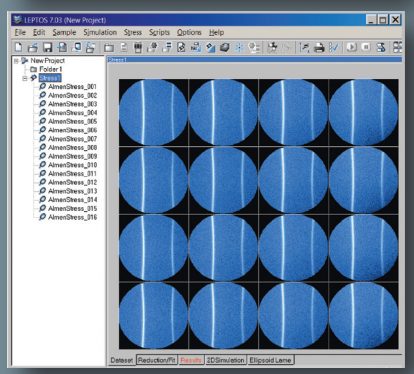
XRD² allows you to analyze the smallest sample features with an X-ray beam collimated down to some 10 microns. With these small beams you can generate 1-D or 2-D stress maps using the high-precision motorized XYZ stages.

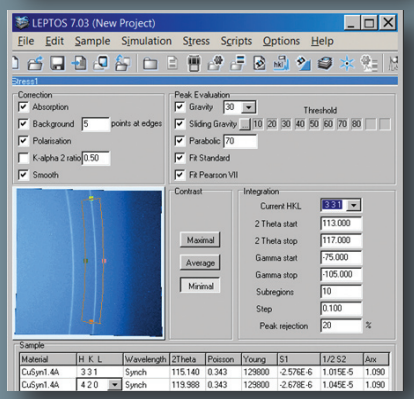
Our 2-D VÅNTEC-500 detector is the obvious choice for stress applications. Its large detector window captures broad residual stress peaks in a single frame.

- Stress measurements in iso-inclination (omega) or side-inclination (psi) mode
- Up to 50 kg of sample load
- Small spot analysis on complex parts such as inhomogeneous or curved samples
- Optimum data quality with the optimum wavelength: Cu, Co, Fe or Cr
- Retained austenite determination

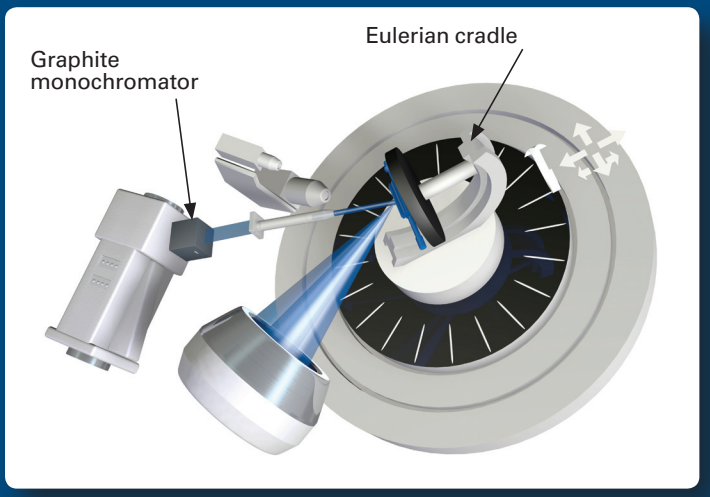
XRD² – the most advanced solution for stress control!



