

## XRD-6100 XRD-6100 OneSight



### Ease of Use and Abundant Functions Herald a New Era of Analysis

The Windows<sup>®</sup>-supported application software ushers this compact, multi-functional, general-purpose X-ray Diffractometer into the networking era of analysis.

X-Ray Diffractometer

## Lab XRD-6100 / XRD-6100 OneSight<sup>™</sup>



In addition to its basic ease of use and abundant functions, the XRD-6100 boasts an integrated design featuring a vertical goniometer and data processing software supporting the Windows<sup>®</sup> user interface.

The XRD-6100 offers solutions encompassing wide-ranging analysis requirements, from routine qualitative and quantitative analysis to state change analysis, including stress analysis, residual austenite quantitation, crystallite size/lattice strain, crystallinity calculation, materials analysis via overlaid X-ray diffraction patterns, enhanced material evaluation and sample heating analysis. Of course, crystalline structural analysis, including precise lattice constant determination, is also supported.

### A General-Purpose X-ray Diffractometer to Address Your Various Analytical Needs

#### Features

#### High-Precision and Reliable Built-in Vertical Goniometer

The goniometer mounted on the XRD-6100 is compact and simple. All the components in the X-ray optical system are precisely assembled and adjusted at the factory and have been designed to ensure that accuracy is maintained. Thus, there is absolutely no need for users to make any adjustments in the future.

#### Windows® 10 Employed as Software Platform

The main unit control and data processing software support the widely used Windows<sup>®</sup> 10 user interface. For this reason, data can be exported to marketed software. Network support and multi-user accessibility are easily achieved.

### Multi-Functional Auto-Search/Match Software (Qualitative Analysis) and Quantitative Analysis Software Equipped as Standard

The XRD-6100 is equipped with auto-search / match software as standard to aid qualitative analysis - the important analysis task of X-ray diffraction. The detailed search parameter settings, second search function, and the comparison display of candidate substances on a raw data profile make analysis easy to understand - even for beginners. What's more, a greater success ratio in results can be achieved with the system. In addition, a simplified quantitative calculation function using the RIR method\* and a function that allows users to create their own database are included in the system as standard.

#### Safe, Compact and Sophisticated Body

The main body (W900 × D700 × H1600 mm) has been massively slimmed. As the rear is a sheer flat surface with no superfluous protrusions, the device can be placed up against walls, which means it does not take up room when installed on site or in the lab. Furthermore, the unit is designed to save energy; the X-ray is OFF when the door is open and the power is turned ON only at the start of measurement (only the filament is always ON; Shimadzu patent). In addition, the door lock mechanism works when sample measurements are taken (when X-rays are emitted) to provide a safe operating environment for protection against X-ray exposure.

#### OneSight Wide-Range High-Speed Detector Available

It is able to achieve qualitative analysis more than 10 times faster than a conventional scintillation detector.

### **Applications of X-ray Diffractometry**

#### Ferrous Metals

#### Steel

Qualitative analysis of steel sheet, measurement of

residual austenite and residual stress, analysis of friction and wear test samples, measurement of iron oxide films and nitride layers, evaluation of plating and texture.

#### Cast Iron

Qualitative analysis of precipitates and additives in cast iron, etc.

#### Surface-Treated Steel

Evaluation of characteristics of surface-treated areas, quality control, residual stress measurement.

#### Non-Ferrous Metals

#### Copper and Zinc

Qualitative analysis of alloys, orientation measurements of foil samples, evaluation of texture, qualitative analysis of plated areas, etc.

#### Aluminum

Qualitative analysis (aluminum, aluminum alloys, oxides and nitrides), evaluation of texture in rolled material.

#### Other Metals

Qualitative analysis (metallic compounds, oxides and nitrides), characteristic evaluation of surface-treated areas, residual stress measurement.

#### Machinery, Automobiles and Shipbuilding

#### Machinery

Qualitative analysis of tool steels, surface condition analysis of machined parts, analysis of austenite layers, qualitative analysis of surface plating, residual stress measurement.

#### Automobiles and Shipbuilding

Qualitative analysis of structural parts, surface quantitative analysis of austenite, residual stress measurement, qualitative analysis of exhaust gas catalysts, etc.

#### Chemicals and Catalysts

#### Chemicals

Qualitative analysis of organic and inorganic chemicals, impurity analysis.

#### Catalysts

Qualitative analysis and measurement of crystalline, measurement of crystallite size to check final product.

#### Ceramics

#### Porcelain and Ceramics

Qualitative analysis of raw materials, final product evaluation, analysis of crystal structures during heating (crystal system, crystallite size, lattice constant).

#### Cement and Glass

Qualitative and quantitative analysis of clinker and cement (free lime, etc.), qualitative analysis of raw materials. Qualitative analysis and orientation measurements of thin film layers formed at the glass surface.





#### Pharmaceuticals and Medical Treatment

#### Pharmaceuticals

Qualitative analysis of pharmaceutical raw materials and identification of impurities. Crystal polymorphism analysis and crystallinity measurements, quality control during pharmaceutical manufacture using crystallite size measurement, final product quality check, crystal polymorphism analysis related to patents.

#### Dental Materials

Qualitative analysis of dental materials such as apatite, etc.

#### Electrical and Electronic Materials

#### **Electrical Components**

Qualitative analysis of corrosion and adhering matter on electrical contacts. Stress measurements in structural parts, qualitative analysis of plated parts, etc.

#### **Electronic Components**

Qualitative analysis and orientation measurements of thin-film electronic materials. Measurement of substrate crystal orientation for magnetic heads and electronic elements.

#### **Battery Materials**

Crystal structure analysis of battery materials.

#### Construction and Civil Engineering

Qualitative/quantitative analysis of asbestos in construction materials, qualitative analysis of construction materials such as tiles and bricks.

#### Environment and Industrial Wastes

#### Environment

Qualitative/quantitative analysis of asbestos and free silicic acids in the work environment. Qualitative analysis of dust.

#### Industrial Waste

Qualitative analysis of residual matter in plating liquids, combustion ash, coal ash, and furnace slag.

#### Resources and Energy

#### Coal, Oil and Natural Gas

Plant-scale qualitative analysis, evaluation of carbon materials, evaluation of catalysts during petroleum refining.

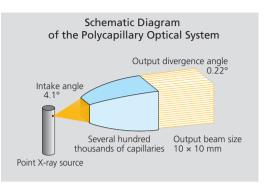
#### **Rocks and Minerals**

Qualitative analysis of raw materials and identification of impurities. Qualitative/quantitative analysis of asbestos minerals (compatible with PRTR method).

### **Polycapillary Optical System**

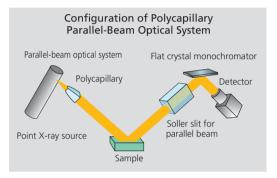
#### Principle of the Polycapillary Optical System

The fine glass capillaries in the order of several microns are arranged in a solid as guides to multiple X-rays. The X-rays pass along each capillary while repeating total internal reflection and exit from the opposite end of the polycapillary system. The capillaries are curved so that repeated total internal reflection is allowed, and the X-rays from the point X-ray source exit the unit as a parallel beam with a large solid angle.

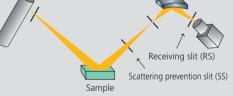


#### Features of the Polycapillary Optical System

Compared with the conventional focused-beam system and the normal parallel-beam system, the polycapillary optical system more efficiently exploits the beam from the X-ray tube, resulting in higher diffraction X-ray intensity. A displacement of the sample in a Bragg-Brentano optical system can move it outside the focus, causing a significant displacement in height in diffraction angle and a dramatic drop-off in diffraction X-ray intensity. Conversely, a displacement of a few millimeters in a parallel-beam system has no effect on the diffraction angle and a small decrease on the diffraction X-ray intensity. Consequently, incorrect loading of the upper and lower sample faces or an irregular surface causes no angular displacement and accurate measurement is possible. The parallel-beam system also allows analysis of curved surfaces, something not possible with conventional optical systems.

