

Materials analysis by X-ray diffraction



www.rigaku.com/en/products/xrd/miniflex



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Materials analysis by X-ray diffraction

Advanced benchtop X-ray diffractometer





6th generation benchtop X-ray diffractometer

Two detector choices

More power More flexibility More results

6th generation MiniFlex 6G retains the characteristics that have made it popular for so many years:

- Compact size allows it to be installed on a lab bench
- ½ the cost of a traditional floor standing diffractometer
- Distinguished scientific literature
 record
- Easy to use, operate, and maintain
- Able to use pre-existing utilities
- 600 W of X-ray tube power

Adding to the new evolution are advanced features that deliver powerful capabilities for the future, including:

- HyPix-400 MF 2D hybrid pixel array detector
 - Acquire data in 2D, 1D or 0D modes
- D/teX Ultra 1D advanced silicon strip detector
 - Uniquely available with receiving monochromator
- ASC-8 unique 8-position
 autosampler

MiniFlex

Rigaku's MiniFlex 6G benchtop XRD redefines X-ray diffraction

X-ray diffraction (XRD) is a powerful and well-established technique for analyzing materials. Industries as diverse as cement, catalysis, petroleum, energy and pharmaceuticals rely on XRD to characterize materials from basic research all the way to quality control. It is also an important scientific technique taught to students who study geology, material science, chemistry and crystallography.

Rigaku MiniFlex 6G is a fully featured, general purpose X-ray diffractometer. It can perform qualitative and quantitative analysis of polycrystalline materials. In qualitative analysis, the instrument is used to identify unknown substances (chemical compounds or "phases") by comparing experimental diffraction data against a database of known phases. In quantitative analysis, it is used to characterize solid mixtures to determine relative abundance of crystalline compounds.



The red pattern illustrates background reduction when using the monochromator.

D/teX Ultra – 1D silicon strip detector

MiniFlex 6G is equipped with the D/teX Ultra high-speed 1D (one dimensional) silicon strip detector to obtain intensity a few tens to roughly 100 times greater than a conventional scintillation counter. D/teX Ultra measures data faster because it can measure a wide range of 20 simultaneously with high angular resolution.

D/teX Ultra may be operated in 0D mode equipped with an optional graphite monochromator (shown above) to maximize sensitivity by optimizing peakto-background ratios. In addition, this option eliminates fluorescence from materials containing Fe, Ni, Co, and Mn.

Choice of optical components for optimal resolution





HyPix-400 MF – 2D hybrid pixel array detector

MiniFlex 6G can also be configured with the HyPix-400 MF 2D (two dimensional) hybrid pixel array detector (HPAD). This new direct photon counting detector enables high-speed, high-dynamic range, low-noise data collection in 0D, 1D, and 2D modes. This highly versatile detector is ideal for the widest range of applications including conventional powder XRD, micro-XRD, and the measurement of complex materials with coarse grain size and/or preferred orientation.



MiniFlex 6G X-ray diffractometer

Options and accessories

Analysis software

PDXL is Rigaku's full-function powder diffraction analysis package. Its modular design and automated flow bar user interface has revolutionized access to the power of XRD for the non-expert user.

The latest version of PDXL includes some important new functions, including a fundamental parameter method (FP method) for more accurate peak calculation, phase identification using the Crystallography Open Database (COD), and a Wizard for ab initio crystal structure analysis.

PDXL's rich feature list includes:

- Search/Match analysis
- Percent crystallinity •
- **Cell refinement** •
- Indexing •
- Ab initio structure solving
- Quantitative analysis •
- Crystallite size and strain .
- Whole pattern profile fitting •
- **Rietveld refinement** .
- Lattice parameter refinement •





D/teX Ultra: 1D Si strip detector and 1D modes.



Graphite monochromator for the D/teX Ultra



HyPix-400 MF: 2D HPAD detector Optional advanced hybrid array pixel detector (HPAD) with zero background noise, an active area of 400 mm², spatial resolution of 100 μ m, and maximum count rate of 10⁶ cps/pixel or more. HyPix-400 MF can operate in 0D, 1D or 2D modes.

ASC-8 automated sample changer Automatic 8-position sample changer with spinner.

ShapeFlex™

BTS 500 and BTS 150 heating and cooling temperature attachments

Sample holders

Various sample holders are available to meet the specific needs of each lab.



High-speed, 1D silicon strip detector standard for fast, high-resolution scanning in 0D

The graphite monochromator optimizes sensitivity by lowering the background level. It improves signal-to-noise by eliminating fluorescence from materials containing Mn, Fe, Co, and Ni containing materials.

Sample holder for large and irregularly shaped samples.

Specimen rotation attachment

The sample rotation stage allows continuous rotation to minimize the effects of preferred orientation.

The high temperature attachment can heat a sample to perform *in situ* powder diffraction measurements under high temperature conditions from ambient to 500°C.



Air-sensitive sample holder

An air-sensitive sample holder is available for users studying materials that might degrade in the presence of air.

PDXL software



PDXL software

PDXL is a one-stop full-function powder diffraction analysis software suite. The modular design, advanced engine and user-friendly GUI have been satisfying both experienced and novice users since PDXL was released in 2007. PDXL provides various analysis tools such as automatic phase identification, quantitative analysis, crystallite-size analysis, lattice constants refinement, Rietveld analysis, *ab initio* structure determination, etc.



