Automated Multipurpose Powder X-Ray Diffractometer

XRDynamic 500
XRDynamic 500: Driving XRD

X-RAY DIFFRACTION REIMAGINED, MARKET LEADERSHIP RECHANNELLED, DECADES OF X-RAY ANALYTICS EXPERTISE REBORN. IT’S FULL BEAM AHEAD, WITH XRDynanic 500.

Behind the instrument is innovative fusion. On the one hand: our experience and market leadership in small-angle X-ray scattering (SAXS) and non-ambient X-ray diffraction, acquired over more than half a century and based on the premium quality and superior performance of our instrument portfolio – trusted by the global X-ray analytics community. On the other, a fresh, bold new design vision, to bring you a diffractometer that breaks new ground in XRD.

THE NEW FRONTIER: HIGH SPEED, GREAT DATA

The natural outcome is a powerful, automated multipurpose powder X-ray diffractometer driven by the TruBeam™ concept, the first to deliver 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. XRDynanic 500 offers 20% better measurement resolution out-of-the-box in a standard Bragg-Brentano configuration when compared with other conventional instruments.

Born out of our long experience and dedication in the field of X-ray analytics, it’s the most cleverly engineered XRD instrument on the market.

FOCUS ON WHAT MATTERS TO YOU:

Intuitive and super-efficient: Automated switching between up to 3 different beam geometries, full automation of all X-ray optics, 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.

FIND OUT MORE

www.anton-paar.com/apb-xrdynamic-500

XRDynamic 500
TruBeam™ – Truly revolutionary, truly unique

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

In one complete package, it combines:
- A LARGE GONIOMETER RADIUS AND EVACUATED OPTICS
- AUTOMATIC INSTRUMENT AND SAMPLE ALIGNMENT ROUTINES
- AUTOMATED SWITCHING OF THE BEAM GEOMETRY AND OPTICS CONFIGURATION
- AN ADDITIONAL TILT AXIS FOR THE PRIMUX 3000 X-RAY SOURCE

With TruBeam™, you know you’ll always achieve outstanding measurement performance for every sample and every user.

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 CHANGE 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 divergent beam, and 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 monochromators to be used with all tube anode types, making Kβ 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
XRDynamic 500: 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 for superior signal-to-noise ratio.

UNBEATABLE PERFORMANCE WITH A NEXT-GENERATION GONIOMETER DESIGN
The compact design of the XRDynamic 500 goniometer uses strain wave gearing which makes counterweights unnecessary and sets new standards in accuracy, measurement range, and resolution.

SAFETY FIRST
Designed with convenience and safety in mind, XRDynamic 500 conforms to the most stringent safety standards so you only need to focus on the sample at hand.

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, even the X-ray tube, and be up and running again in no time thanks to the intelligent design and auto-alignment – you’ll always be 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)
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 $q_{	ext{min}} = 0.05 \text{ nm}^{-1}$.

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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 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 µm x 55 µm pixel size
- 0D and 1D detection modes
- Energy filtering
- Quantum efficiency >97 % for Cu Kα (Si sensor) and >99 % for Mo / Ag Kα (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:
- Vertical theta/theta geometry
- 360 mm or 400 mm radius
- Measurement range up to 162.5° with all optics configurations
- Guaranteed 2theta linearity ≤0.01°
- Excellent angular resolution with a FWHM of 0.021° for the 1st peak of LaB₆ (Cu radiation)

Sample stages for every application
1. Sample spinner stage
2. Capillary spinner
3. XY stage with autosampler
4. EVAC module for high-resolution XRD and SAXS
5. Non-ambient attachments

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

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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.

**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

**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 qmin = 0.05 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° 2theta
- EVAC module with fully evacuated beam path for unparalleled data quality
- CdTe detectors for excellent quantum efficiency with hard X-rays

**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 and 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
Dedicated software: For novices and experts, a results-oriented user-centered interface

The XRDdrive and XRDanalysis 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: MAXIMUM USER ORIENTATION**

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

- A simple, user-friendly interface reduces the required user training time allowing everyone to collect the best quality XRD data.
- Easily set up complex experiments consisting of multiple measurement configurations and sample types that can run without user interaction to maximize instrument usage and efficiency.
- Intelligent features such as automatic instrument/sample alignment and component recognition reduce the risk of user error.

**XRDanalysis: STATE-OF-THE-ART EVALUATION**

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 ICDD or load structures directly from CIFs.
- Database filtering options to ease phase identification.
- Streamlined batch analysis of ambient and non-ambient experiments.
- Customizable reporting with the possibility to export data and graphics directly into Microsoft Word/Excel or export data in a simple ASCII format.
Quality & experience you can trust

EXPERIENCE IN DESIGN AND DEVELOPMENT

As a global leader in analytical instrumentation, Anton Paar provides 170 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. More than 3,400 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.

“Quality & experience you can trust”

We are confident in the high quality of our instruments. That’s why we provide full warranty for three years.

All new instruments* include repair for 3 years.
You avoid unforeseen costs and can always rely on your instrument.
Alongside the warranty we offer a wide range of additional services and maintenance options.

*Due to the technology they use, some instruments require maintenance according to a maintenance schedule. Complying with the maintenance schedule is a prerequisite for the 3-year warranty.

X-RAY SOURCE

<table>
<thead>
<tr>
<th>Source type</th>
<th>Primux 3000</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-ray generator</td>
<td>Up to 3 kW</td>
</tr>
<tr>
<td>Tube voltage / current</td>
<td>20 kV to 60 kV / 2 mA to 50 mA</td>
</tr>
</tbody>
</table>

GONIOMETER

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Vertical Theta/Theta geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measurement radius</td>
<td>360 mm or 400 mm</td>
</tr>
<tr>
<td>Maximum usable angular range</td>
<td>-95° to 162.5° (with all optics configurations)</td>
</tr>
<tr>
<td>Minimum step size</td>
<td>0.0001°</td>
</tr>
<tr>
<td>2theta linearity</td>
<td>≤0.01°</td>
</tr>
<tr>
<td>Maximum angular speed</td>
<td>15° / sec</td>
</tr>
<tr>
<td>Maximum angular resolution</td>
<td>0.021° (FWHM of 1st LaB6 peak in Bragg-Brentano configuration)</td>
</tr>
</tbody>
</table>

SAMPLE STAGES AND ATTACHMENTS

- Fixed sample stage
- Sample spinner stage (reflection/transmission)
- XY stage (with autosampler option)
- Capillary spinner stage
- EVAC module

Non-ambient attachments
- HTK 1200N
- HTK 16N/2000N
- TTK 600
- XRK 900
- CHC plus+
- BfS 150/500

DETECTORS

- Solid-state hybrid pixel detectors
  - Pixos 1000 (0D mode)
  - Pixos 2000 (0D and 1D modes)
  - Pixos 2000 CdTe (0D and 1D modes) for hard X-rays

SOFTWARE

- XRDdrive: system control and data acquisition software
- XRDanalysis: data processing and analysis software for qualitative and quantitative phase analysis, microstructure analysis, and Rietveld refinement

GENERAL SPECIFICATIONS

| Exterior dimensions (width x depth x height) | 1350 mm x 1160 mm x 1850 mm |
| Weight (not including optional accessories) | 750 kg                      |
| Power supply                                 | 3-phase: 3/NPE 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-6 bar, Temperature 20 – 25 °C |