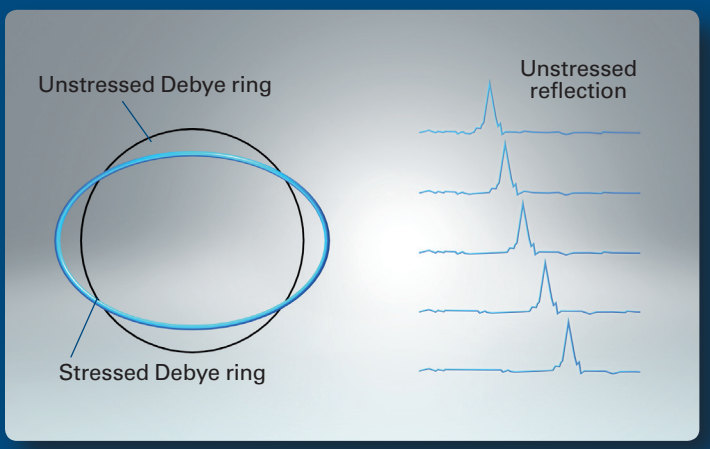


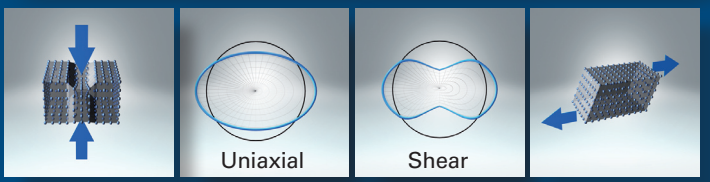


With the XRD² method you directly measure stress-induced deformation of single or multiple Debye cones. This improves the sampling statistics and data quality because you are simultaneously collecting a large number of measurement points from multiple inclination angles. The unreliable data points due to large grain size or texture can be automatically eliminated from the stress evaluation. Therefore, the XRD² method can obtain more accurate stress values, especially for samples with large grains or texture. With DIFFRAC.LEPTOS, measuring a stress component, stress tensor and principal stresses is a straightforward and intuitive operation.



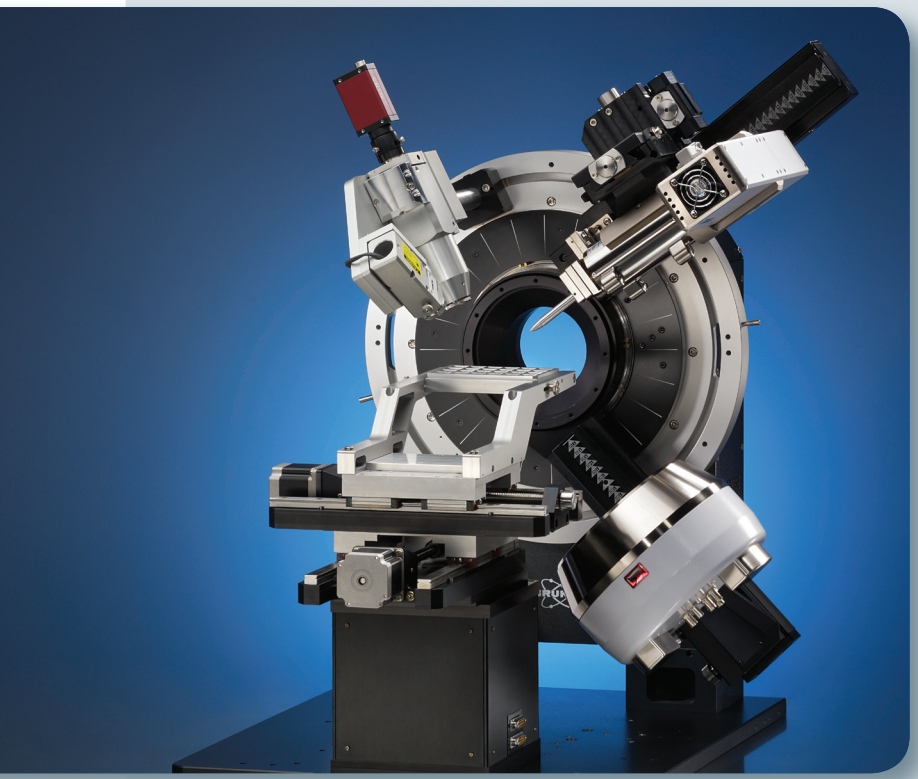
- Extended XRD² method for stress evaluation of 2-D data
- Multi *hkl* evaluation method, reducing the effects of anisotropy and texture
- From normal and shear stress up to the complete stress tensor





Master the flood of samples – XRD²





High-throughput screening systems can probe hundreds of samples rapidly and nondestructively.

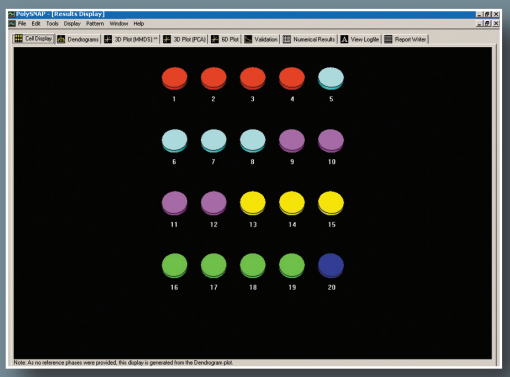
High-precision sample positioning, automated data acquisition, handling, and evaluation are indispensable. XRD² has the capability to simultaneously and unambiguously determine sample properties such as phase composition, polymorphism, structure, percent crystallinity, particle size, texture, and residual stress.

