

# Automated Multipurpose Powder X-Ray Diffractometer

**XRDynamic 500**





# XRDynamic 500: Driving XRD

**XRDynamic 500 drives unbeatable XRD data quality with maximum efficiency. Driven by the TruBeam™ concept, this automated multipurpose powder X-ray diffractometer delivers both outstanding measurement speed and resolution, without any compromises.**

With TruBeam™, you get full automation of beam geometries and X-ray optics, as well as instrument and sample alignment, in combination with flexible instrument setups for an array of applications.

Most importantly, you get best-in-class data quality. XRDynamic 500 offers 20 % better measurement resolution out-of-the-box in a standard Bragg-Brentano configuration when compared with other conventional instruments.

Enjoy the benefits of a versatile platform, with fully automated optics and alignment routines. This allows everyone, from novices to experts, to collect top-quality XRD data quickly while minimizing errors. XRDynamic 500: Driving XRD.

- **Intuitive and super-efficient:** Automated switching between up to three different beam geometries, full automation of all X-ray optics, automated sample handling of up to 105 samples, and completely automated instrument and sample alignment
- **Best-in-class data quality:** A large measurement radius and evacuated beam path; zero compromise on measurement speed or resolution with outstanding signal-to-noise ratio
- **Maximum flexibility:** Versatile instrument setups for every application with optimized solutions for powder XRD, non-ambient XRD, PDF analysis, and SAXS

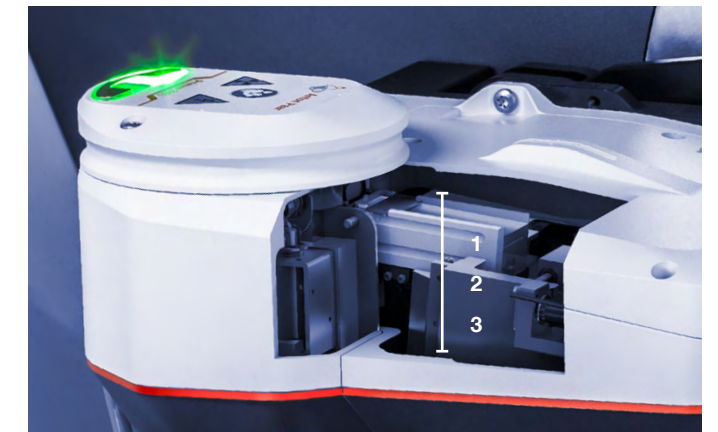




# Truly Revolutionary, Truly Unique

The revolutionary TruBeam™ concept is truly unique on the market, bringing higher resolution, increased efficiency, and more options.

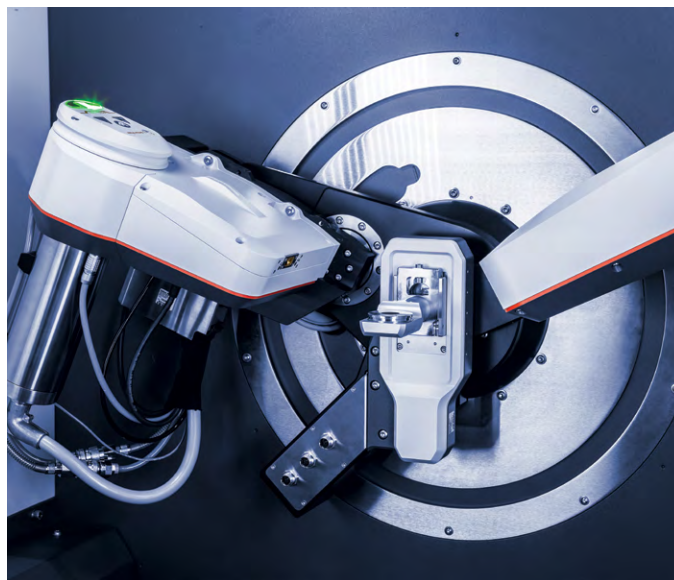
Up to three beam geometries at a click



**Position 1:** Bragg-Brentano

**Position 2:** Flat monochromator

**Position 3:** X-ray mirror (parallel beam or focusing)



## Large goniometer radius and evacuated beam path for better resolution

- Standard goniometer radius of 360 mm or 400 mm for the highest resolution data in classic Bragg-Brentano geometry
- Unique evacuated beam path with all optical components plus detector under vacuum for maximum signal-to-noise ratio
- No need to compromise between measurement speed and measurement resolution – now you can have both
- Minimal measurement background due to air scattering when a larger goniometer radius is being used

