Rigaku

SmartLab

X-RAY DIFFRACTOMETER

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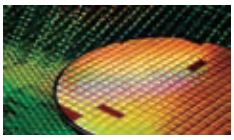
Introduction

SmartLab: Advanced measurements with simple operation

Powered by Rigaku's proprietary Guidance software system, SmartLab incorporates intelligent, application-specific protocols in all measurement types, enhancing new or inexperienced users' abilities to make quality measurements with a minimal learning curve. For advanced users, the automated methods offer greater throughput and productivity.

CBO technology: Modularity without the modules

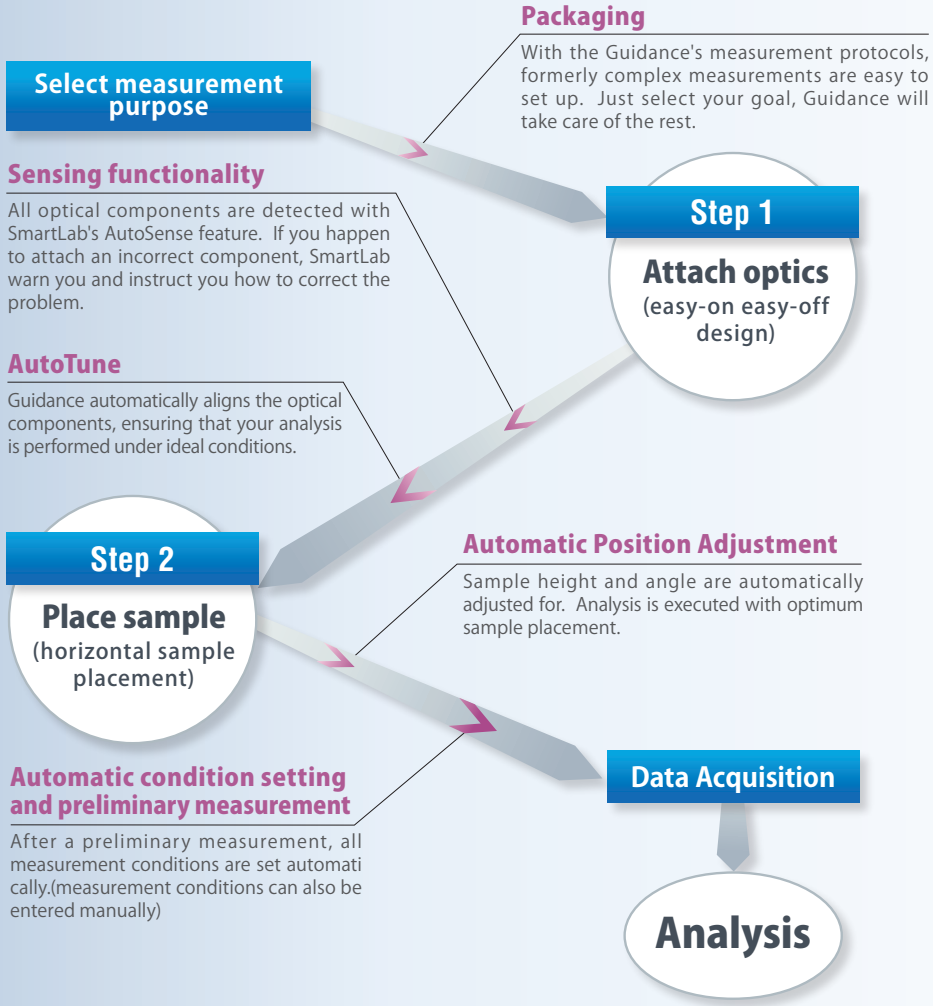
SmartLab includes as standard Rigaku's patented Cross Beam Optical (CBO) technology. CBO technology uses simultaneously mounted, simultaneously aligned optical components for both focusing (Bragg-Brentano) and parallel beam diffractometer geometries. Users can switch between the two geometries without the need to remove, replace, or realign optical components.




SmartLab Guidance: Start saving time

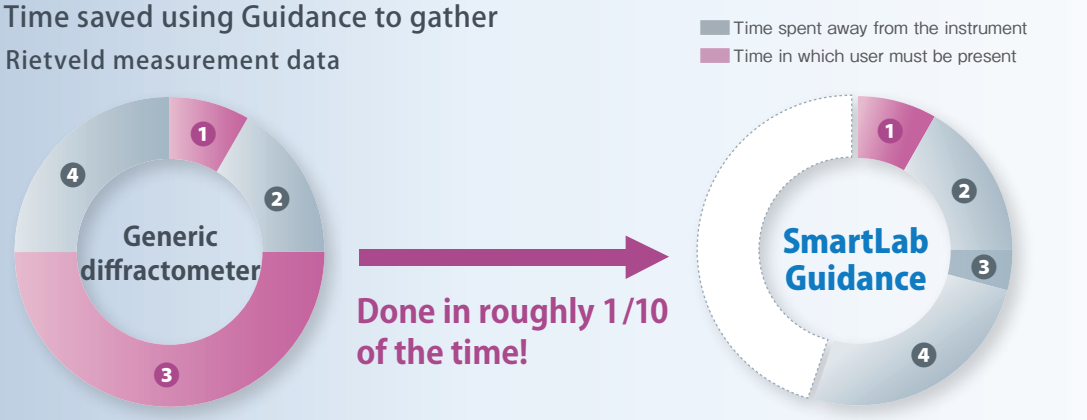
Fast, precise and easy to use... Utilizing Rigaku's industry-first Guidance technology, the SmartLab will advise you on the optimum conditions and settings. The program will determine which optics units are most appropriate for your application, determine the instrument settings and execute the measurement, offering a completely automated measurement sequence.

Measurement Flow



Case Study:

Time saved using Guidance to gather Rietveld measurement data



❶ Input measurement range
❷ Make preliminary measurement
❸ Calculate and set measurement conditions such as step size, scan rate slit conditions etc.
❹ Perform measurement.

❶ Input measurement range
❷ Make preliminary measurement
❸ SmartLab Guidance will automatically set the optimum measurement conditions using the preliminary measurement data.
❹ Perform measurement

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Powder Diffraction

SmartLab makes powder diffraction easy

Automatic alignment, CBO, and SmartLab's Guidance software engine combine to create an extremely flexible, intelligence-based data collection platform. SmartLab gathers information about your sample, suggests measurement configurations, helps you set the diffractometer, and executes measurements, all with the help of user-friendly dialog screens. CBO technology allows simple selection of focusing and parallel beam geometries on demand for the widest possible range of applications.