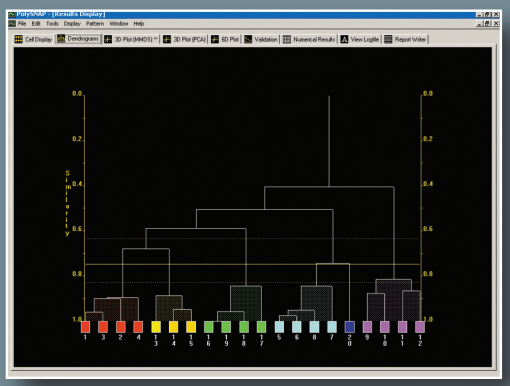
The D8 DISCOVER with XRD² is the unique solution for high-throughput screening in terms of speed, sensitivity, and data quality.

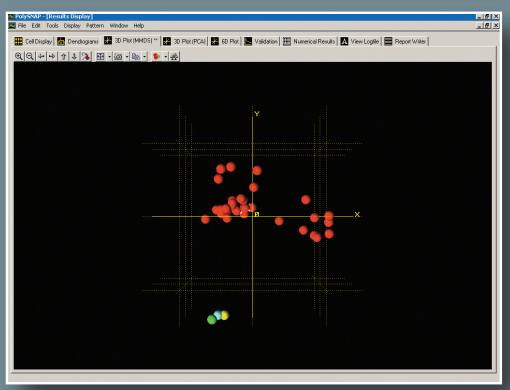
The D8 DISCOVER can also be integrated into large workflows and plays in concert with other analytical methods. Rapid screening with the D8 DISCOVER with XRD² is the optimum solution to master your high-throughput needs.

- Reflection and transmission geometry with the same setup
- Vertical Theta-Theta configuration for horizontal sample loading
- Large scan range up to 150 mm x 150 mm in X and Y
- Boost intensity with the IμS and MONTEL optics
- Patented Laser-Video microscope for exact sample positioning

XRD² – the optimum solution to master your high-throughput needs!