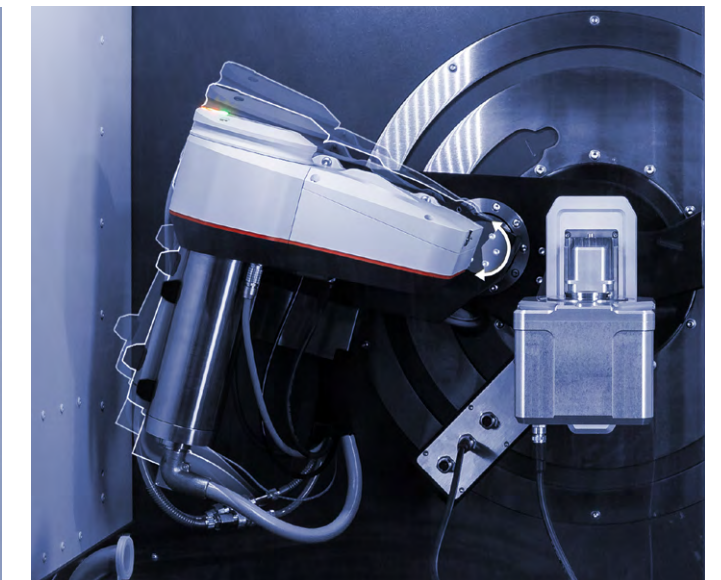
## Keep it simple with auto-alignment

- Automatic alignment of every beam and measurement geometry with all mirrors and monochromators
- Precise alignment of the X-ray source to all optics with an optimized take-off angle under all conditions
- Instrument self-alignment can be triggered at any time without the need for a service visit – delivering maximum uptime and reduced ownership costs
- Fully automated sample alignment under both ambient and non-ambient conditions to avoid measurement errors



## Easy geometry and optics changes with just one click

- Fully automated optics to completely change the measurement configuration in an instant with no user intervention required
- Automation of all optics as standard, including absorbers/filters, beam mask, Soller slits, divergence slits, anti-scatter slits, and parallel plate collimators
- Use up to three beam geometries within a single measurement batch, with all mirrors and monochromators fitted in a motorized optics stack
- Choose from Bragg-Brentano, a monochromatic  $K\alpha$  divergent beam, or an X-ray mirror (parabolic or elliptical) in reflection or transmission