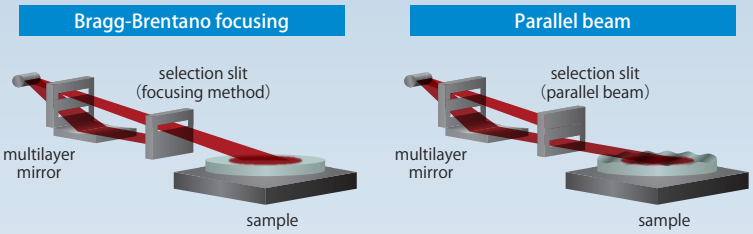
Supported powder diffraction applications include:

- **Phase identification**
- **Quantitative analysis**
- **Percent crystallinity**
- **Crystallite size/lattice strain analysis**
- **Precise lattice parameter determination**
- **Rietveld refinement**

SmartLab identifies peak locations and intensities, and searches for the best matches from the ICDD Powder Diffraction File. Multi-phase mixtures are routinely identified. Quantitative phase information is readily available from standard calibration, semi-quantitative, whole pattern fitting and Rietveld methods.

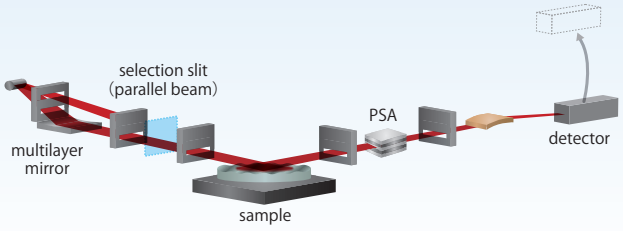
Cross Beam Optical (CBO) technology

Change and adjust optics easily, whether you are using focusing optics in the direct beam path, or a multilayer mirror optic for high-brilliance, monochromated parallel beams.



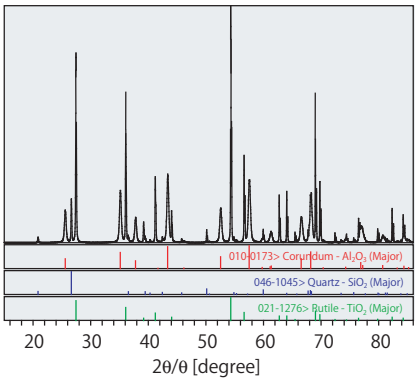
High resolution parallel beam optics

By combining the parallel beam from a multilayer mirror with a long slit PSA (parallel slit analyzer), you can obtain exceptionally accurate, high-resolution data with high repeatability without the influence of sample shape or measurement environment. The effectiveness of this configuration is particularly notable for in-situ analysis, powder structure determination, and the analysis of clay minerals and organic materials.

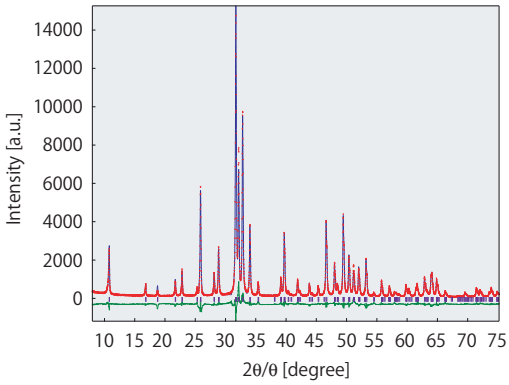


Rietveld refinement of hydroxyl apatite showing difference plot, crystal structure, and calculated electron density map. Information from focusing and parallel beam data sets can be combined to yield excellent refinements for complex molecular structures.

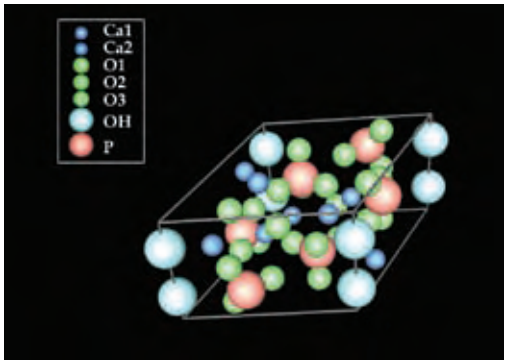
Phase identification mixture of corundum, quartz, and rutile



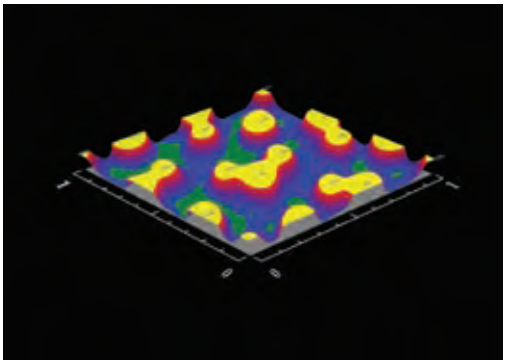
Rietveld analysis of hydroxyl apatite



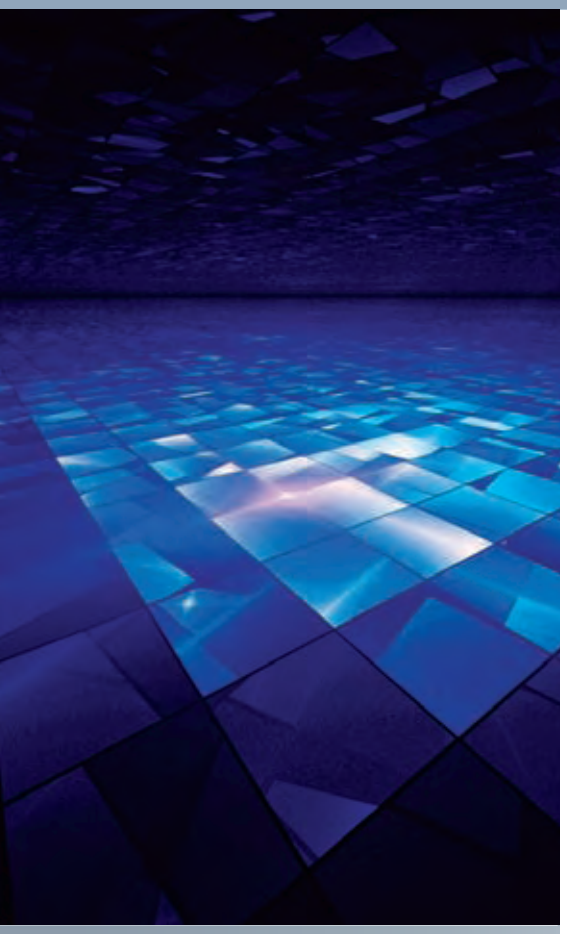
Crystal structure



Electron density map
ab-plane, c=0.25 maximum entropy method



SmartLab standard sample stage



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Thin film analysis

SmartLab makes thin film analysis flexible

Measurement of advanced thin film materials using XRD and X-ray reflectivity (XRR) techniques can be a challenge for X-ray users.