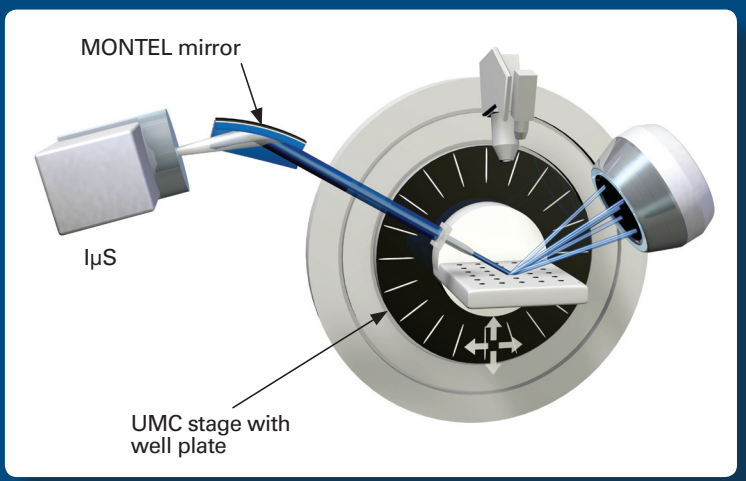


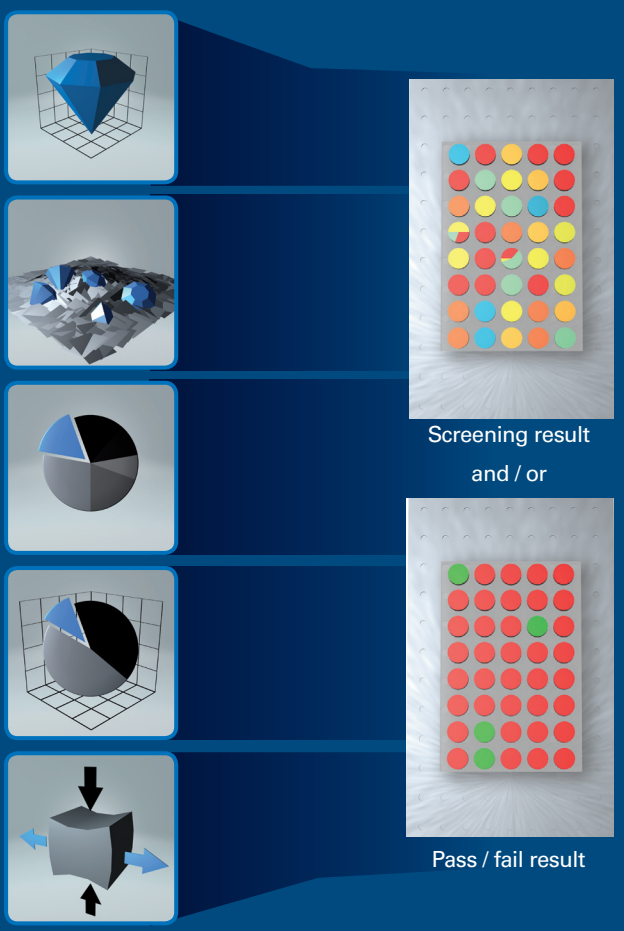




DIFFRAC.POLYSNAP is a powerful cluster analysis tool with clean, elegant and informative graphic displays. It allows for high-throughput analysis of any kind of numeric data, and makes getting a handle on your dataset – large or small – a breeze .

For quality control, samples can be automatically flagged based on a given pass/fail criterion.





Micro – Nano – Å – pick your scale with XRD²



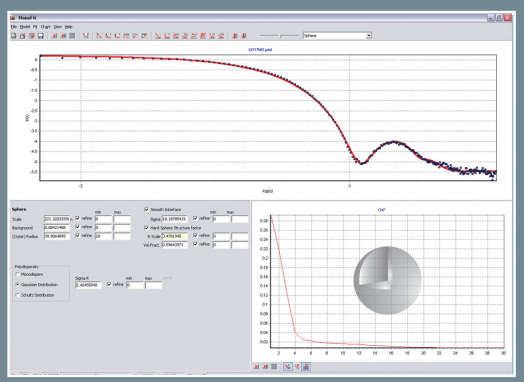


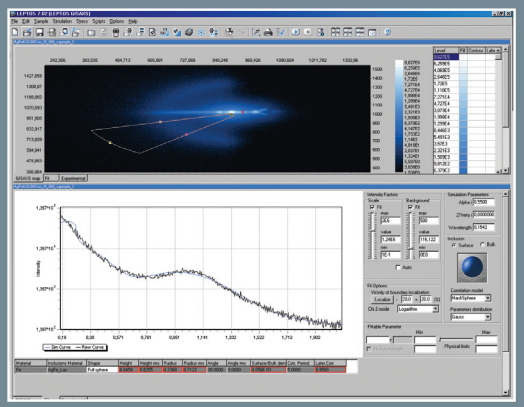
Modern materials research and nanotechnology rely on structural investigations to design and optimize new materials. The detailed knowledge of structural properties allows you to understand and predict electrical, optical, and mechanical properties that affect the material performance.

XRD² provides a broad and comprehensive picture of structural aspects from atomic positions to particle sizes, from epitaxial relationships to particle shapes. It covers the whole range of length scales: large-scale features that result in Small Angle X-ray Scattering (SAXS) signals, up to arrangement of individual atoms in a single crystal that result in Bragg diffraction signals. Consequently, the D8 DISCOVER with XRD² can characterize structures in the nano-range, molecular structures in single crystals, and heterostructures in thin films.