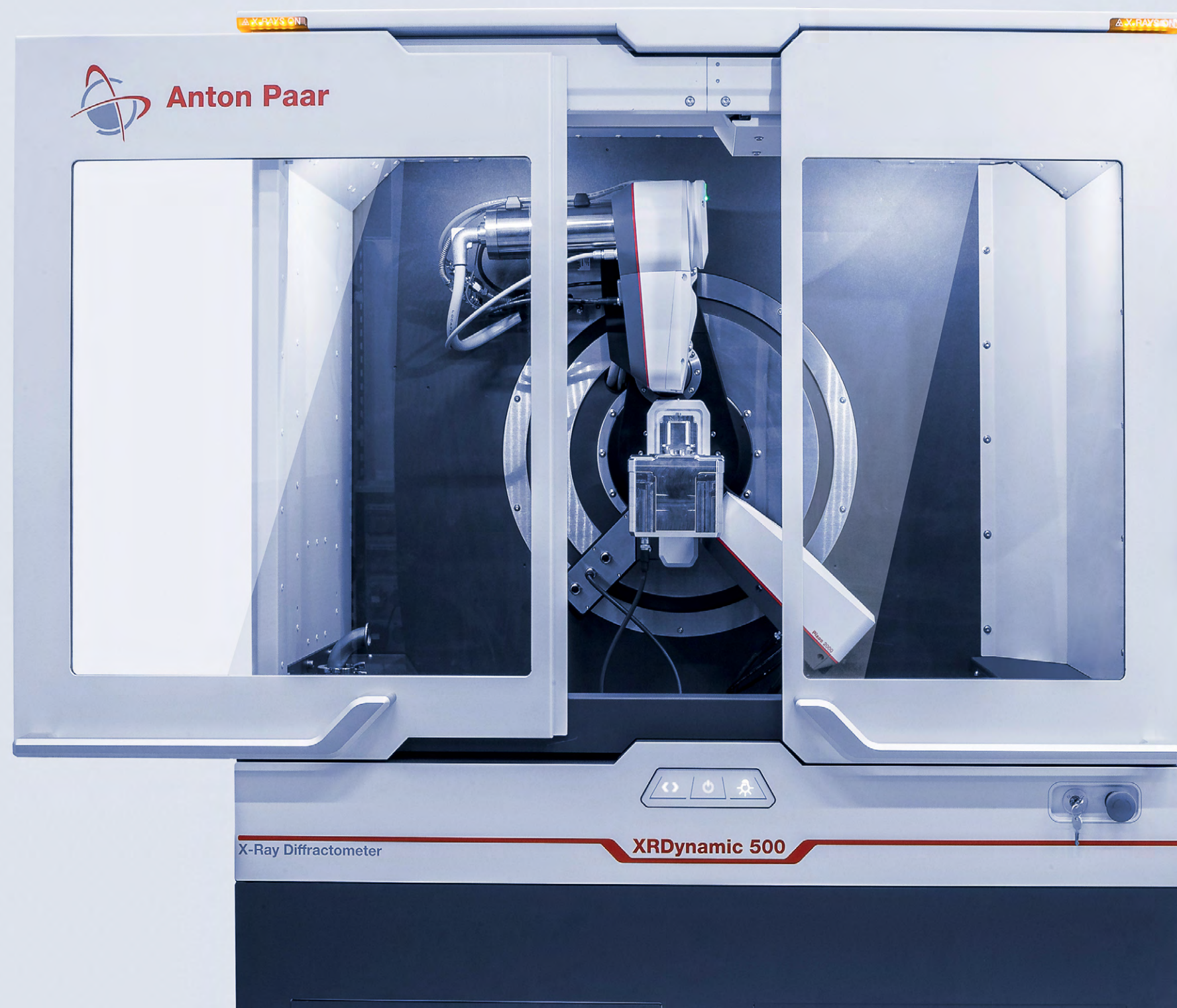


## The optimal, all-purpose X-ray beam

- Patented source pitch concept with an additional tilt axis for precise alignment of any optical component with the X-ray source
- Maximum primary beam intensity thanks to optimized take-off angle of the X-ray source to all mirrors and monochromators
- Pitch concept allows multilayer  $K\alpha_{1,2}$  monochromators to be used with all tube anode types, making  $K\beta$  filters redundant and maximizing measurement quality
- Easy switching of the tube focus and fast exchange of the X-ray tube to overcome issues such as sample fluorescence



# One Instrument, a World of Possibilities



## **Excellent data quality as standard**

A goniometer radius of 360 mm or 400 mm means that unrivalled measurement resolution can be achieved without the use of monochromators, while evacuated optics keep the measurement background to a minimum (up to 50 % less) for superior signal-to-noise ratio.

## **The latest in high-end pixel detectors**

The Si- or CdTe-based pixel detectors from Advacam feature the latest CERN technology in the form of the integrated Timepix3 chip. The 0D and 1D measurement modes offer unparalleled performance and measurement speed for all powder XRD applications.

## **Unbeatable performance with a next-generation goniometer design**

The compact design of the XRDynamic 500 goniometer uses strain wave gearing. This makes counterweights unnecessary and sets new standards in accuracy, measurement range, and resolution.

## **Autosampling for maximum throughput**

The XRDynamic Autosampler maximizes sample capacity (up to 105), integrates seamlessly, and performs flexibly. Automated measurements for all sample types ensure consistently reliable results.

## **A sample stage for every application**

Whether you use it for reflection, transmission, or non-ambient studies, XRDynamic 500 offers sample stages and holders for every eventuality. Quickly change configuration, including the X-ray tube, and be up and running again in no time thanks to the intelligent design and auto-alignment – ensuring you're always working with the optimal setup.

## **Reduce set-up time and errors with component recognition**

Automatic and easy connection of all optics and stages allows fast exchange between setups while always ensuring the correct instrument configuration.