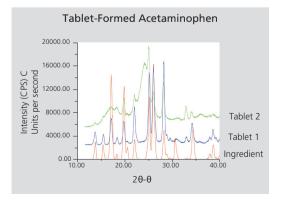


# Configuration of Bragg-Brentano Optical System Divergence slit (DS)



## Sample Measurement Using the Polycapillary Optical System

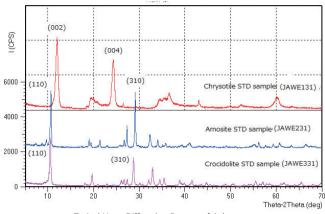
This example shows measurements of the raw drug acetaminophen and its tablets during the process of manufacturing. Tablets can be directly analyzed to evaluate the degree of crystallinity and crystal polymorphism. The XRD-6100 is able to perform accurate, highly sensitive measurements on irregular surfaces or curved surfaces like this.



### Qualitative and Quantitative Analysis of Asbestos and Free Silicic Acids

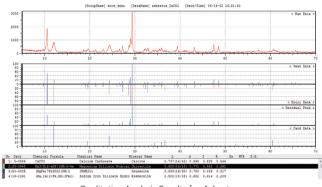
The content of asbestos in construction materials is measured using phase dispersion microscopes and X-ray diffractometers. After pulverizing the sample acquired from the site in a pulverizer, a phase dispersion microscope and X-ray diffractometer are used respectively to qualitatively analyze the sample. If the sample is determined to contain asbestos at this stage, then it is guantitatively analyzed using the X-ray diffractometer. In actual practice, asbestos analysis (JIS A 1481-3) requires sensitivity sufficient to determine 0.1 % content by weight in 100 mg of acquired sample. To increase sensitivity so that such trace asbestos levels can be detected, formic acid is used to dissolve matrix components in the pulverized sample. Then the residue after formic acid treatment is recovered in a fluorocarbon polymer binder filter using a suction filtration system for use in quantitative analysis. The quantitative analysis is performed using an X-ray diffractometer, where the absorption of diffracted X-rays must be corrected to compensate for the asbestos itself and the undissolved matrix components. This correction process (base standard absorption correction method) involves first measuring the metal plate (base plate) for a blank filter, placing the filter with the formic acid-treated asbestos in the diffractometer, and measuring the asbestos together with the metal base plate to determine a correction factor from the diffraction intensity ratio of the metal plate. Then that correction factor is used to determine the corrected asbestos diffraction intensity. Note that this method was originally developed for measuring the free silicic acid content in mineral particulates during work environment measurements. The XRD-6100 X-ray diffractometer environmental measurement package includes a filter holder and rotational sample stage for use in the base standard absorption correction method, and environmental quantitation software for performing quantitative calculations that correct for absorption. This environmental quantitation software incorporates Shimadzu's proprietary measurement expertise cultivated from many years in this field, which is especially valuable when guantitating particularly trace levels of asbestos.

In addition, this XRD-6100 X-ray diffractometer environmental measurement package is compliant with methods specified in the Notification No. 0828001 by the Director of the Chemical Hazards Control Division, Industrial Safety and Health Department, Labour Standards Bureau, Ministry of Health, Labour and Welfare of Japan, such as for analyzing asbestos in natural minerals or measuring the free silicic acid content in mineral particulates during work environment measurements.

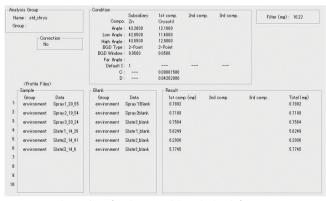


Typical X-ray Diffraction Pattern of Asbestos

The major types of asbestos are serpentine asbestos (chrysotile) and amphibole asbestos (amosite and crocidolite). The characteristic peaks of these types can be quantitatively analyzed by X-ray diffractometry.







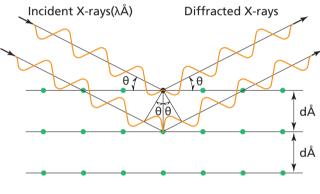
Screenshot of Environmental Quantitation Software

Note: Please obtain the ICDD database separately for analysis of asbestos and free silicic acids.



#### **Principle of Operation**

The XRD-6100 analyzes crystalline states under normal atmospheric conditions. Furthermore, this method is non-destructive. X-rays hit a sample loaded in the center of the goniometer and are diffracted by the sample. The changes in the diffracted X-ray intensities are measured, recorded and plotted against the rotation angles of the sample. The result is referred to as the X-ray diffraction pattern of the sample. Computer analysis of the peak positions and intensities associated with this pattern enables qualitative analysis, lattice constant determination and/or stress determination. Qualitative analysis may be conducted on the basis of peak height or peak area. The peak angles and profiles may be used to determine crystalline size and degree of crystallization, and are useful in conducting precise X-ray structural analysis.



 $\lambda = 2d \cdot sin\theta$ 

#### Applications

Ferrous metals, non-ferrous metals, machinery, shipbuilding, welding, automobiles, ceramics, cement, glass, catalysts, electrical parts, electronic materials, magnetic materials, battery materials, fibers, paper, pulp, food products, chemicals, agricultural chemicals, dies, pigments, paints, pharmaceuticals, dental materials, biological matter, petroleum, coal, power generation, natural gas, mining ore, soil, rocks, clay, minerals, construction, civil engineering, environment, and industrial waste.

#### Construction

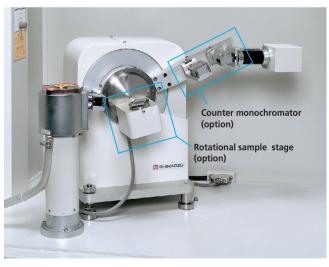
#### Compact, X-ray-Protected Housing

The compact construction (W900xD700xH1600mm) minimizes installation space requirements.

The front door is mounted on guide rollers, enabling light and smooth opening of the door. Therefore, it is easy to facilitate the installation/exchange of samples and attachments. A magnet latch assures the door closes; to further ensure safety, a door interlock mechanism is automatically activated whenever X-rays are generated.

#### High-Precision, Vertical $\theta\text{-}\theta$ Goniometer

High-speed rate (1000°/min) and high-precision angle reproducibility (±0.001°) provide fast measurement and highly reliable data. The  $\theta$ - $\theta$  Vertical goniometer unit allows analysis of samples in various states, substantially widening the application range. The drive mechanism features an independent dual axis  $\theta$  -2 $\theta$  linkage drive, and independent 2 $\theta$ and  $\theta$  axis drives, freely selectable for efficient thin film and various other types of analysis.



Vertical Goniometer

#### High-Voltage Transformer for High Output X-ray Tube

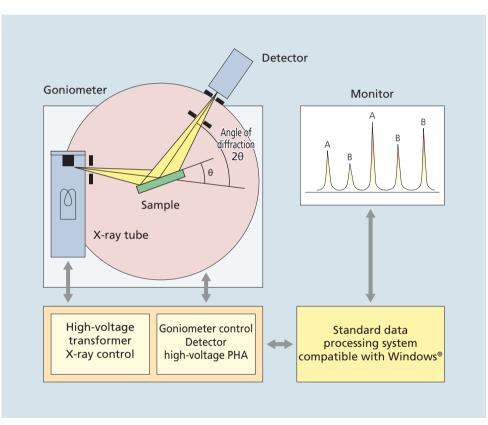
The high-voltage transformer supports either the 2.2kW high output fine focus X-ray tube or 2.7kW high output broad focus X-ray tube.