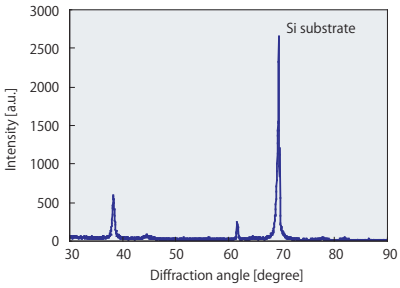
SmartLab's approach to this problem is to aid users in choosing the specific measurement conditions, experimental geometries, and application methods best suited to their particular sample. SmartLab does not ask how long to scan, over what range, or at what step size. Instead, intelligent dialog screens ask about possible composition, thickness and perfection. Measurement conditions are proposed along with user-friendly instructions on how to proceed.

Guidance software provides analytical methods and measurement capabilities for determination of:

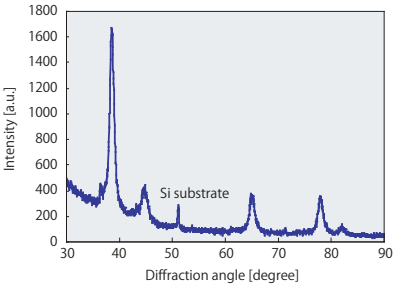
- **Composition**
- **Orientation/texture**
- **Perfection**
- **Relaxation**
- **Strain/stress**
- **Thickness**
- **Interface roughness**
- **Density**
- **Surface uniformity**

For gold nanoparticles deposited on silicon, normal and grazing incidence geometries (above) allow the user to optimize measurement conditions for either substrate or thin film properties. Grazing incidence limits the beam penetration depth into the sample, enhancing signal from the thin film.

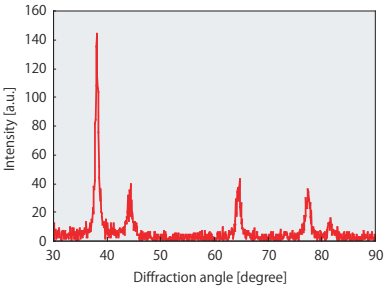
Symmetric scan



Grazing incidence scan



In-plane scan

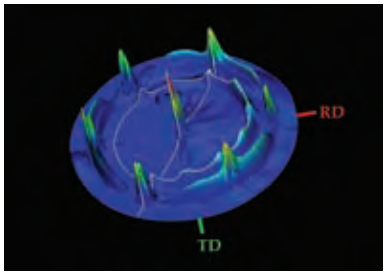


For semiconductor wafers, the horizontal sample mount does not cause the sample to bend or bow, and is ideal for high-resolution rocking curves, reciprocal space maps, and XRR where strain-free sample handling is crucial.

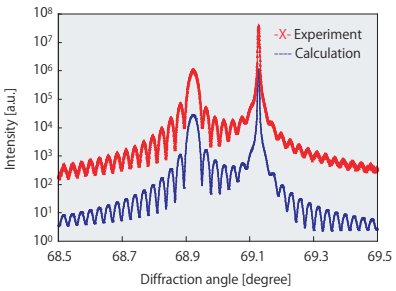
Orientation information can be obtained from pole figure measurements.
Pole figures represent the way in which individual crystallites are oriented within the film. The ability to collect data in theta-theta mode using Rigaku's patented in-plane geometry allows the user to collect an entire pole figure ($\alpha = 0 - 90°$) of a thin film.

XRR provides accurate measurement of thin film thickness, roughness, and density. XRR analysis software provides interactive modeling and automated curve fitting capability.

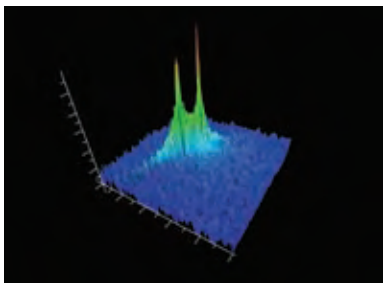
Pole figure Bi_2O_3 film (111)



Rocking curve SiGe/Si (004)



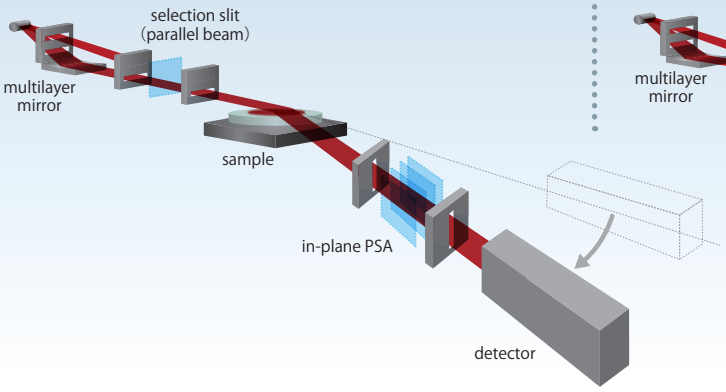
Reciprocal space map SiGe/Si (224)



Precise measurements are aided by Guidance software, which provides automated sample alignment and simulation of reciprocal space.