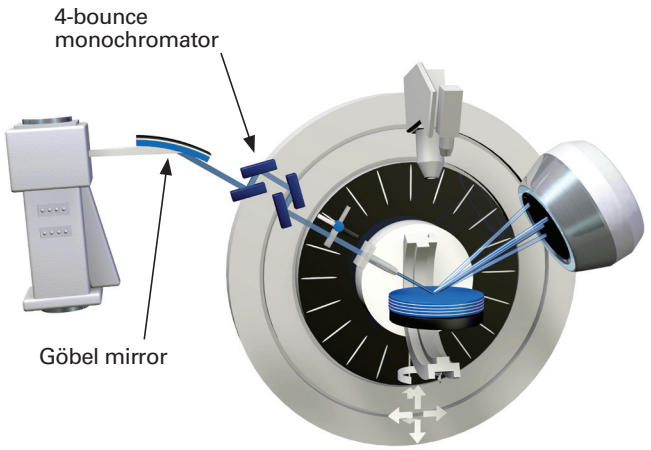
Due to the unique combination of large angular coverage with extremely low background and single-photon detection, the VÅNTEC-500 detector enables collection of 2-D SAXS patterns from anisotropic samples in real time. In GISAXS mode, the detector covers a wide range in the out-of-plane direction and probes the nanostructure of a layered sample in a single shot. Maps of large reciprocal space sections can be acquired in a very short time due to the high spatial resolution and the large active area of the detector.

XRD² analyzes every structural aspect of your sample - pick your scale with the D8 DISCOVER!

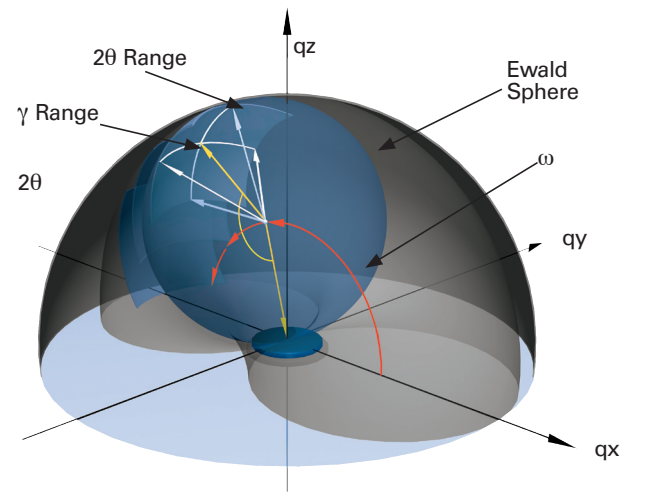




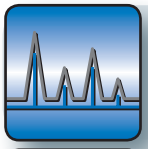
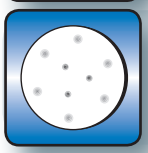
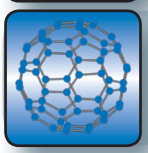
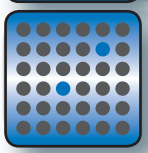
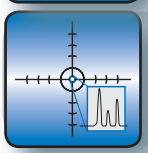
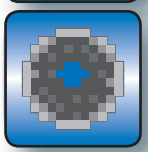
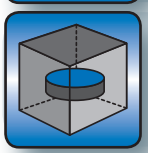
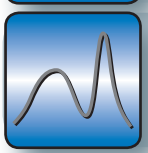
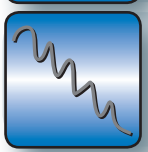
DIFFRAC.SUITE provides all the tools to map the nanoworld. With DIFFRAC.NANOFIT, nanoparticles can be modeled by means of geometrical shapes or by dedicated polymer models, whereas DIFFRAC.LEPTOS provides a sound physical basis for the comprehensive evaluation of 2-D GISAXS data.



- Variety of 2-bounce and 4-bounce channel-cut monochromators for HRXRD
- Helium beam path to reduce air scattering in SAXS measurements
- Boost intensity for SAXS measurements with IμS and MONTEL mirror