#### X-ray Tubes

The XRD-6100 will accept various types of X-ray tubes, including the normal focus (NF) 2kW type and broad focus (BF) 2.7kW type, which are standard accessories, as well as the optional long fine focus (LFF) 2.2kW type. By attaching the optional counter monochromator, all types of samples, including Fe samples, can be analyzed using the standard Cu X-ray tube.

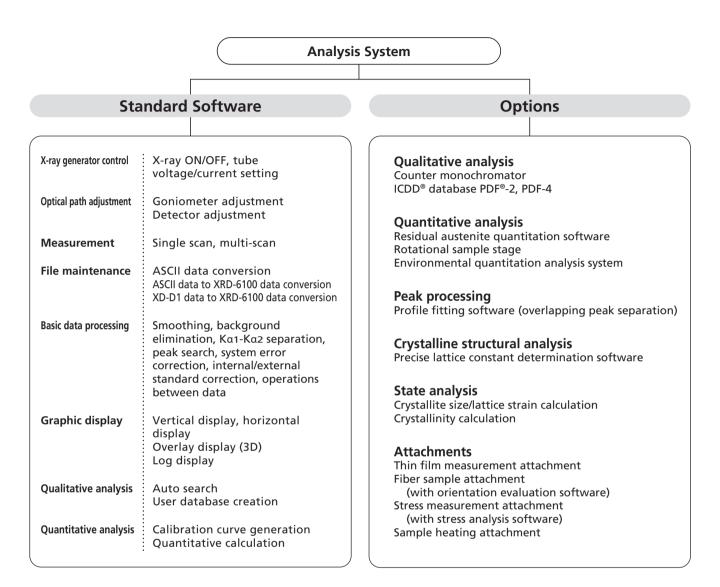
#### Highly Stable X-ray Generator

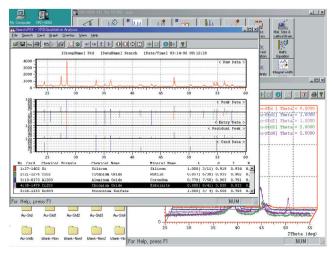
Shimadzu's extensive experience in producing high-performance X-ray generators has enabled the production of a highly stable X-ray generator, with tube voltage and tube current both stable to within  $\pm 0.01\%$  with respect to 10%voltage fluctuation. This stability is unaffected during fluctuation of source voltage or ambient temperature, ensuring high reliability of data even during prolonged periods of data acquisition.



XRD-6100 Relational Diagram

### Providing a Complete Analysis System



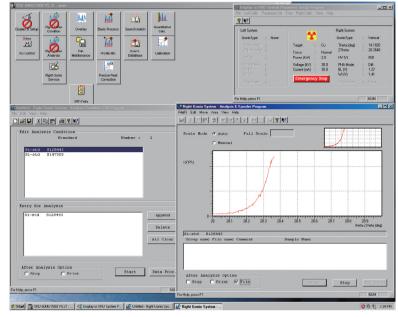


Auto Search Results and Thin Film Sample Overlay Display

### Automatic Measurement, Easy Operation

#### **Measurement Display**

Sample measurement conditions can be set easily. The scheduling and the progress condition of the measurement can be confirmed in one view by the analysis & spooler.

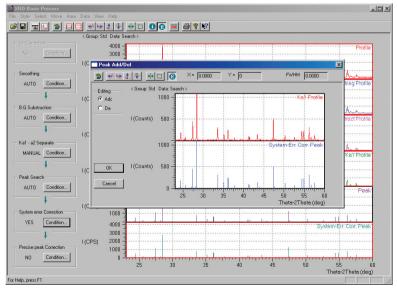


Measurement Screen

### Multitasking for Enhanced Analysis Efficiency

#### **Basic Data Processing**

The multitasking capability provided with the Windows® (OR Windows®10) operating environment allows measurement and data processing to be conducted simultaneously, enhancing the efficiency of analysis operations.



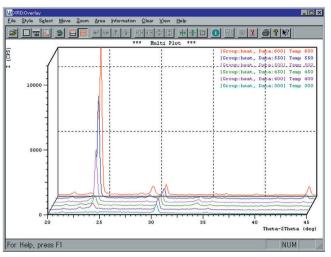
Basic Data Processing Screen

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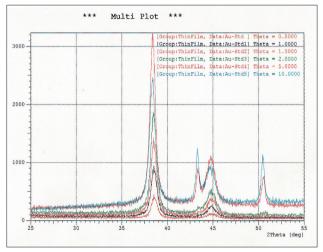
### **Comfortable Data Processing Environment**

#### **Graphic Display**

Data can be freely zoomed with a click of the mouse, so profile comparison of thin film data or heating measurement data can be easily accomplished using a combined 2-dimensional or 3-dimensional display. The software also features a variety of other useful graphic functions, such as intensity Log conversion display and hidden-line processing on the 3-dimensional display. Each type of data can be output to a color printer, so differences between samples can be recognized at a glance.



3-Dimensional Screen of Thin Film Sample



2-Dimensional Output of Thin Film Sample

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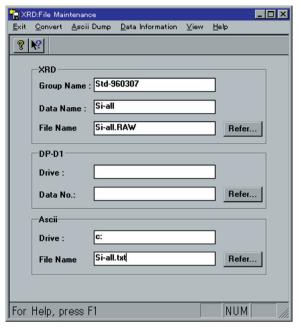
### Addition/Subtraction Operations

Data manipulation functions such as deletion of unnecessary peak profiles and addition of duplicate measurement data to obtain a summed profile are some of the invaluable tools available for conducting efficient data analysis. Profile calculations are conducted in the window displayed on the right.



#### File Maintenance ~Data Format Conversion~

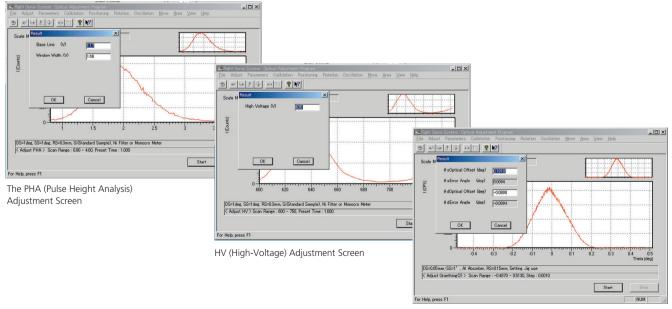
With the XRD-6100, data measured by other x-ray diffractometers can be converted into files to enable analysis using this data processing software. In the case of other x-ray diffraction data,  $2\theta$  angle and x-ray intensity text files (ASCII data) can be converted into XRD-7000 data format. In reverse, raw data measured by the XRD-6100 also can be converted into text files or files formatted to enable Rietveld analysis. Furthermore, processed data including peak data, as well as raw data, can be converted to text format, facilitating data processing in customized formats.



File Conversion Window

#### **Optical System Adjustments**

The XRD-6100 system makes fully automatic optical adjustments to the goniometer from the computer screen, even for optional attachments. In addition to completely automatically adjusting all settings, such as the zero angle for the  $\theta$  and  $2\theta$  axes, the x-ray detector high-voltage settings, the PHA baseline and window width settings, it automatically saves the settings information. This feature can be utilized for routine maintenance.



θ-Axis Adjustment Screen

### **Enhanced Auto Search System**

[ Auto Search, General Quantitation Software Provided as Standard ]

#### Identification work can be performed efficiently on screen.

#### Detailed search parameters can be set.

To obtain correct results with automatic search/match, search parameters that conform to each sample must be set. The XRD-6100 enables the setting of detailed search parameters such as selection of files to be used in the search and three levels of element data input.