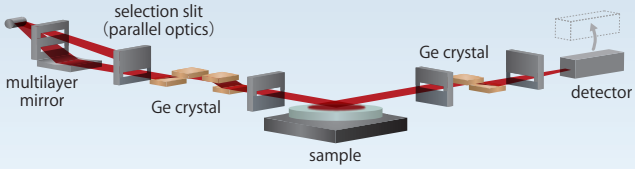
In-plane geometry

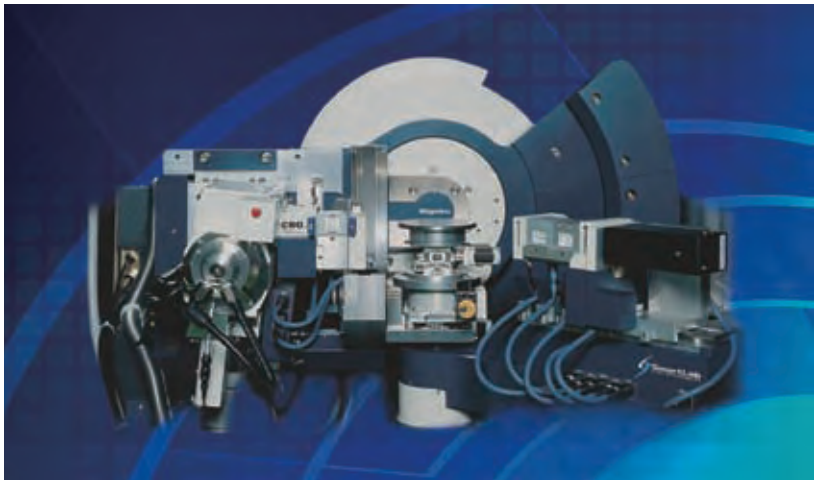
With the addition of Rigaku's proprietary in-plane attachment, it is possible to evaluate structures perpendicular to the sample surface and perform depth profiling without base information. Our pole figure measurement function enables you to obtain perfect pole figures from thin film samples that were previously unmeasureable, opening the door for sophisticated orientation studies.



High resolution/triple-axis

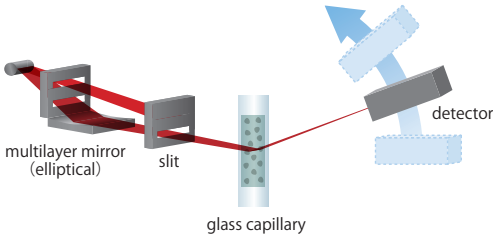
Adding a channel cut crystal to an intensity-focused multilayer mirror it is possible to make high-resolution reflectivity, rocking curve and reciprocal lattice measurements. Dedicated software provides fine-grain control over the 4-axis thin film sample stage and rotary attenuator, automatically optimizing the sample position.





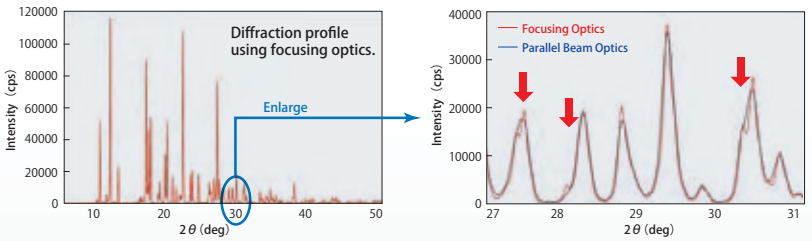
SmartLab with 9 kW rotating anode

Focusing mirror and Bragg-Brentano switch system



With the combination of a focusing mirror at the detector position and a 1D high-speed detector, it is possible to obtain high resolution, high intensity data with the transmission method. Suitable for nanoscale samples, oriented samples, and closed-atmosphere samples. With CBO-E it is possible to change to the standard reflection method (Bragg-Brentano) at the press of a button. Not solely for focusing optics, this multi-purpose instrument demonstrates exceptional versatility.

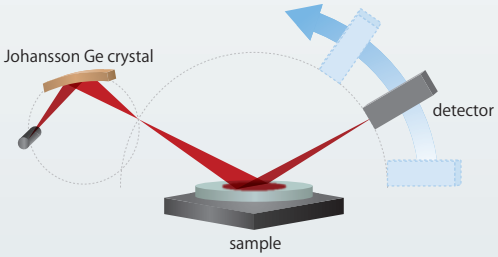
Comparison of diffraction profiles using focusing optics and high resolution parallel beam optics from Indometacin, an analgesic anti-inflammatory drug

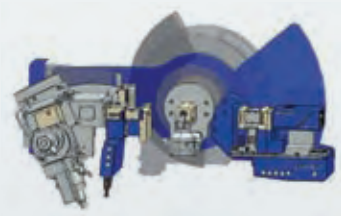


Comparing the angular resolution (normalized intensity) of focusing and parallel beam optics, the improvement in peak separation is evident.

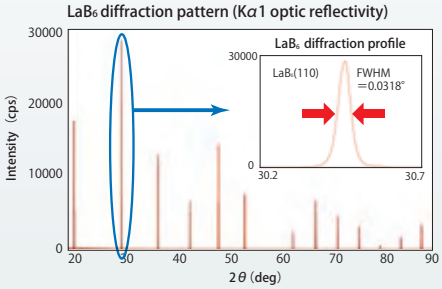
Kα1 Optics

The above shows symmetric Johansson Kα1 optics. Along with high intensity for microfocus, the symmetric Johansson configuration provides high resolution. And, when paired with CBO or CBO-E, it is possible to create focusing and thin film optics with the Kα1 (singular) characteristic line. Free yourself from time-consuming optics exchanges while continuing to employ the optimum optics configuration for a wide range of samples.



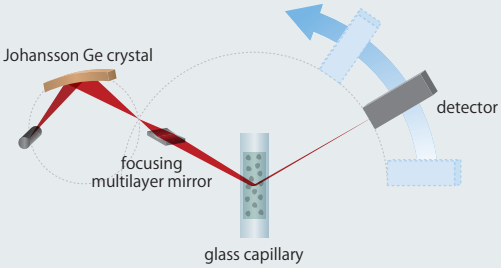


NIST SRM 660a LaB_6 diffraction profile and half-width

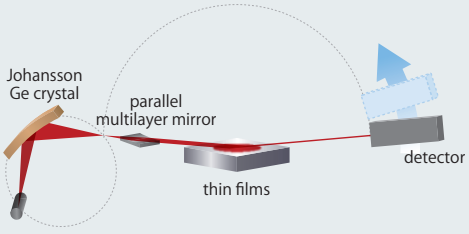


Completely eliminate Kα2 and achieve high resolutions with a half-width of 0.04°

Transmission measurement

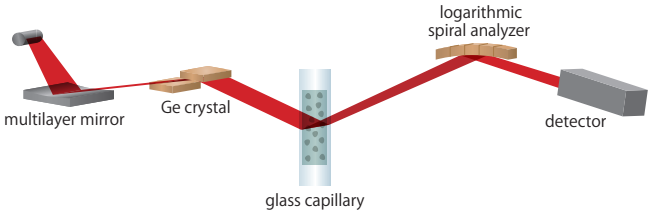


Thin film measurement

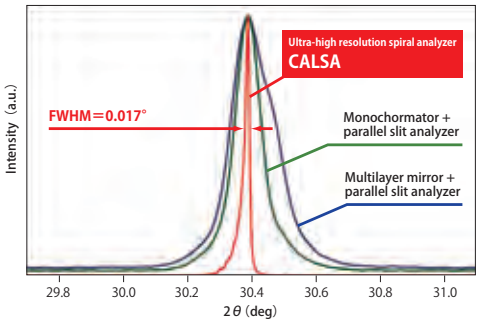


CALSA Ultra-high resolution spiral analyzer

An ultra high resolution Ka1 parallel beam optic developed with proprietary Rigaku technology. Two Ge crystals on the incident optic side ensure that the sample is only exposed to Kα1 characteristic rays. The combination of a multi-crystal Ge analyzer and a high-speed 1D detector provides high-resolution measurement capabilities comparable to those achieved with synchrotron lightsources.