Applications

Applications	Task	Measurement
 **Phase Identification**	Crystalline phase identification	Measure intensity distribution of XRD² pattern
 **Phase Quantification**	Crystalline phase quantification	Measure relative intensities of XRD² pattern
 **Texture**	Orientation identification and quantification of crystallites in solid samples	Collect intensity distribution in XRD² patterns as a function of sample orientation
 **Stress**	Residual stress determination	Measure shifts in XRD² patterns as a function of sample orientation
 **Microstructure Analysis**	Size and arrangement of crystalline or amorphous particles	Measure the intensity distribution in an XRD² pattern
 **Small Angle X-ray Scattering**	Nanostructure analysis including particle shape, size, distribution, and particle orientation	Measure small angle X-ray scattering signals in XRD² patterns
 **High-Throughput Screening**	Rapid analysis of multiple samples in combinatorial research, development and quality control	Automatically collect XRD² patterns from sample libraries and arrays
 **Micro Diffraction**	Microanalysis of small or inhomogeneous samples	Measure XRD² pattern with micron accuracy
 **Mapping**	Mapping of inhomogeneous and structured samples	Automatically collect XRD² patterns from multiple locations
 **Reciprocal Space Mapping**	Orientation and quality of epitaxial layers	Measure diffraction patterns as a function of incident and exit angle
 **Non-Ambient**	Change of structural properties as a function of sample environment	Collect XRD² patterns under varying conditions
 **High Resolution X-ray Diffraction**	Thickness, composition, mismatch, relaxation, and defects for epitaxial layers	Measure rocking curves, radial scans, and reciprocal space maps Absolute lattice parameter using Bond method
 **X-ray Reflectometry**	Thickness, roughness, and density of crystalline and amorphous layers down to 0.1 nm. Lateral and vertical roughness correlation	Measure specular scans, diffuse scans, and reciprocal space maps
 **Grazing Incidence Diffraction**	Phase identification, parallel mismatch, crystal quality, symmetry, and orientation of very thin layers	Measure in-plane reflections with very small incident and exit angle

Evaluation	Key Features
Identify crystalline phases by matching with known data sets	▪ Super speed phase identification in milliseconds ▪ Excellent data quality even from non-ideal samples due to 2-D sampling ▪ Enhanced match qualification using 2-D diffraction details
Quantify the volume fractions from the ratio of the diffracted intensities	▪ Super speed phase quantification in milliseconds ▪ Obtain accurate results for any sample geometry from non-ideal samples
Determine orientation distribution	▪ Simultaneously record multiple high-resolution pole figures and full background ▪ Intuitive modeling of texture using the component method ▪ Descriptive and graphical presentation of individual texture components
Determine the stress and strain tensor	▪ Simultaneously record multiple reflections and full background ▪ Better statistics by monitoring the shape of the Debye ring ▪ Easy stress determination on curved samples with micron spot sizes
Crystalline size by γ and 2θ profile analysis. Evaluate GISAXS data using geometrical shape, correlation and distribution models	▪ Partical size up to microns with γ integration ▪ Accurate alignment of sample with tilt stage
Model the data and determine nano structural properties	▪ Straightforward determination of anisotropic sample parameters ▪ Capillary mode for liquids ▪ He beam-path for minimized air scattering
Extraction and screening of specific sample parameters	▪ Sample alignment using the Laser-Video microscope ▪ Horizontal sample mount for reflection and transmission geometry ▪ Operator-ready display of the results
Integrate spotty data and extract desired sample information	▪ Evidential results from traces for forensic and archeology studies ▪ Micro spot analysis ▪ Valuable diffraction information even from a small number of grains
Extraction and mapping of specific sample properties	▪ Mapping of samples up to 300 mm x 300 mm ▪ 1-D and 2-D sampling using free grids ▪ 1-D and 2-D mapping display using LEPTOS
Determine layer structure and epitaxial relationship	▪ Large set of reflections covered simultaneously with 2-D detector ▪ Collect a large section of reciprocal space with only one sample rotation ▪ Full picture of reciprocal space without blind spots or missed reflections
Determine structural parameters as a function of sample environment	▪ Domed temperature stage for maximum angular coverage ▪ Software-controlled temperature profiling ▪ Comprehensive graphical display and report
Simultaneous evaluation of several reflections	▪ Tool-free switch of optics with SNAP-LOCK ▪ Optimized beam divergence depending on sample ▪ Adjustable detection resolution with PATHFINDER
Unified evaluation of XRR and HRXRD	▪ Nine orders of magnitude dynamic range using a Göbel mirror and knife edge collimator ▪ Göbel mirror with prefigured substrates for perfect incident beam conditions
Determine lattice parameters and phases	▪ Alignment of lattice planes with tilt stage ▪ Characterization of layers down to 1 nm ▪ Depth profiling by changing the incident angle