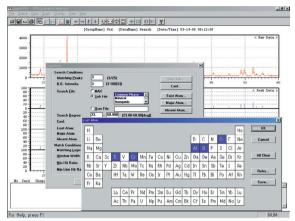
## Replete with second search function for authoritative identification of a small amount of components.

Identifying a small amount of components with a primary search is difficult; a second search is often needed after the maior components have been identified. The XRD-6100 is equipped with a second search function to provide easy identification of a small amount of components.

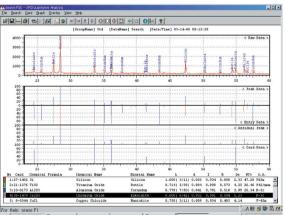
#### Various search result data can be displayed.

Search results can be stack-displayed with each standard data display over raw data. Also, for easy comparison, standard substance names, chemical equations, ore names, Miller indices, and ICDD numbers can be displayed on each peak. Furthermore, an easy quantitative calculation function using a corundum ratio for candidate substances (Intensity ratio for the α-Al<sub>2</sub>O<sub>3</sub> strongest peak) is included in the equipment.\*

\* When using this function, please obtain the ICDD database separately.



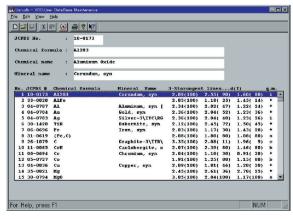
Search Parameter Setting Screen



Search Result Screen

#### Dedicated user database can be created.

The user's own database file - separate from the sub-file supplied by ICDD (International Center for Diffraction Data) can be created. Data obtained through measurements by the XRD-6100 and manually entered data can be registered in the database file, which means that the user's basic samples can be registered, and comparisons made with those substances to provide an extra dimension to quality control.



User Database Creation Screen

### Sophisticated Quantitation Software

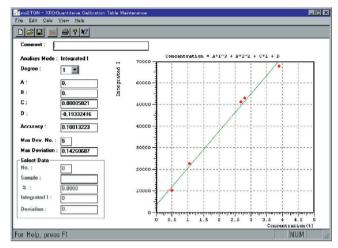
#### Satisfies your analysis objectives.

#### **Creating Calibration Curves**

Calibration curves are created with a standard sample of known concentration, based on the fact that the mass concentration and X-ray diffraction intensity of a crystal are proportional. Three methods are available for creating calibration curves: the external standard method, in which no matrix absorption correction is made; the internal standard method in which absorption correction is made; and the standard addition method. The software supports all three methods.

With the software, intensity (X-ray diffraction line height), integrated intensity, or intensity ratio modes can be selected for the axis displayed. The mass concentration unit can be switched between mg and %.

In addition, displaying the correlation coefficient (R) allows the accuracy of the calibration curve to be evaluated.



Calibration Curve Screen for Integrated Intensity

#### **Quantitative Analysis**

The three methods indicated above are available to satisfy most of the application needs.

Further, up to 5 peaks may the specified for quantitation and up to 10 sets of data may be calculated simultaneously.

ii XRD:Quantitative Calculation		
<u>File Edit View Calo</u> In	formation <u>P</u> eak List	Help
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Analysis Group Name : st Si,25deg Comment : Hollow Worl Analysis Mode Integrated 1 (Peak Files) Group Data 1 envqnt 053 2 envqnt 055 4 5 6 7 8 9 10:	Condition Compo. temp d: 3.3480 Error: 2.0000 Curve: sio2.TQN A: 0. B: 0. C: 0.000058 D: -0.193324 4.23 2.80 1.37	Concentration (%)
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Integrated Intensity Quantitation Results Screen

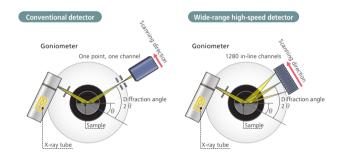
Note: Residual austenite quantitation and environmental quantitation software packages are optional.

### OneSight Wide-Range High-Speed Detector for High-Speed and High-Sensitivity Measurement

The OneSight is a wide-range high-speed detector consisting of a number of semiconductor devices. The wider angle of acquiring diffraction lines allows measurement to be performed with the goniometer fixed. By offering high-speed, high-sensitivity measurements, the time required for qualitative and quantitative analysis can be significantly reduced. The OneSight can be mounted on existing XRD-6100/7000 units installed at customers' sites.

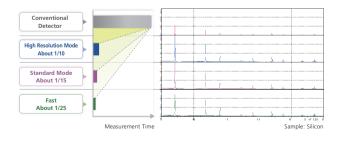
#### Wide-range array detector with 1280 channels

A conventional scintillation detector has only one channel at one point whereas the OneSight has 1280 channels on a wide-range array. Thus, compared with scintillation detectors, this detector can acquire diffraction lines over a wide angle at one time.



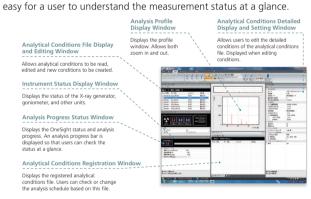
### High-speed quantitative analysis using three measurement modes

The OneSight features three kinds of measurement modes: High resolution, Standard, and Fast. It enables measurement speeds that are 10 times faster (High resolution), 15 times faster (Standard), and 25 times faster (Fast) than those attained with a conventional scintillation detector.





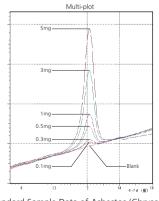
Advanced user interface enhances operational efficiency. The measurement software for the OneSight has been redesigned. The analytical profile is located in the center, the analytical conditions list and instrument status display are indicated on the left, the analysis schedule is displayed on the bottom center, and the detailed analysis conditions display is shown on the right. The window layout can also be changed. By displaying necessary information in one window, the new design makes it



### ONE SHOT mode achieves simultaneous measurement of diffraction profiles at a specific angle range.

The OneSight can perform a simultaneous diffraction profile measurement over a range of more than 10 deg. with a fixed-position goniometer.

This is useful in quantitative analysis using a specific diffraction peak.



Standard Sample Data of Asbestos (Chrysotile) (30 sec. measurement time per sample)

### Options

#### **OneSight Wide-Range High-Speed Detector** (FD-1001 1D high-speed detector P/N S215-24320-93)

It is an optional detector that can be mounted on existing XRD-6100/7000 units. The wide-range detector consists of 1280 semiconductor devices, and achieves qualitative analysis more than 10 times faster than conventional scintillation detectors. It also features a ONE SHOT mode that takes advantage of the wide measurement angle to perform analysis with a fixed goniometer. Operability is improved by using software that supports measurements made using the OneSight.

Number of Channels	1280
Strip Width	50 µm
Sensor Area	W64 × L8 mm
Dimensions	W70 × D22 × H62 mm



#### **Qualitative Analysis**

#### **Counter Monochromator**

Installed in the X-ray detector unit, the counter monochromator transforms X-rays which have passed through the entrance slit into monochromatic X-rays, allowing only the characteristic X-rays (K $\alpha$  X-rays) to be detected. Exclusion of all other X-rays from the sample, including continuous X-rays and K $_{B}$  X-rays as well as fluorescent X-rays, ensures diffraction patterns with a high signal-to-noise ratio.

Part Description	Application	P/N
Counter Monochromator CM-3121	Cu X-ray tube	215-22360-02
Counter Monochromator CM-3131	Co X-ray tube	215-22360-03
Counter Monochromator CM-3141	Fe X-ray tube	215-22360-04
Counter Monochromator CM-3151	Cr X-ray tube	215-22360-05

Note: It is not possible to be used in combination with OneSight wide-range high-speed detector.