NIST SRM 660 aLaB6110



CBO-f Micro-area measurement optics unit

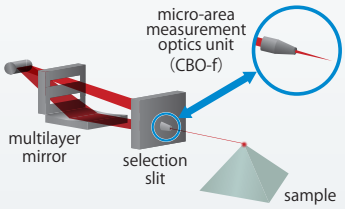
■ No need to switch between line- and point-focus modes

With the addition of CBO-f, Rigaku's newly developed optic for micro-area measurement, it is no longer necessary to reconfigure the system to point- or line-focus modes. CBO-f makes micro-area measurements fast.

■ High S/N Ratio Measurement

Achieve a high signal-to-noise ratio with monochromated, focused, high-brilliance X-rays.

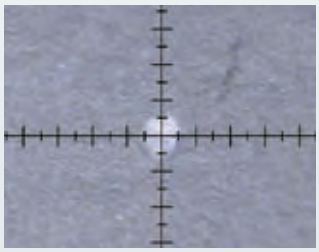
Explore the full potential of small spot measurement.



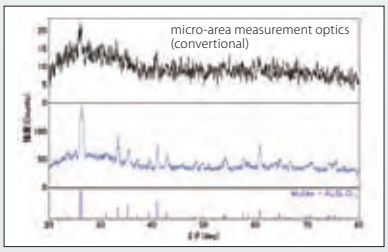
Micro-area measurement

CBO-f can take X-rays directly from a line-mode light source, focusing them to ϕ0.4 mm to irradiate the sample. It is possible to obtain over ten times the intensity of existing optics. CBO-f adjustment is automatic.

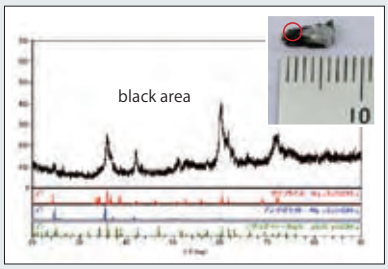
Serpentine, a mineral group that is pulverized for the mortar additive used in plaster is, has three major polymorphs: non-asbestos antigorite, lizardite, and chrysotile (found in asbestos). The X-ray diffraction patterns in the images above are the results of measurements taken from the black and white areas seen in the photos, each one smaller than 1 mm in diameter.
By comparing the measurements with a database, it was found that the white area is primarily composed of calcite, a polymorph of calcium carbonate, whereas the black area includes chrysotile, antigorite and lizardite.

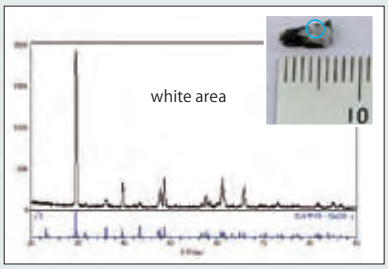


CCD view



Insulator (φ0.4 mm)





Optics
Stage & Attachment

SmartLab
X-RAY DIFFRACTOMETER

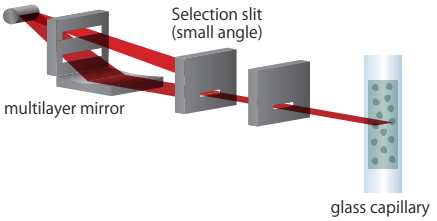
SAXS Small Angle X-ray Scattering

Small Angle X-ray Scattering (SAXS) is fast becoming an important tool in the study of the structure of nanomaterials. Usually reserved for specialists working on dedicated instruments, SAXS data can be difficult to collect and interpret.

SAXS applications include:

- **Particle size distributions of nanoparticles suspended in solution**
- **Particle/pore size distributions in deposited or bulk solid nanomaterials**
- **Particle shape analysis**
- **Correlation function analysis of irregular electron density distributions**

SAXS

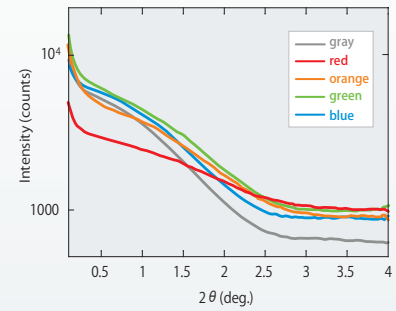


Features from 1 - 100 nm in size may be studied using the SmartLab in SAXS mode. SmartLab's optional rotating anode power makes the measurement extremely sensitive, allowing measurement of dilute or weakly contrasting scatterers.

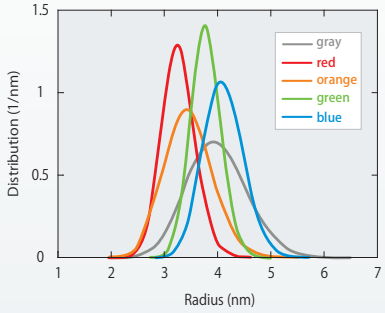
NANO-Solver provides size distribution functions of nanoscale pore/particles and correlation length functions for materials with density fluctuation based on the non-linear least square curve fitting analysis of X-ray small angle scattering profiles.

※Data provided courtesy of Assoc. Proff. Takahisa OMATA,Osaka University, Japan and Dr. Hideaki MAEDA and Dr. Hiroyuki NAKAMURA, AIST, Japan

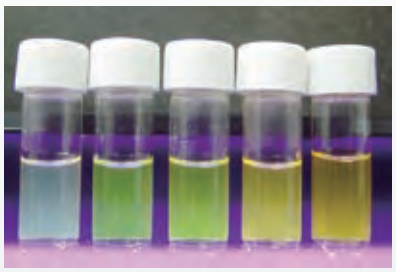
Small angle scattering profile
nano size Cd-Se particles (※)



Particle size distribution (※)



Nano size Cd-Se particles during
UV radiatin (※)

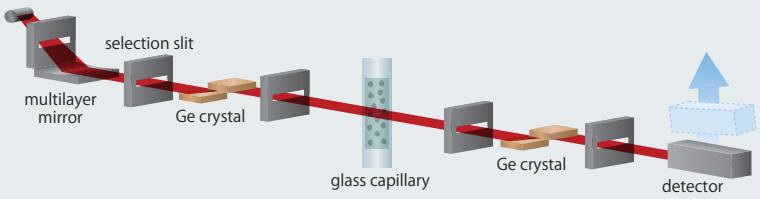


Ultra SAXS

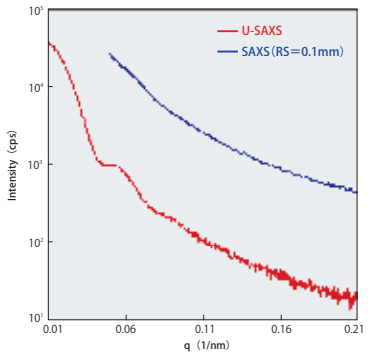
With the crystal spectrum, Rigaku was able to develop a high resolution transmission method optic for use in SAXS.