## **Non-ambient XRD made easy**

All of the necessary connections for non-ambient experiments are located directly in the diffractometer housing for ultimate user convenience. The option of an integrated non-ambient control unit (CCU) makes working with and switching between different non-ambient attachments effortless.

## **Best-in-class nanostructural analysis (SAXS) on a diffractometer**

XRDynamic 500, in combination with the EVAC module, is unique in allowing you to collect small-angle X-ray scattering (SAXS) data with the quality of a stand-alone line-focus SAXS instrument. The completely evacuated beam path, combined with dedicated optics and state-of-the-art pixel detectors, results in an outstanding resolution with  $q_{\min} = 0.05 \text{ nm}^{-1}$ .



# Quality Components for Quality Data

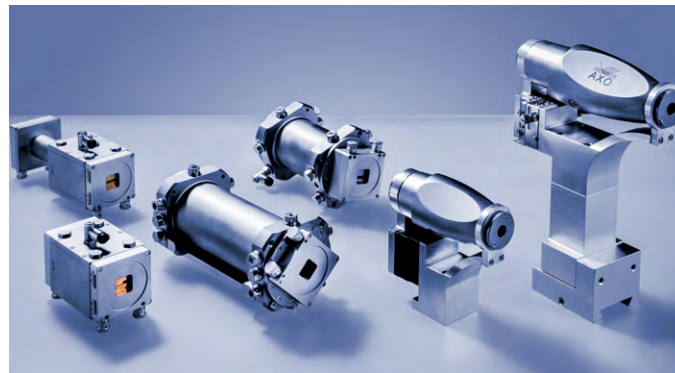


## Primux 3000 – the ideal source for any task

Primux 3000 is a high-performance sealed-tube X-ray source providing a brilliant line or point focus beam for all applications.

It features:

- Simple and straightforward tube exchange so you always work with the most suitable tube type for your application
- A variety of different available anodes
- Easy switching between line and point focus
- Automatic recognition of the tube type and tube focus to minimize setup errors



## Advanced X-ray optics from AXO DRESDEN (an Anton Paar company)

The X-ray optics used in XRDynamic 500 are produced by AXO DRESDEN, a global leader with more than 20 years of experience in applied X-ray optics and high-precision deposition techniques.

You benefit from:

- High-performance optics which ensure the highest quality and intensity of the X-ray beam, regardless of source type or beam geometry
- Options for various X-ray mirrors and  $K\alpha_{1,2}$  monochromators that can all be placed in the automated optics unit of XRDynamic 500

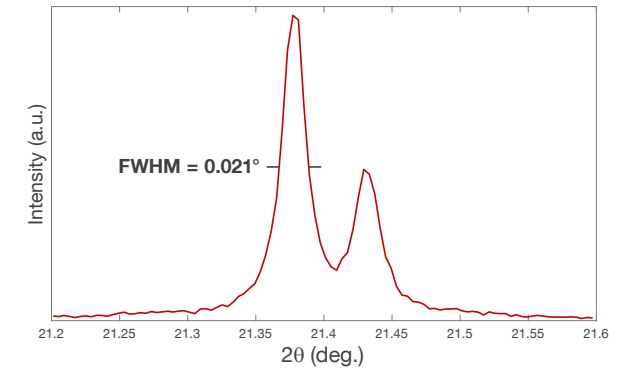


## Pixos™ – the latest in pixel detector technology

The evacuated Pixos™ detection units feature solid-state hybrid pixel detectors from Advacam based on the Timepix3 chip developed by CERN.

They provide:

- Si or CdTe sensors (14 mm x 14 mm)
- 55  $\mu\text{m}$  x 55  $\mu\text{m}$  pixel size
- 0D and 1D detection modes
- Energy filtering
- Quantum efficiency >97 % for Cu  $K\alpha$  (Si sensor) and >99 % for Mo / Ag  $K\alpha$  (CdTe sensor)