(please use KB X-ray cut filters as a substitute.)



### Options

#### **Qualitative Analysis**

#### ICDD PDF-2

This is the powder X-ray diffraction database provided by ICDD. PDF-2 contains substance name, chemical formula, d-I data. Furthermore, it also contains miller indices, lattice constants, space groups and other crystallographic information. Using the special PDF-2 Automatic Search Software, unknown substances can be easily identified via the registered crystallographic information.

#### PDF-2 Data Mining Software

Searches can be performed from the card No., as well as based on multiple elements using "AND" or "OR" conditions, with analyte identification and crystalline structure obtained simultaneously.

Note: Included in PDF-2 Database.

ICDD PDF-2	P/N for Educational Institutions	P/N for Other Uses
Single License	239-50002-12	239-50002-11

Note: The license (before 2017) is valid for five years. It can be extended for five more years for free at the time the license period ends. The license since 2017 is not available for extending for five more years.

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47.302		55	2	2	0	100
56.121		30	3	1	1	60
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Search Result Screen by Searching Card Number

#### **ICDD PDF-4**

In addition to the functions of PDF-2, database PDF-4 features the display of 3D structural charts, various lattice parameters, simulation wave form by the calculation, and the import of the measurement data. There are two databases: PDF-4+ (for general) and PDF-4/Organics (for organics).

ICDD PDF-4+	P/N for Educational Institutions	P/N for Other Uses
Single License (New, 1-year license)	239-50015-02	239-50015-01
Single License (Renewal, 1-year license)	239-50015-04	239-50015-03
Single License (Renewal, 3-year license)	239-50015-06	239-50015-05
Single License (Renewal, 5-year license)	239-50015-08	239-50015-07

ICDD PDF-4 / Organics	P/N for Educational Institutions	P/N for Other Uses
Single License (New, 1-year license)	239-50015-22	239-50015-21
Single License (Renewal, 1-year license)	239-50015-24	239-50015-23
Single License (Renewal, 3-year license)	239-50015-26	239-50015-25
Single License (Renewal, 5-year license)	239-50015-28	239-50015-27

#### Quantitative Analysis

#### **Rotational Sample Stage RS-1001**

The RS-1001 performs in-plane rotation of the sample in combination with oscillation around the goniometer sample axis ( $\theta$ ). It is available to minimize the variation in diffraction pattern intensities attributable to the sample crystalline orientation, and thereby enhance the precision in most types of guantitative analysis.

#### Main specifications

Operation Modes

Rotation	
----------	--

Rotation Speed 1

Minimum Step Width

ß axis (sample in-plane)
1 to 60rpm
0.1°
Constant speed rotation, oscillation sample
in-plane rotation scan (continuous, step)

• Measuring angle range 20 5° to 163°

 Part Description
 P/N

 Rotational Sample Stage (without option driver)
 215-21766-01



Note: Please arrange the option driver at the same time. Please refer to the special accessories on page 29.

#### Environmental Measurement Stage RS-2001

A complete environmental analysis system, this comprises a special environmental guantitative analysis stage, filter holder and guantitation software. A special filter holder is provided which allows measurement using an asbestos and free silicic acids imbedded filter as is. The main specifications of the environmental stage are the same as those of the general-purpose rotational sample stage. The calibration curve correction is based on Zn; however, when the diffraction line of the sample overlaps with that of Zn, an Al filter holder (optional) is also available. The sample stage option driver can also be used with the rotational sample stage. Zn filter folder ( $\varphi$ 25) is one of the standard accessories of RS-2001.

#### Main specifications

Measuring angle range 2θ 5° to 163°

Part Description	P/N
Environmental Analysis Stage (with S/W)	215-21767-03
Al Filter Holder (ø25)	215-23765-92
Aluminum Sample Holder (5pc)	215-22507-06
Aluminum Sample Holder (5pc, with plated through hole)	215-22507-10

Note: Please arrange the option driver at the same time.

Please refer to the special accessories on page 29.

#### **Environmental Quantitation Software** (P/N 215-00421-92)

Even if a sample such as airborne dust in the work environment is collected by a filter, the amount is small, and even if a general-purpose guantitative analysis method is applied, a reliable calibration curve cannot be obtained due to the effect of matrix substances, and thus, good results cannot be obtained. The environmental quantitation software employs the substrate standard mass absorption correction method to eliminate the effect of X-ray absorption of matrix substances, and provides a calibration curve analysis method with good linearity and high accuracy. Used in combination with the filter holder shown in the table above.

#### Automatic Analysis

#### Auto 5 Position Sample Changer ASC-1001

This stage is used in order to automatically measure a maximum of 5 samples. The ASC-1001 performs in-plane rotation of the sample in combination with oscillation around the goniometer sample axis ( $\theta$ ) to minimize the variation in diffraction pattern intensities attributable to the sample crystalline orientation. Also, it is possible to use the filter holder (option) with the Environmental Measurement Stage RS-2001.

#### Main specifications

- Sample Amount Max. 5
- Powder Sample Holder 25mm ø, 5pc (standard)
- Sample Size Powder:25mm ø
- Filter: 25mm ø (option) Rotation Speed 1 to 60rpm
- Measuring Angle Range 2θ 5° to 163°

Part Description	P/N
Auto 5 Position Sample Changer (with an option driver unit)	215-23175-01
Zn Filter Holder (25mm ø) 5pc/set	215-23760-91
Al Filter Holder (25mm ø) 5pc/set	215-23760-92

Note: Please arrange the option driver at the same time. Please refer to the special accessories on page 29.



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4:												
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10:												

Environment Quantitation Screen



#### Sample Plates for RS-2001 and ASC-1001

Part Description	P/N
Aluminum Sample Holder (5pc)	215-22507-06
Glass Sample Holder (5pc)	215-22507-07
Glass Micro Sample Holder (5pc)	215-22507-08
Non-reflective Sample Holder (2pc)	215-22507-09



### Options

#### Attachments

#### Thin Film Analysis Using Attachment THA-1101

This specialized attachment includes the thin film sample stage, monochromator and suction pump.

Employing the fixed incidence angle, parallel X-ray diffractometry method, penetration of incident X-rays into the substrate sample is limited as much as possible, providing low background, thin film X-ray diffraction patterns.

Samples are easily set in place using the suction pump. The sample stage option driver can also be used with the rotational sample stage.

#### Main specifications

RotationRotation speed

ß axis (sample in-plane)

eed 1 to 60rpm ncidence angle 0.1°

Minimum incidence angleSample suction pump

Operation modes

0.1° AC100V, 10W (1 pump) Constant speed rotation, oscillation, sample in-plane rotation scan, (continuous, step)

Part Description	P/N
Thin Film Analysis Attachment (without option driver)	215-21765-01

Note 1: Please arrange the option driver at the same time. Please refer to the special accessories on page 29.

Note 2: It is not possible to be used in combination with OneSight wide-range high-speed detector.



#### Fiber Sample Attachment

Used in combination with the Rotational Sample Stage (RS-1001), this system measures the degree of orientation for fibers. The acquired data is then processed using the provided fiber sample attachment software to calculate the degree of orientation.

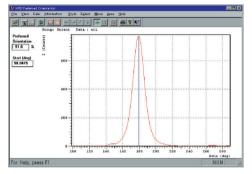
Part Description	P/N
Fiber Sample Attachment (with S/W)	215-22624

Note: It is not possible to be used in combination with OneSight wide-range high-speed detector.

### Orientation Evaluation Software (P/N 215-00428-92)

This software evaluates the degree of orientation for fiber samples, using the data of peak width at half height acquired from orientation measurement (sample in-plane ß axis measurement).