With high resolution at 0.03° (q=0.02nm^{-1}), this configuration is ideal for the analysis of photonics crystals with large particle diameters and lattice constants.

U-SAXS



Comparison of U-SAXS and SAXS profiles



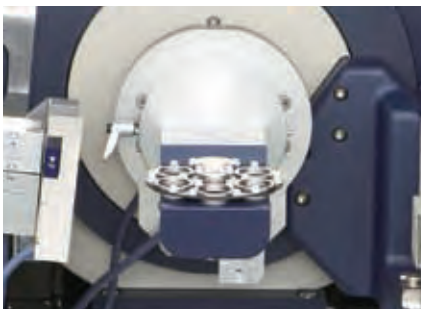
Sample: Colloidal silica 200 nm

sample	USAXS		Light scattering	
	average	FWHM*	average	FWHM*
200 nm	193	51	198	37
750 nm	728	95	747	162

With high resolution at low angles, it becomes possible to analyze particles with diameters in the hundreds of nanometers

Sample stages and attachments

6 position auto sample changer

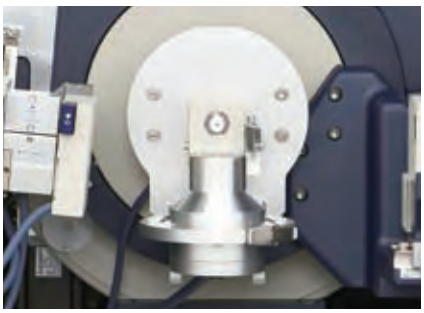


This sample changer makes it possible to perform consecutive measurements on up to 6 sam-ples with the ability to make reflectivity and transmission measurements.

Specifications

Samples	Max. 6
Sample rotation rate	60rpm to 120rpm
Sample (plate)	Reflection method holder Transmission method holder

Capillary Rotation Attachment



When measuring crystals in a capillary it is possible to reduce the effects of orientation by rotating the crystal during trans-mission measurement.

Specifications

Sample rotation rate	60rpm to 120rpm
Capillary Holder	For 1.0mm / For 0.7mm / For 0.5mm For 0.3mm

$\alpha\beta$ Stage

Pole figures, thin films, distor-tions... perform all of these mea-surements.
Avoid time-wasting attachment changes.

Specifications

α-axis range	−5° to 95°
β-axis range	360° Max. 30rpm
Pivot shaft	±10mm (back and forth toward 45° direction)

β-rotation Stage

By in-plane rotation of the sample, the number of diffract-ing crystallites increases and the effect of coarse crystal surfaces can be reduced.

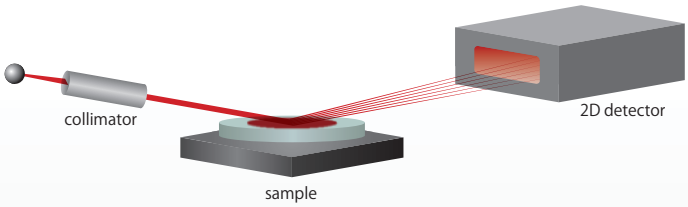
Specifications

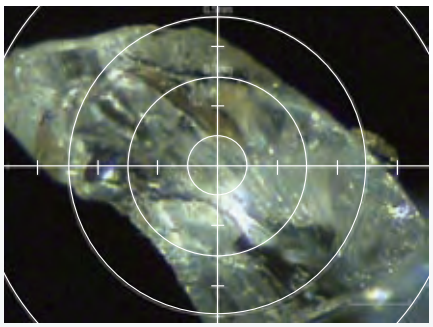
Sample rotation rate	60rpm to 120rpm
Attachment	Standard XY 20mm, XY 4", RxRy

PILATUS 100K/R

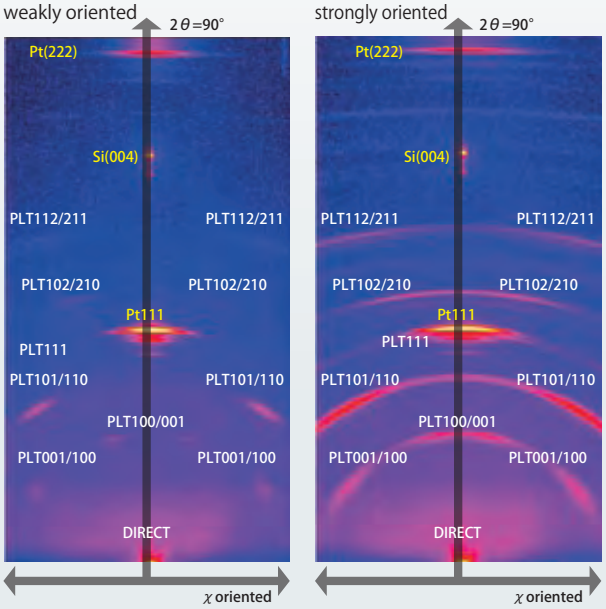
2D silicon detector

Perform microscopic or trace qualitative analysis, thin film structure determination, comprehensive 2D residual stress measurements, crystal orientation and alignment studies and more. With horizontal sample placement for SAXS measurements, this high-speed high-sensitivity system combines a point focus X-ray source and a low-noise CMOS hybrid 2D detector.