## A new class of goniometer

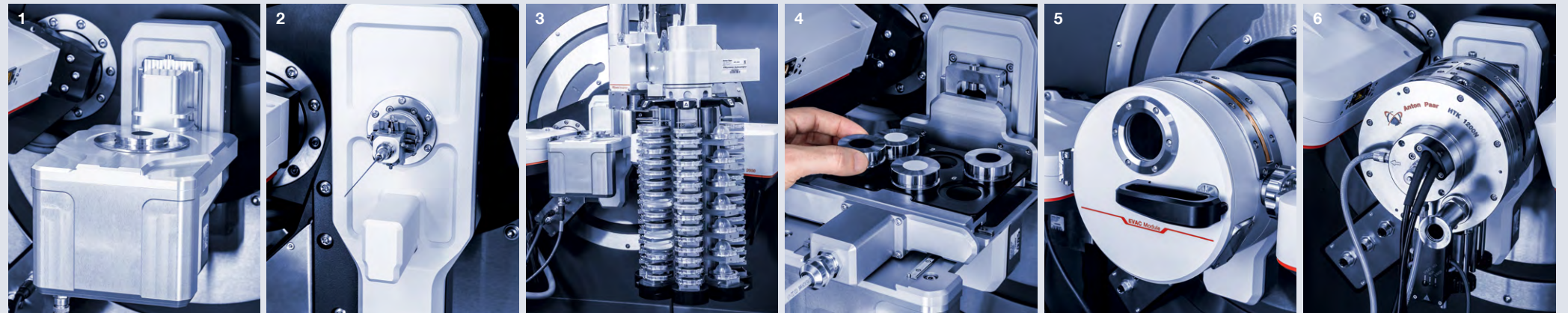
Using high-precision strain wave gearing instead of worm gear units makes for one of the most innovative goniometers on the market and a robust and maintenance-free solution.

It offers:

- Vertical  $\theta/\theta$  geometry
- 360 mm or 400 mm radius
- Measurement range up to 162.5° with all optics configurations
- Guaranteed 2θ linearity  $\leq 0.01^\circ$
- Excellent angular resolution with a FWHM of 0.021° for the 1st peak of  $\text{LaB}_6$  (Cu radiation)

## Sample Stages for Every Application

- 1 Sample spinner stage
- 2 Capillary spinner
- 3 XRDynamic Autosampler
- 4 XY stage with autosampler
- 5 EVAC module for high-resolution XRD and SAXS
- 6 Non-ambient attachments





# All Manner of Measurement

Powder X-ray diffraction is an essential characterization technique for an almost infinitely wide spectrum of materials and applications. X-ray diffraction data reveal valuable information about the phase composition, crystal structure, and microstructure of samples. In addition to diffraction, X-ray scattering experiments can provide information about properties such as the nanostructure or the short-range order present in materials.

- Minerals
- Pharmaceuticals
- Chemicals
- Metals and alloys
- Building materials
- Nanomaterials
- Batteries
- Food samples
- Colloids and biological samples



## High-quality powder diffraction

XRDynamic 500 is perfectly adapted to characterize even the most complex phase mixtures. Quantitative phase analysis and structure analysis are possible using the Rietveld method implemented in the XRDanalysis software. Typical powder XRD applications include:

- Phase identification
- Phase quantification
- Crystal structure analysis
- Microstructural analysis (crystallite size, stress/strain)
- Amorphous phase quantification

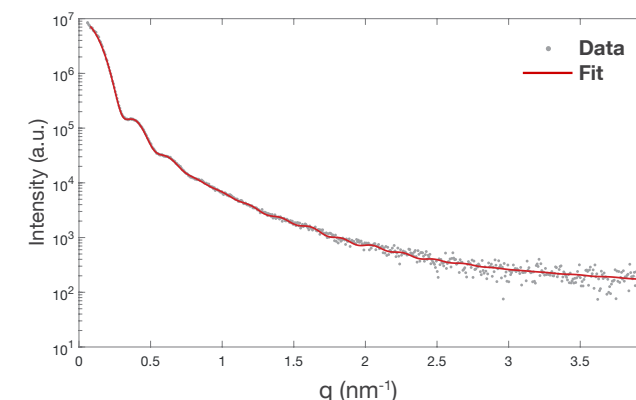


## Non-ambient diffraction

Non-ambient conditions are increasingly required in XRD, as sample properties can drastically change with varying temperature, pressure, gas atmosphere, or humidity. Coming from the world leader in non-ambient diffraction, XRDynamic 500 is designed with non-ambient measurements in mind.