Degree of Orientation Evaluation Screen

### Options

#### Attachments

#### Stress Analysis Attachment

This specialized stress analysis system using the side-inclination method includes the stress analysis sample stand, X-ray tube and stress analysis software.

X-ray stress analysis is widely used to measure the level of stress in substances. In the X-ray diffractometry of stress extremely small changes in the lattice space are measured from the X-ray diffraction pattern profile. The use of the special stress analysis stand associated with the side-inclination method allows the precise measurement of the residual stress. This technique is free of absorption error. The software includes the following functions: as measurement, width at half height, peak position calculation and stress calculation. Depending on the type of sample and reflective plane, either the Cr X-ray tube or Co tube is necessary.

#### Main specifications

- Inclined Axis
- Inclined Angle Range 0 to 50°
- Operation Modes Oscillating, fixed

α axis

Part Description	P/N
Stress analysis attachment SA-1101 compatible with scintillation detector (with Cr tube)	215-21769-01
Stress analysis attachment SA-1111 compatible with scintillation detector (with Co tube)	215-21769-03
Stress analysis attachment SA-2101 compatible with OneSight detector (with Cr tube)	215-21769-95
Stress analysis attachment SA-2111 compatible with OneSight detector (with Co tube)	215-21769-96

Note 1: Please arrange the option driver at the same time. Please refer to the special accessories on page 29.

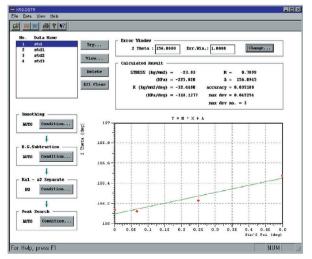
Note 2: Stress analysis software (compatible with scintillation detector/OneSight detector) equipped.

#### Stress Analysis Software

#### (Compatible with scintillation detector/OneSight detector) (P/N 215-00429-92)

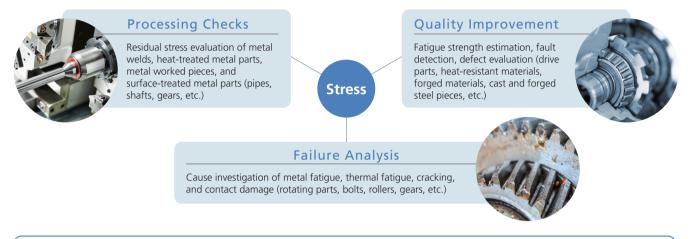
This software can analyze data obtained using either a parallel-beam (fixed  $\psi$  or fixed  $\psi_0$ ) or orthogonal-beam method.





Residual Stress Analysis Result Screen

### Powerful Tool for Processed Part Checks of Metal Products, Quality Improvement, and Failure Analysis



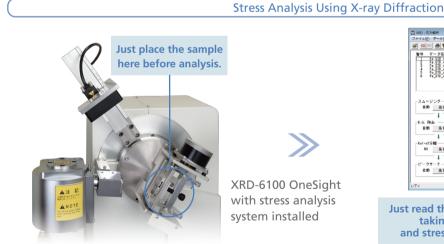
#### Features of Stress Measurement Using X-ray Diffraction

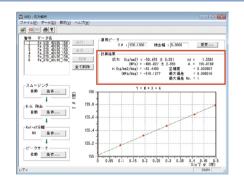
#### Enables non-destructive testing.

Users can repeat residual stress measurements without the need for destructive machining.

#### No special skills required.

Anyone can take measurements since there is no need for sample processing or advanced adjustments that may have an effect on the results.





Just read the data into the analysis software after taking measurements, and the graphs and stress values are displayed automatically.

A graph line moving up to the right indicates compression stress, and a downward-sloping line indicates tensile stress.

#### Merits of Adoption

#### High-Speed Measurements

Makes measurements about 10 times faster compared with a conventional scintillation detector.

### Simultaneous Measurement with ONE SHOT Mode

Measurements can be done all at once with the goniometer fixed for each  $\Psi$  angle

#### Significantly Reduced Analysis Time

Qualitative analysis to determine whether stress is compressive or tensile can be completed in 1 minute only and quantitative analysis that includes calculation of possible stress can be done within 5 minutes.



### Options

#### Attachments

#### Polycapillary Attachment PCL-1002

The polycapillary unit is a new optical X-ray element that splits a single X-ray beam emitted from a point's light source into multiple X-ray beams using three-dimensionally arranged capillary optics. This creates a powerful parallel beam output that covers a large area.

1) Compared to conventional methods, this unit uses the X-ray more effectively and increases the intensity of the diffracted X-ray, allowing more sensitive analysis.

2) With conventional methods, variations in sample surface height are directly translated into variations in X-ray diffraction angles. This polycapillary unit uses parallel beams, so it is not affected by variations in sample surfaces.

Part Description	P/N
Polycapillary Attachment PCL-1002	215-24375-91
CM-4121 Counter Monochromator Assembly (for parallel beams)	215-22360-06
X-Ray Tube (Long fine focus, with Cu target)	210-24100-11

Note 1: If an LFF type X-ray tube is used in the XRD-6100 system, the X-ray tube listed above is not required.

Note 2: It is not possible to be used in combination with OneSight wide-range high-speed detector.

#### Sample Heating Attachment HA-1001

The system is used to heat the sample during X-ray diffractometry to study the influence of heat on the crystalline structure. It consists of a special sample heating furnace and temperature controller. The atmosphere in the furnace, consisting of air, an inert gas or a vacuum, may be heated to 1500°C during measurement. The measurement results are output in multiple data formats to enable comparison of X-ray diffraction patterns obtained at various temperatures.

#### Main Specifications

Thermocouple	Pt-Pt/Rh
Measurement Temperature	1500°C max. in vacuum, air
	1200°C max. using inert gas (N <sub>2</sub> )
Control Functions	PID value setting, fixed temperature control
	(temperature increase, decrease, hold, stop)
Power Supply	Single phase 200/220V±10% 10A

Part Description	P/N
Sample Heating Attachment (with temperature controller)	215-23000

Note: It is not possible to be used in combination with OneSight wide-range high-speed detector.



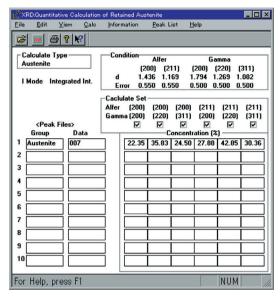


### Various Optional Software

#### **Quantitative Analysis**

### Residual Austenite Quantitation Software (P/N 215-00430-92)

A common method to quantify residual austenite is to apply the method for samples consisting of 2 components such as tempered copper  $\alpha$ -iron and  $\gamma$ -iron. Special software allows the determination without the need of a standard sample. The software directly uses the intensity ratio of the measured X-ray peaks of the  $\alpha$ -iron and  $\gamma$ -iron components to theoretically perform the calculation. The five-peak average method is used to make the determination, so scattering due to the matrix effect is reduced, enhancing the reliability of the results. Using the rotational sample stage (P/N 215-21766-01) for measurement further helps to overcome data scattering.



Quantitation Results Screen

#### **Peak Processing**

### Overlapping Peak Separation Software (P/N 215-00423-92)

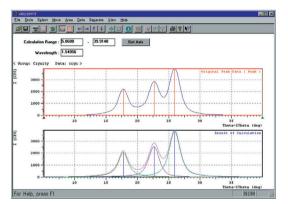
Using the Gauss and Lorentz models, overlapping peaks are separated one by one, with information including position, intensity, width at half height and integrated intensity calculated for each diffraction peak.

These are then utilized to conduct quantitative analysis and crystalline structure analysis.