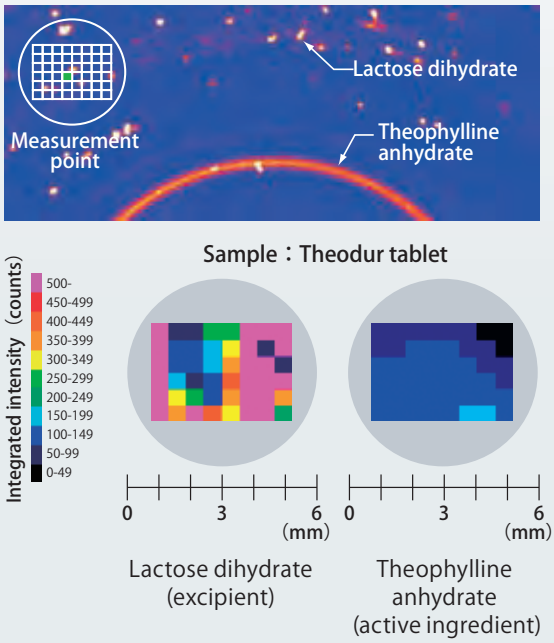


CCD View



※PLT is (Pb,La) TiO_3
Samples: 2 types of PLT, (Pb,La)TiO_3/Pt/Si-Sub
Measurement range: 2θ =0～90°
Measurement time: 90 sec.
Instrument: SmartLab

Tablet Mapping Measurement



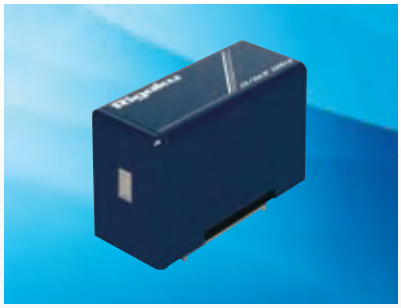
Lactose dihydrate (excipient)

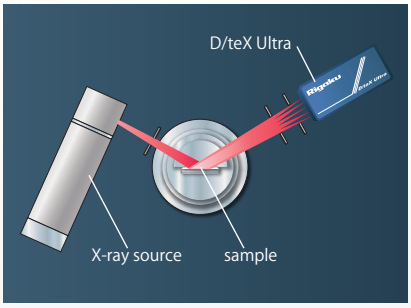
Theophylline anhydrate (active ingredient)

D/teX Ultra
1D high-speed detector

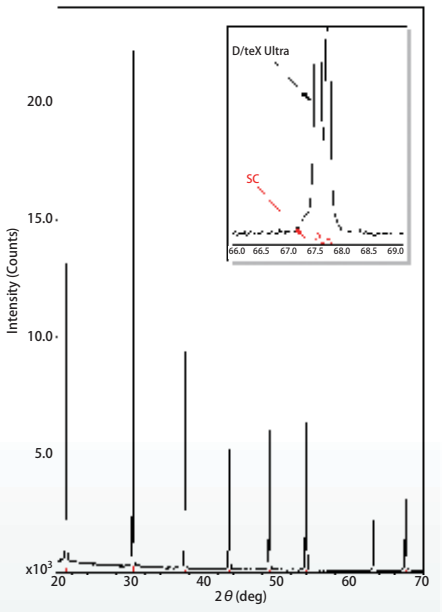
■ Rapid measurement and high energy-resolution
Compared to existing detectors, D/teX Ultra can give you approximately 100 times the speed or intensity. With its best-in-class energy resolution, you can even reign-in the climbing background seen when measuring ferrous samples with Cu target sources.

■ Combine speed with sensitivity
Wide-angle powder diffraction profiles can be measured in minutes. Analyze low quantity samples and detect trace components.





High sensitivity measurement

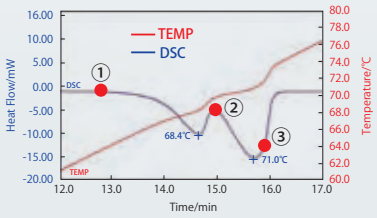


With 100x the sensitivity of existing detectors (compared to our standard model), analyzing trace components is easy.

X-ray DSC Simultaneous X-ray diffraction and differential scanning calorimetry measurements

During phase changes, dehydration, melting and solidification, a material's crystalline state changes constantly. With XRD-DSC, it is possible to analyze changes to the crystalline state with X-ray diffraction while simultaneously monitoring thermal changes with DSC. The instrument is well suited to a wide range of applications, including the evaluation of organic and inorganic compounds, pharmaceutical products, polymer macromolecules, ceramics, electronics materials etc. Simultaneous measurement ensures that the sample, temperature and atmospheric conditions are all identical, dramatically improving the credibility of analysis results and increasing (R&D and quality control) efficiency

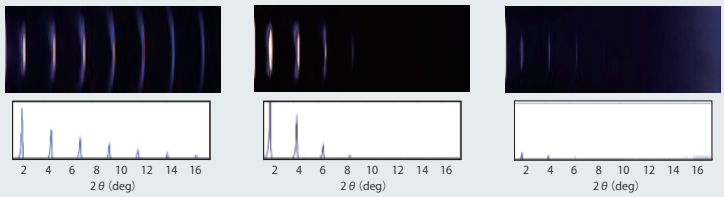
Transition, melting and crystallization over rising and falling temperature in straight-chain hydrocarbon dotriacontane (n-C32 H66)



Sample weight: 5.92mg
Heating rate: 3℃/min

When combined with the PILATUS 100K/R, changes in the diffraction pattern during transition and melting can be observed in real time.

① pretransition：63.1℃ ② post-transition：70.5℃ ③ fusing OR melting：71.2℃



PDXL Integrated powder diffraction analysis software

■ Increase your qualitative capabilities with hybrid search matching !

Combining the advantages of peak based and profile based qualitative analysis, Rigaku's proprietary Hybrid Search Match technology will improve your qualitative analysis results.

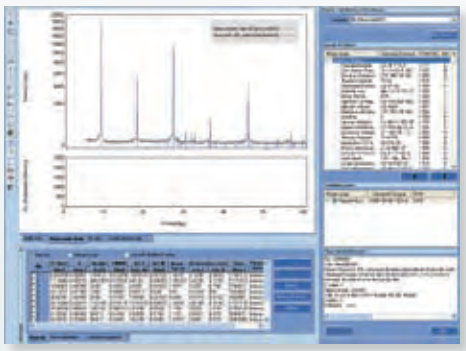
Previously difficult tasks like the identification of crystal phases with preferred orientation or complex lattice distortions are made easy.

■ Simplified quantitative analysis with the Rietveld method

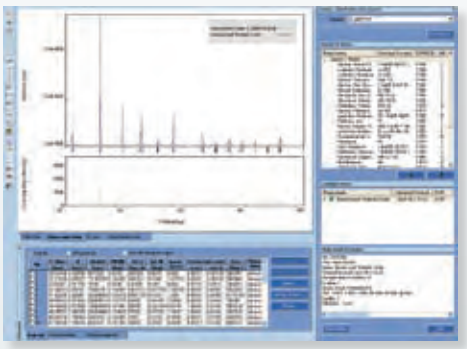
Until now, X-ray diffraction-based quantitative analysis was a complex process involving mixing the sample with a standard reference material, measuring it, using those results to create a calibration curve and then determining quantity. Using the Rietveld method it becomes easier to perform quantitative analyses and there is no need to create a calibration curve.