It provides:

- Plug-and-play mode for all Anton Paar non-ambient attachments
- Integrated control unit for all Anton Paar non-ambient attachments
- Built-in non-ambient connections in the diffractometer housing
- Control software designed to simplify non-ambient XRD measurements



## Small-angle X-ray scattering (SAXS)

SAXS data with the quality of a stand-alone line-focus SAXS instrument on a diffractometer? With XRDynamic 500 and the EVAC module it's finally possible, thanks to a fully evacuated beam path and dedicated SAXS optics.

- Line collimation SAXS with  $q_{\min} = 0.05 \text{ nm}^{-1}$
- Particle size and shape analysis
- Pore size and distribution
- Analysis of isotropic, colloidal, and biological samples (BioSAXS)
- State-of-the-art SAXSanalysis software package



## Pair distribution function (PDF) analysis

XRDynamic 500 is not only perfectly suited to the measurement of crystalline samples, but also ideal for amorphous materials. PDF analysis is the go-to method for analysis of the local ordering present in amorphous samples.

- Easily switch to a Mo or Ag source to maximize q-range
- Transmission measurements with capillaries up to  $162.5^\circ 2\theta$
- CdTe detectors for excellent quantum efficiency with hard X-rays



# Dedicated Software

**The XRDynamic 500 software packages are the keys to collecting and evaluating X-ray powder diffraction data for both expert and novice users. The user-oriented approach simplifies every step of the data collection and analysis process.**

## XRDdrive

**The XRDdrive software allows you to exploit the full potential of XRDynamic 500 and the TruBeam™ concept.**

- Easily set up complex experiments consisting of multiple measurement configurations and sample types
- Run up to 105 samples without user interaction using the XRDynamic Autosampler to maximize instrument usage and efficiency
- Intelligent features such as automatic instrument and sample alignment and component recognition reduce the risk of user error
- A simple-to-use interface ensures complex non-ambient experiments can be handled just like standard ambient ones
- HDF5-based data format combines the results of complex measurement batches into single hierarchical files containing all relevant information for export to the XRDanalysis software or any other analysis software package

## XRDanalysis

**XRDanalysis is a next-generation software package for powder diffraction analysis that allows you to effortlessly perform phase identification/quantification and microstructure analysis for ambient and non-ambient experiments.**

- Optimized analysis workflow to guide inexperienced users without placing any restrictions on advanced users
- Search/match functionality based on advanced algorithms for identification of even minor phase impurities
- Rietveld refinement for quantitative phase and structure analysis while accounting for all instrument and sample microstructure effects
- Full integration of PDF databases from the International Centre for Diffraction Data (ICDD) and the Crystallography Open Database (COD), with the option to load structures directly from CIFs
- Streamlined batch analysis of ambient and non-ambient experiments
- Export data and graphics directly into Microsoft Word and Excel

## XRDview

**XRDview is the ultimate data visualization and reporting tool for XRDynamic 500.**

- The same user-friendly interface and workflows as XRDdrive
- Peak search and fitting based on advanced algorithms (optional)
- Quantification of unknown samples using user-created calibration curves (optional)
- Automatic comparison to reference samples and standard reference materials
- Advanced data visualization including axis scaling, data offset, heat map, and normalization
- Audit log to ensure full traceability (optional)
- Reporting and high-resolution image exporting

## XRDynamic 21 CFR Part 11

**Collect compliant XRD data quickly while minimizing errors.**

- XRDdrive and XRDview in regulated environments (e.g., pharmaceutical industry)
- User management, roles and permissions, audit trail, electronic signature, and data evaluation, to ensure compliance and traceability



# Quality and Experience You Can Trust

## Experience in design and development

As a global leader in analytical instrumentation, Anton Paar provides measurement solutions for a wide variety of analytical tasks and applications in both laboratory and process environments.

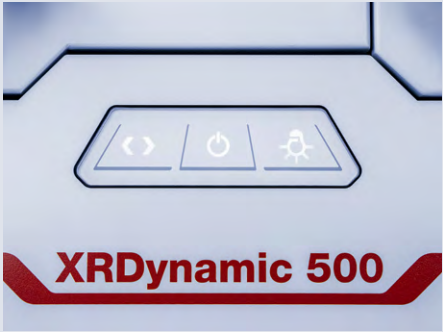
Our long tradition as a manufacturer of precise scientific instruments has been characterized by continuous innovation and integration of the latest technologies in our design and manufacturing concepts.