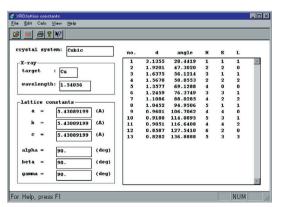
#### **Crystalline Structure Analysis**

#### Precise Lattice Constant Determination Software (P/N 215-00424-92)

In X-ray diffractometry, higher accuracy is often required to determine the lattice constant, which is a fundamental parameter for determining a substance's crystalline structure. This is most often used for quantitating solid solution metal. This software corrects the raw diffraction angle data calculated via basic data processing to determine enhanced precision lattice constants for up to 7 crystals concurrently, employing the least squares method to further minimize error in diffraction angles. In addition, the Miller index is applied to each peak.



Peak Separation Screen



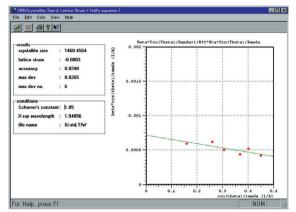
Precise Lattice Constant Determination Calculation Result Screen

### Various Optional Software

#### **State Analysis**

### Crystallite Size & Lattice Strain Software (P/N 215-00426-92)

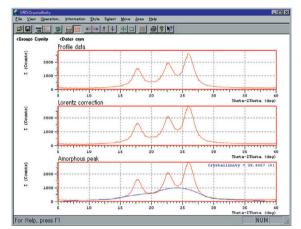
Samples normally consist of crystallites ranging in size from several µm to tens of µm. However, in the case of catalyst crystallites, which may measure several hundred Å, X-ray diffraction is insufficient, resulting in diffraction peak spreading. This software quantitatively determines that spread, and applies the Scherrer's equation to calculate the crystallite size. When there is involvement of lattice strain, the diffraction spread is determined for a number of diffraction peaks, and from the resultant line slope and intercepts, the size of each of the crystallites and the lattice strain are calculated. (Hall's Method)



Hall's Equation Calculation Result Screen

### Crystallinity Calculation Software (P/N 215-00427-92)

The degree of crystallization of a mixture of crystalline and amorphous substances, such as found in high polymer samples, is an important parameter of substance characterization. This software automatically or manually separates the measured diffraction patterns into those of crystalline components and those of amorphous components. Then, it calculates the integrated intensity of the two types of substances, called degree of crystallization using the peak area ratio of the two classes of components.



Crystallinity Calculation Result Screen

### Other Accessories

#### **Sample Holders**

The following sample holders, including five pieces of an aluminum sample holder, which is supplied as standard with the diffractometer, are available for different applications.



Part Description	Sample Area	Application	Remarks	P/N
Aluminum Sample Holder	ø25 (dia.) x 1mm (d)	General purpose	Made of aluminum, 5pc	215-22507-01
Glass Sample Holder	ø25 (dia.) x 1mm (d)	Lattice constant, contamination prevention	Made of glass, 5pc	215-22507-02
Glass Micro Sample Holder	ø15 (dia.) x 0.5mm (d)	Micro samples	Made of glass, 5pc	215-22507-03
Non-reflective Sample Holder		Ultramicro samples	Made of silicon, 2pc	215-22507-05

#### **Cooling Water Circulator**

With its built-in cooler, the Cooling Water Circulator cools the X-ray tube and X-ray generator by circulating cooled, clean water. The unit is recommended when no tap water is available or the available water is of poor quality.

#### Main specifications

Power Supply Three phase 200V ±10% 10A (RKE1500B-V-G2-SP)
 Ambient Temperature 5 to 40°C

Cooling Capacity

5.3kW (50/60Hz) (RKE1500B-V-G2-SP)

Part Description	P/N
RKE1500B-V-G2-SP	239-15049-02



RKE1500B-V-G2-SP

### **Specifications**

#### XRD-6100

	Max. output	3kW
	Output stability	±0.01% (for 10% power fluctuations)
	Max. tube voltage	60kV (50kV)*1
	Max. tube current	80mA (50mA)*1
X-ray Generator	Voltage step width	1kV
	Current step width	1mA
	Overload limit setting	Setting changeable with tube type
	X-ray tube protection	Against undervoltage, overload, overvoltage, overcurrent and/or failure of water supply
	Safety mechanisms	Door interlock mechanism (X-ray can be generated only after the door is closed) Emergency stop
	Туре	Vertical type
	Scanning radius	185mm
	Min. step angle	0.002° (20), 0.001° (0)
	Angle reproducibility	0.001° (20)
	Scanning angle range	-6° to 163° (2θ), -180° to 180°(θ)
	Scanning system	$\theta/2\theta$ linkage mode, $\theta$ , 2 $\theta$ independent mode
Goniometer	Operation mode	Continuous scan measurement, step scan measurement, calibration, positioning, $\theta$ axis oscillation (when using 2 $\theta$ continuous scan or step scan)
	Max. speed	1000°/min (20)
	Scanning speed	0.1° to 50°/min (2θ), 0.05° to 25°/min (θ)
	Divergence slit (DS)	0.5°, 1°, 2°, 0.05mm
	Scattering (SS)	0.5°, 1°, 2°
	Receiving slit (RS)	0.15mm, 0.3mm

\*1 When using OneSight wide-range high-speed detector.

#### X-ray Tubes and X-ray Filters

Focus Type	Type NF	Type BF	Type LFF* <sup>3</sup>	
Focus Size	1 x 10mm	2 x 12mm	0.4 x 12mm	
Tube Voltage, Current	60kV, 50mA	60kV, 60mA	60kV, 55mA	
Target	X-ray Tube Maximum Load & P/N			
Cu	2.0kW (239-24014-01)*2	2.7kW (210-24016-21)	2.2kW (210-24100-11)	
Со	1.8kW (062-40003-04)	2.7kW (210-24016-24)	1.8kW (210-24100-14)	
Fe	1.5kW (062-40003-05)	2.2kW (210-24016-25)	1.0kW (210-24100-15)	
Cr	2.0kW (062-40003-06)	2.7kW (210-24016-26)	1.9kW (210-24100-16)	

X-Ray Filter			
Part Description	P/N		
Ni filter (for Cu)	(215-22500-02)		
Fe filter (for Co)	(215-22500-03)		
Mn filter (for Fe)*4			
V filter (for Cr)	(215-22500-05)		

\*2 When using it as a point focus, combine a X-ray tube and a point focus head of following P/N.

1) X-ray tube (Cu target, 2.0kW, NF) P/N 210-24016-11 2) Point focus head P/N 239-16047

2) Point focus head PIN 239-160 \*3 When using the polycapillary system, use LFF type. \*4 Custom support.

#### Detectors

### **OneSight Wide-Range High-Speed Detector** (FD-1002 1D High-Speed Detector P/N 215-24320-93)

(PD-1002 TD high-speed Detector PN 215-24520-95)				
Scan Range 0-148° : Radius of Goniometer 185 mm				
Operation Mode	Step-scan mode, One-shot mode			
Sensor	Reverse biased pn-junction array			
Detection Principle	Photon counting method			
Weight	280 g			
Active Area	64 × 8 mm			
Number of Channels	1280			
Width of One Channel	50 μm			

#### **Scintillation Detector**

SC-1001 P/N 215-24385-91

Scintillator	Na I
Scaler	Preset time: 0.1 to 1000sec; digits: 7
HV/PHA	500 to 1200 V high-voltage power supply, baseline and window auto-controlled

#### **Data Processing Unit**

Casing	g W900 x D700 x H1600	
OS Windows® 10		
Controlled Elements	d Elements Goniometer, X-ray generation, tube voltage, tube current, detector high voltage*5, PHA*5, scaler	
Basic Data Processing Smoothing, BG elimination, Kα1-Kα2 separation, peak searching, peak width at half height, integrated intensity, systematic error correction, internal/external standard correction, operations between data, graphic display		
Qualitative Analysis Database (library) creation, automatic library search (ICDD PDF-2/PDF-4 options)		
Quantitative Analysis	titative Analysis Calibration curve generation, quantitative calculation	

\*5 When using scintillation detector.