APPLICATIONS


Perfect match

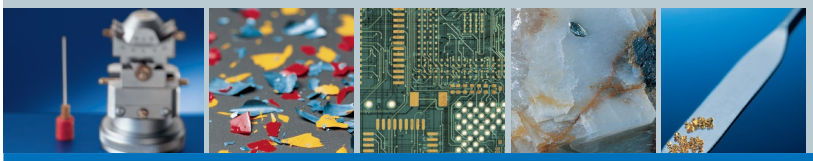

Match


No Match, Physical limitations

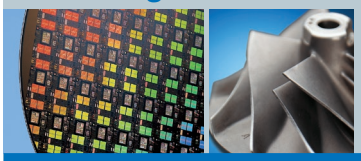
- Phase Identification
- Phase Quantification
- Texture
- Stress
- Microstructure Analysis
- Small Angle X-ray Scattering (SAXS)
- High-Throughput Screening (HTS)
- Micro Diffraction
- Mapping
- Reciprocal Space Mapping (RSM)
- Non-Ambient
- High-Resolution X-ray Diffraction (HRXRD)
- X-ray Reflectometry (XRR)
- Grazing Incidence Diffraction (GID)

Power & Versatility for all Samples Types

Small



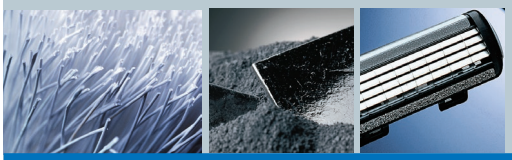
Large



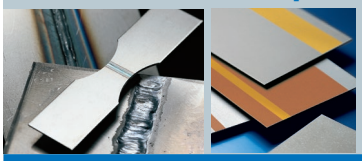
Inhomogeneous



Preferred Orientation



Process Samples



Weakly Diffracting



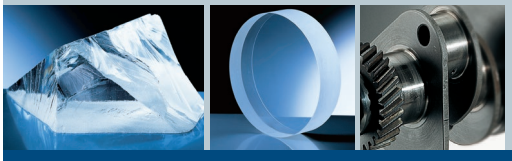
Powder



Complex Geometries



Heavy



Technical Data	
Configurations	Horizontal or vertical goniometer, Theta/2Theta and Theta/Theta geometry
Measuring circle diameter	Any intermediate setting between 500 mm and 1,080 mm (depending on setup)
Angular range (without accessories)	360°
Max. 2θ angle (depending on configuration and accessories)	Up to 168°
Angle positioning	Stepper motors with optical encoders
Smallest addressable increment	± 0.0001°
Max. angular speed (depending on configuration and accessories)	± 20°/s
VÅNTEC-500 detector **Microfocus X-ray source**	Huge detection area covering more than 15,000 mm² Noise-free operation with less than 0.0005 cps/mm² Variable detector positioning Proven radiation hardness Maintenance-free design Guaranteed to have no dead or defective areas
X-ray sources	Sealed tube TWIST-TUBE: fast and easy switching between line and spot focus Microfocus X-Ray Source (IμS) TURBO X-RAY SOURCE: from 1.2 kW up to 18 kW, (depending on focus size and anode type)
General space and infrastructure requirements:	
Exterior dimensions (h x w x d)	202 x 168 x 129 cm 79.5 x 66.0 x 50.6 inch
Weight (without optional electronics)	945 kg (without optional accessories) 2,085 lbs
Cooling water supply (without optional internal water chiller)	Min. 4 l/min, pressure 4 bar to 7.5 bar, no pressure on outlet side, temperature: 10 °C to 20 °C
Power supply	Single phase: 208 to 240 V Three phases: 120 V, 230 V, 240 V 47 to 63 Hz
Maximum power consumption (without controllers for optional equipment)	6.5 kVA

TWIST-TUBE: US 7,421,064 patent; EP 1 923 900 B1 patent. Laser Video: US 5,359,640, MIKROGAP technology, VÅNTEC-500: US 6,340,819 B1 patent.

D8 DISCOVER door: DE 102 008 020 729 patent, DE 102 008 020 730 patent.

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