Anton Paar's ISO-certified quality management system guarantees unbeatable quality in our products and services no matter where you are in the world.

## A global network known for quality

The Anton Paar Group is active in more than 110 countries, and has manufacturing hubs located throughout Europe and North America. Our employees make up a worldwide network covering research and development, manufacturing and production, sales, and support.

Our mission as your partner is to ensure we're there for you throughout the entire after-sales process. This includes technical and service support via our global network as well as support from our experienced application specialists via application notes, regular user training courses, and online support.



## Highest Safety as Standard

- Clearly visible X-ray warning lamps
- Interlock mechanisms for maximum user safety
- Compliance with the most stringent safety guidelines on X-ray, machinery, and electrical safety
- Maximum X-ray protection with a leakage X-ray dosage <0.1 µSv according to EURATOM regulations

XRDynamic 500	
X-ray source	
Source type	Primux 3000
X-ray generator	Up to 3 kW
Tube voltage / current	20 kV to 60 kV / 2 mA to 50 mA
Goniometer	
Configuration	Vertical $\theta/\theta$ geometry
Measurement radius	360 mm or 400 mm
Maximum usable angular range	$-95^{\circ}$ $2\theta$ to $162.5^{\circ}$ $2\theta$ (with all optics configurations)
Minimum step size	0.0001°
$2\theta$ linearity	$\leq 0.01^{\circ}$
Maximum angular speed	15° / sec
Maximum angular resolution	0.021° (FWHM of 1st LaB <sub>6</sub> peak in Bragg-Brentano configuration)
Sample stages and attachments	
Ambient sample stages	<ul style="list-style-type: none"><li>– Fixed sample stage (reflection/transmission)</li><li>– Sample spinner stage (reflection/transmission)</li><li>– XY stage (with autosampler option)</li><li>– XRDynamic Autosampler</li><li>– Capillary spinner stage</li><li>– EVAC module</li></ul>
Autosampling options	<ul style="list-style-type: none"><li>– XRDynamic Autosampler (up to 105 samples)</li><li>– Autosampler option for XY stage (3, 6, 12, 48 samples)</li></ul>
Non-ambient attachments	<ul style="list-style-type: none"><li>– HTK 1500</li><li>– HTK 1200N</li><li>– HTK 16N/2000N</li><li>– TTK 600</li><li>– XRK 900</li><li>– CHC plus+</li><li>– BTS 150/500</li></ul>
Detectors	
	<p>Solid-state hybrid pixel detectors</p> <ul style="list-style-type: none"><li>– Pixos 2000 (0D and 1D modes)</li><li>– Pixos 2000 CdTe (0D and 1D modes) for hard X-rays</li></ul>
Software	
	<ul style="list-style-type: none"><li>– XRDrive: System control and data acquisition software</li><li>– XRDanalysis: Data processing and analysis software for qualitative and quantitative Phase analysis, microstructure analysis, and Rietveld refinement</li><li>– XRDview: Data plotting and visualization package</li><li>– XRDynamic 21 CFR Part 11 package: Supporting work in regulated environments and compliance with US FDA 21 CFR Part 11 regulations (for XRDrive and XRDview)</li></ul>
General specifications	
Exterior dimensions (width x depth x height)	1,350 mm x 1,160 mm x 1,850 mm
Weight (not including optional accessories)	750 kg
Power supply	3-phase: 3/N/PE AC 400/230 V, 50...60 Hz, 25 A 1-phase: 208...240 VAC, 50...60 Hz, 36 A
Maximum power consumption (without additional controllers for optional equipment)	5.5 kW
Cooling water supply	Flow rate >3.6 L/min, pressure 4.5 bar to 6 bar, temperature 20 °C to 25 °C

Trademarks: TruBeam 018100679, UK00918100679; XRDynamic 017957955, UK00917957955; PIXOS 018289393



**Our well-trained and certified technicians are ready to keep your instrument running smoothly.**

Maximum uptime | Warranty program | Short response times | Global service network