### Accessories

Special Accessories ©:Absolutely required O:Required •:Required depending on object							ctive								
Analysis Objective	Part Description	P/N	Iron and steel related	Non-ferrous metals, precious metals	Machinery, automotive, shipbuilding, welding	Brickmaking, ceramics	Cement and glass	Electrical, electronic materials	Foodstuffs, textiles, paper, pulp	Chemicals, catalysts. dyes, paints	Medical, dental materials, biological organisms	Natural resources, energy	Construction, engineering	Industrial waste	Environment (Asbestos)
1 BG Reduction, Especially Iron Samples	Counter Monochromator CM-3121	215-22360-02	0	0	0	0	0	O	0	0	0	0	0	0	0
2 Qualitative Analysis PDF-2 Search	ICDD PDF-2 file	239-50002-11,12	$\odot$	0	0	0	0	$\odot$	0	0	0	0	0	0	O
3 Qualitative Analysis PDF-4 Search	ICDD PDF-4 + file	239-50015-01,02	$\odot$	0	0	0	0	$\odot$	0	O	0	O	0	$\odot$	O
4. Concret Durness Quantitative Analysis	*Rotational Sample Stage RS-1001	215-21766-01	0				0		0					0	0
4 General Purpose Quantitative Analysis	*Auto 5 position sample changer ASC-1001	215-23175-01		$ ^{\circ}$	$ \circ $	0		0		0	0	$ \circ $	$ \circ $		
	Residual austenite quantitation S/W	215-00430-92	0		0										
5 Residual Austenite Quantitation	*Rotational Sample Stage RS-1001	215-21766-01	0		0										
6 Environmental Quantitative Analysis System	*Environmental Quantitative Analysis Stage RS-2001 (Filter holders Zn, with S/W)	215-21767-03												O	0
Analysis System	Filter holder Al (ø 25mm)	215-23765-92												0	O
7 Multiple Peak Separation	Multiple peak separation S/W	215-00423-92													
8 Crystal Structure Analysis	Rietveld analysis, RIETAN software	215-00433-92													
9 Crystallite Size / Lattice Stress	Crystallite Size / Lattice Stress S/W	215-00426-92							0	0	0				
10 Degree of Crystallization	Degree of Crystallization S/W	215-00427-92							0	0	0				
11 Heating Analysis	Sample Heating Attachment HA-1001	215-23000													
12 Thin Film Analysis	*Thin Film Analysis Attachment THA-1101 (stage, monochromator, suction pump)	215-21765-01	•	•	•	•	•	•							
	*Rotational Sample Stage RS-1001	215-21766-01							0						
13 Fiber Degree of Orientation Analysis	Fiber Sample Attachment (with S/W)	215-22624							0						
	*Stress analysis attachment SA-1101 compatible with scintillation detector (with Cr tube)	215-21769-01	0	0	0	•	•	•							
	*Stress analysis attachment SA-1111 compatible with scintillation detector (with Co tube)	215-21769-03	0	0	0	•	•								
14 Residual Stress Analysis	*Stress analysis attachment SA-2101 compatible with OneSight detector (with Cr tube)	215-21769-95	0	0	0	•	•	•							
	*Stress analysis attachment SA-2111 compatible with OneSight detector (with Co tube)	215-21769-96	0	0	0	•	•	•							
	Stress analysis software (compatible with scintillation detector/OneSight detector)	215-00429-91	0	0	0	•	•	•							
15 Strong Parallel Beam X-ray Source	poly-capirally unit PCL-1002	215-24375-91													
Neter Discourse and and an Ac	SV(P/NO1E 21764) at the same time when you are	l 	- 6 + 1-		l.			1	1	I			<u> </u>		

Note: Please arrange optional driver ASSY(P/N215-21764) at the same time when you arrange the accessories of the asterisk. Moreover, even when two or more accessories are arranged, the option driver ASSY and optional additional ASSY can be combined with one unit.

The following attachment software cannot be used in combination with OneSight wide-range high-speed detector. • Counter Monochromator CM-3121

Counter Monochromator CM-3121
 Sample Heating Attachment HA-1001
 Thin Film Analysis Attachment THA-1101 (can be used as rotational sample stage)
 The following analysis objectives are unmeasurable.
 Heating analysis, 12 Thin film analysis, 13 Fiber degree of orientation analysis, 16 Constant Irradiation Width Analysis, 15 Strong parallel beam X-ray source.
 Please contact us for further information.

### Installation Requirements

#### Installation Site

This instrument uses X-rays for measurement and analysis. Accordingly, before installing the instrument, be sure to consult local regulations regarding measures associated with X-ray generation, and comply with all necessary regulatory procedures.

#### **Power Requirements**

For Main Unit	Single phase 200/220V ±10%
	2kW type: 30A
	3kW type: 50A
Data Processing Unit	Single phase 100V ±10% 10A
Ground	Independent, at least 100 $\Omega$ resistance
Ground	Independent, at least 100 $\Omega$ resistance

#### Installation Site Environment

The following ambient temperature and humidity are required.

Temperature	23°C ± 5°C
Humidity	Less than 75%

Avoid any sudden changes in temperature, which might cause condensation to form on the surfaces of internal parts. Heat generated from the instrument is approximately 1kW. When the cooling water circulator is installed in the same room, this is increased by 2.6kW for the NF type X-ray tube, 2.9kW for the LFF type X-ray tube and 3.9kW for the BF type X-ray tube.



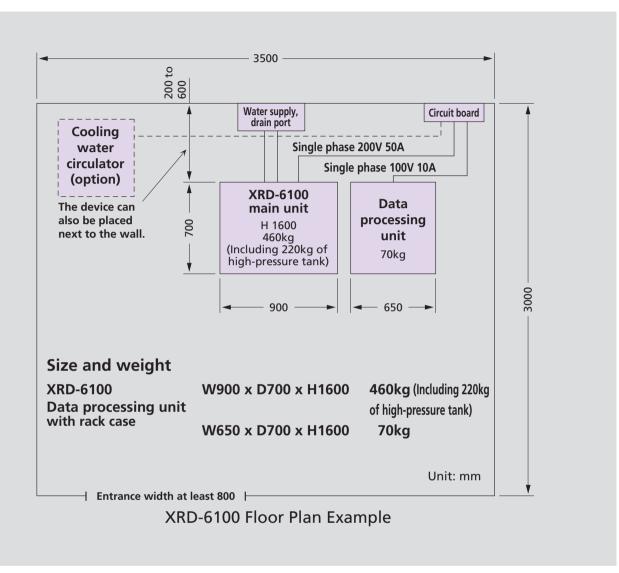


#### **Cooling Water Supplied to Instrument**

When cooling water supplied to the instrument becomes dirty due to piping corrosion, etc., this causes clogging of the X-ray tube filters. Cooling water should be supplied using the following conditions.

Flow Rate	At least 4.0L/min
Water Pressure	0.3 to 0.5 MPa
Water Quality	pH6 to 8, hardness less than 80ppm
Particulates	Less than 0.1mm
Supply Water Port Diameter	12.7mmø
Drain Water Port	Natural drainage

If the flow rate is lower than 4.0L/mim, the safety circuit for protection of the X-ray tube is active, disabling the X-ray generation circuit. When minimum conditions of the flow rate cannot be fulfilled, use the cooling water circulator, available as an option.



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