Quantitative analysis with the Rietveld method is generally perceived as difficult to do correctly, but PDXL's easy-to-use interface makes it a simple task for both beginner and expert alike.

Orientation

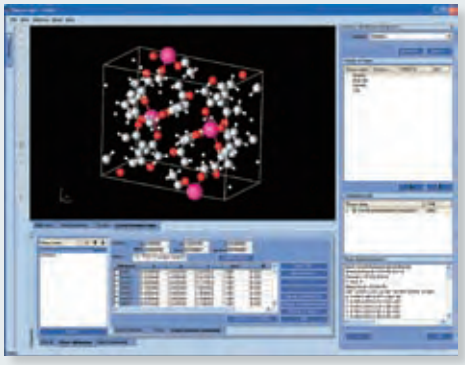


Solid Solutions



PDXL Rietveld Analysis Profile

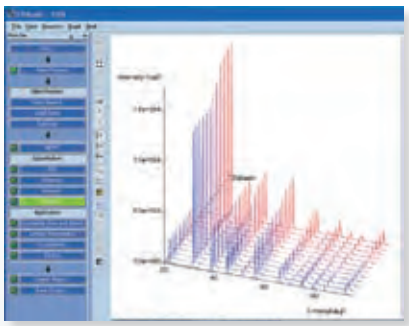
Organic Crystal Structure Refinement



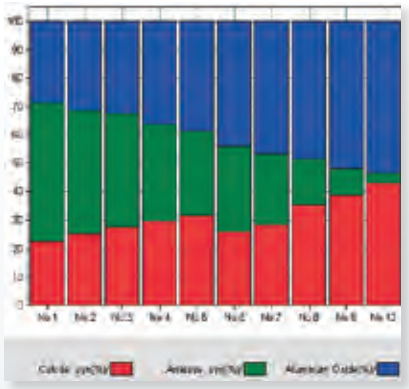
■ Drastically reduce operation time with automated analysis, private report generation

Use PDXL's automated analysis functionality to process multiple data sets under the same conditions, or to compare the analysis results from samples measured under different conditions. Then, let PDXL save you even more time by automatically generating reports from the saved analysis results.

Automated analysis using the PDXL Flow Bar



Graph quantitative results from varied synthesis conditions

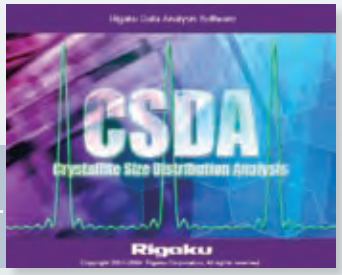


Create analysis reports

Extensive software library

Crystallite Size Distribution Analysis

CSDA



3 D Display & Analysis

3D Explore

Nanoscale Pore/ Particle Size Distribution

NANO-Solver

General Purpose 2 D Data Processing

2DP

Specifications

X-ray generator	Maximum rated output	3kW	9kW
	Rated tube voltage	20 to 45kV (60kV optional)	20 to 45kV
	Rated tube current	2 to 60mA	10 to 200mA
	Type	Sealed tube	Rotating anode
	Target	Cu (Other targets available)	
	Focus size	0.4×8mm (line/point) (others optional)	0.4×8mm (line focus)
Goniometer	Scanning mode	θs/θd coupled, θs, θd independent encoder controlled	
	Goniometer radius	300mm (Options available)	
	Min. step size	0.0001°	
	Sample height (Z-axis)	Z：−4～+1mm	
	Sample stage (optional)	χ：−5～+95° φ：0～360° X, Y：20mm, φ100mm Rx, Ry：−5～+5°	
	Sample size	Max. φ150mm×3mmt (24mmt optional)	
Optics	Incident side	CBO,automatic variable divergence slit Ge 2-bounce and 4-bounce monochromators (optional)	
	Receiving side	Automatic variable scattering slit Automatic variable receiving slit PSA, Ge 2-bounce analyzer (optional)	
Detector	Scintillator NaI	Scintilation counter：Scintilator (NaI) D/teX Ultra (optional) PILATUS 100K/R (optional)	

Installation Requirements

		3kW	9kW
Power	Instrument	3φ AC200V±10% 50/60Hz 28A [30A]	3φ AC200V±10% 50/60Hz 50A [60A]
	Computer	1φ AC100V±10% 50/60Hz 5A [15A] (grounded socket)	
Earth		D-type, ground resistance under 100Ω, used for 1 system only	
External dimensions		Standard：1200 (W)×960 (D)×1930 (H) mm	
		In-Plane：1200 (W)×1230 (D)×1930 (H) mm	
Mass		Approx. 750kg	Approx. 850kg

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Rigaku

Rigaku Corporation Tokyo Branch
4-14-4, Sendagaya, Shibuya-ku, Tokyo 151-0051, Japan
Phone:+81-3-3479-0618 Fax:+81-3-3479-6112 e-mail:rinttyo@rigaku.co.jp **www.Rigaku.com**

Rigaku Corporation
Head Office
3-9-12, Matsubara-cho, Akishima-shi, Tokyo 196-8666, Japan
Phone:+81-42-545-8189 Fax:+81-42-544-9223
e-mail:rinttyo@rigaku.co.jp

Rigaku Americas Corporation
9009 New Trails Drive,The Woodlands, Texas 77381-5209, USA
Phone:+1-281-362-2300 Fax:+1-281-364-3628
e-mail:info@rigaku.com

Rigaku European SE
Gross-Berliner Damm 151, 12487 Berlin, Germany
Phone:+49-30-6264035-0 Fax:+49-30-6264035-10
e-mail:rese@rigaku.co.jp

Rigaku Corporation
Osaka Factory
14-8, Akaoji-cho, Takatsuki-shi, Osaka 569-1146, Japan
Phone:+81-72-693-7990 Fax:+81-72-693-6746
e-mail:rinttyo@rigaku.co.jp

Rigaku Beijing Corporation
2601A, Tengda Plaza, No. 168, Xizhimenwai Avenue,
Haidian District, Beijing 100044, P.R.China
Phone:+86-010-8857-5768 Fax:+86-010-8857-5748
e-mail:info@rigaku.com.cn

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