Phase identification using COD

The Crystallography Open Database (COD) is a free, public-domain database of the crystal structures published in International Union of Crystallography, Mineralogical Society of America and so on. PDXL can incorporate both ICDD/PDF-2 and COD to perform automatic phase identification, adding the COD library of over 150,000 crystal structures to PDXL's already substantial capabilities.

Fundamental parameter method

The peak shape in a powder diffraction pattern would appear to be a delta function if measured under ideal conditions. In reality, the peak shape changes depending on a number of measurement conditions: wavelength distribution of the source, optical systems, slit conditions, crystallite size and strain, and so on. The peak shapes obtained from measurements made under real-world conditions are described using an empirical function such as a split pseudo-Voigt function, or a split Pearson VII function, which has a good agreement with the obtained peak shapes. The fundamental parameter method (FP method) is a method to calculate peak shape by convolution of the shapes caused by all the instrumental and sample conditions.



Wizard for *ab initio* crystal structure analysis

Recently, there have been many published examples of *ab initio* crystal structure analysis performed on powder diffraction data. This development is attributed primarily to significant improvements in PC processing speed and in the efficiency of the algorithms used for structure determination. PDXL has so far provided all of the functions required for *ab initio* crystal structure analysis, such as indexing, structure determination and structure refinement by the Rietveld method. Now the "Structure Analysis Wizard" is available in PDXL to provide support and guidance for users undertaking the complicated procedure of structure analysis, particularly of organic compounds. This wizard system will make it possible for even the beginner to achieve analytical success.

Clustering function

The PDXL clustering feature can group multiple scan data based on the similarity of powder diffraction patterns and peak positions, and displays the grouped data in an easy-to-read tree. This is particularly effective when it comes to classifying and screening the data from a large number of scans.

The proof is in the results

A Google Scholar search (excluding patents) referencing the "Rigaku MiniFlex" finds over 13,000 articles. Journals as prestigious and diverse as the Journal of the American Chemical Society, Journal of Orthopedic Research, Thin Solid Films, Vibrational Spectroscopy, Biotechnology Letters, Catalysis Communications, and Materials Letters reference the MiniFlex.

A Google patent search indicates over 500 patents include reference to the Rigaku MiniFlex. These patents cover a wide range of inventions, including polymorphs, lithium electrochemical cells, nanocomposites, conductive ink, wire coating, pharmaceutical co-crystal compositions of drugs, tires, conductive materials, cement, ceramics, pharmaceutical formulations, solar cells, polymers, thin films, super capacitors, phosphors, coatings, catalysis, and medical devices.





Legacy of innovation

The Rigaku MiniFlex X-ray diffractometer is historically significant in that it was the first commercial benchtop (tabletop) X-ray diffraction instrument. When introduced in 1973, the original Miniflex[™] XRD was about one-tenth the size of, and dramatically less expensive than, conventional X-ray diffraction (XRD) equipment of the period. The original instrument (Gen 1), and its successor that was introduced in 1976 (Gen 2), employed a horizontal goniometer with data output provided by an internal strip chart recorder. The third generation (Gen 3) instrument, introduced in 1995, was called Miniflex+. It provided a dramatic advance in X-ray power to 450 W (by operating at 30 kV and 15 mA) and Windows® PC computer control. Both the Miniflex+ and the succeeding generation products employ a vertical goniometer and allow the use of an automatic sample changer. The fourth generation (Gen 4) MiniFlex Il instrument was introduced in 2006 and offered the advance of a monochromatic X-ray source and a D/teX Ultra 1D silicon strip detector. The fifth generation (Gen 5) MiniFlex600 system, introduced in 2012, built upon this legacy with 600 W of available power and new PDXL powder diffraction software.



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Specificat	ions and ultility requ	irements

Software	Control	MiniFlex Guidance
	Data analysis	PDXL Basic Analysis package
		PDXL Qualitative Analysis package
		PDXL Quantitative Analysis package
		PDXL Comprehensive Analysis package
		PDXL Rietveld Analysis package
		PDXL Structure Analysis package
		ICDD, ICSD, and COD databases available
Generator	Maximum power	600 W
	Tube voltage	40 kV
	Tube current	15 mA
	Shutter	Rotary shutter linked to interlock
	X-ray tube	Cu, Co, Fe, or Cr
Optics	Divergence slit	Fixed or Variable
	Scattering slit	Fixed
	Receiving slit	Fixed
	Filter	Kβ Foil filter
	Monochromator (optional)	Graphite for D/teX Ultra
Goniometer	Туре	Vertical
	Radius	150 mm
	Scanning range	-3 to 145° (θ-2θ)
	Scanning speed	0.01 to 100°/min (2θ)
	Minimum step width	0.005° (2 0)
	Accuracy	±0.02°
Detector	D/teX Ultra	1D High speed silicon strip detector
Dimensions	Main body	620 W x 722 H x 460 D (mm)
Weight	Main body	Approx. 80 kg
Power	Main Body	1¢ AC100 to 240V ±10%
		50/60Hz ±1% 0.7 kVA
	PC	1¢ AC100V ±10%
		50/60 Hz ±1% 0.7 kVA

Options			
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Attachments	Specimen rotation attachment		
	Automatic sample changer for 8 samples		
	HyPix-400 MF 2D hybrid pixel array detector		
	Diffracted beam monochromator		
	Air-sensitive sample holder		
	ShapeFlex sample holder		