

XRD-6000

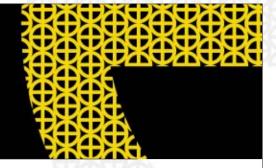
Shimadzu X-ray Diffractometer







XRD-6000



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Ease of use and abundant functions herald a new era of analysis

The Windows XP-supported application software usher this compact, multi-functional, general purpose X-ray Diffractometer into the networking era of analysis.

With its basic ease of use and abundant functions, the XRD-6000 boasts an integrated design featuring a vertical goniometer and data processing software supporting the Windows XP user interface.

The XRD-6000 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. And, of course, crystalline structural analysis is also supported, including precise lattice constant determination and crystal system determination.

Features

High-precision built-in vertical goniometer

This can measure various samples including hard-to-secure samples like powders and thin films as well as highly soluble samples.

Windows XP employed as software platform

The main unit control and data processing software supports the widely used Windows XP user interface. For this reason, data can export to marketed software, network support, and multi-user accessibility is easily achieved.

Multi-functional auto-search/match software (qualitative analysis) equipped as standard

The XRD-6000 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 raw data profile make analysis easy to understand for even the beginner, and - what is more - a greater success ratio in results can be achieved with the system. In addition, an easy quantitative calculation function and a function that incorporates element data from the X-ray fluorescence spectrometer are also included in the system.

Routine performance maintenance for device is easy

Adjustments to the optical system are performed by automatic setting function. And as the XRD-6000 has a function to automatically save the system's adjustment parameters, system status can be monitored and recorded. Consequently, routine performance maintenance can be easily controlled,

Distinguished body that is safe and compact

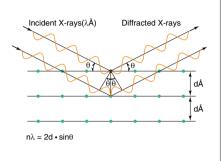
The main body has been massively slimmed down (30% reduction in installation surface area compared to previous Shimadzu diffractometers), and as the rear is a sheer flat surface with no superfluous protrusions, the device can placed up against walls, which means it does not take up room when installed on site or in the lab. The unit is also specifically designed to promote ease of handling in sample loading and positioning, and together with the door lock mechanism engaged during X-raying, provides a safe operating

Contents	P 04 - XRD-6000 Features and Applications	P 14 - Options	P 23 - Main Specifications
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A general purpose X-ray diffractometer

Principle of operation

The XRD-6000, an X-ray diffractometer analyze crystalline states under normal atmospheric conditions. This method is non destructive. X-rays focused on a sample fixed on the axis of the spectrometer (goniometer) 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 of the sample. Qualitative analysis may be conducted on the basis of peak height or peak area. The peak angles and profiles may be used to determine particle diameters and degree of crystallization, and are useful in conducting precise X-ray structural analysis.



Applications

Steels, non-ferrous metals, machinery, shipbuilding, welding, automobiles, ceramics, cement, glass, catalysts, electrical parts, electronic materials, magnetic materials, superconductive 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

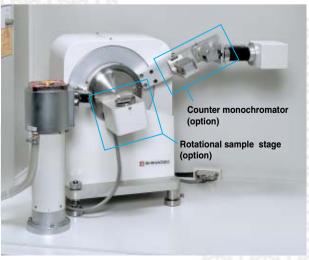
Compact, X-ray-protected housing

The compact construction (W900xD700xH1600mm) minimizes installation space requirements.

The front door is mounted on guide rollers to enable extremely light-touch and smooth door opening for facilitative installation/exchange of samples and attachments. A magnet latch assures certain door closing, and to further ensure safety, a door interlock mechanism is automatically activated whenever X-rays are generated.

High-precision, vertical goniometer

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



Vertical Goniometer

to fulfill your varying analytical needs

Construction

High voltage transformer for high output X-ray tube

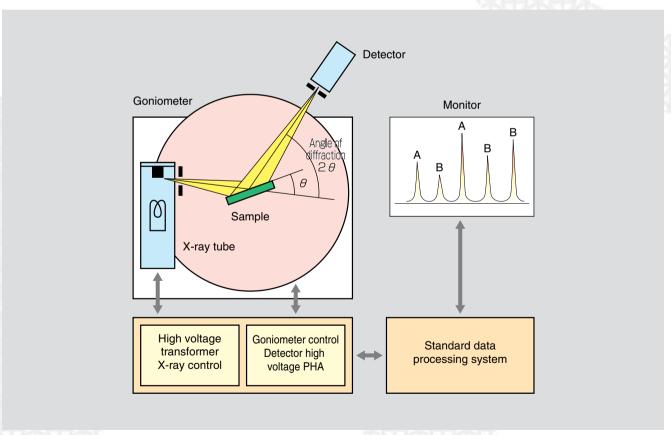
The high voltage transformer supports either the 2.2kW high output fine focus X-ray tube or 2.7kW high output broad focus X-ray tube.

X-ray tubes

The XRD-6000 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 long experience in producing high-performance X-ray generators has provided an X-ray generator of high stability, with tube voltage and tube current both stable to within $\pm 0.01\%$. 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-6000 Relational Diagram

Providing a Complete Analysis System

Analysis System

Standard Software

X-ray generator control : X-ray ON/OFF, tube voltage/current setting

Optical path adjustment Goniometer adjustment

Measurement Single scan, multi-scan

File maintenance : ASCII data conversion

ASCII data to XRD-6000 data conversion XD-D1 data to XRD-6000 data conversion

Basic data processing : Smoothing, background elimination,

 $K\alpha_1$ - $K\alpha_2$ separation, peak search,

system error correction.

internal/external standard correction,

operations between data

Graphic display Vertical display, horizontal display

Overlay display (3D)

Log display

Qualitative analysis : Auto search

User database creation

Quantitative analysis Calibration curve generation

Quantitation

Options

Qualitative analysis

Counter monochromator ICDD database PDF2, PDF4 PDF2 search software

Quantitative analysis

Residual austenite quantitation software

Rotational sample stage

Environmental quantitation analysis system

Peak processing

Overlapping peak separation

Crystalline structural analysis

Precise lattice constant determination software Rietveld method analysis software

State analysis

Crystallite size/lattice strain calculation

Crystallinity calculation

Thin film measurement attachment

Fiber sample attachment

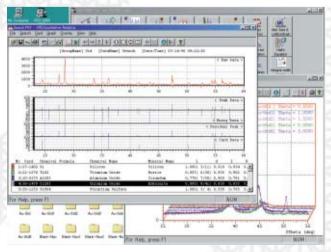
(with orientation evaluation software)

Stress measurement attachment

(with stress analysis software)

Sample heating attachment

Micro-measuring attachment



Auto search results and thin film sample overlay display

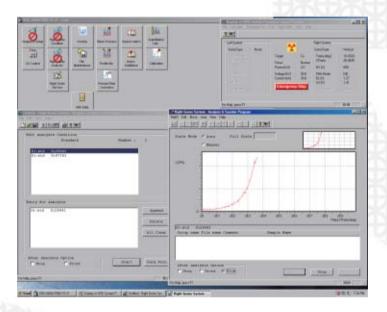
Automatic Measurement, Easy Operation

[Goniometer optical system adjustment and saving of adjustment data are both fully automated.]

Measurement Display

Wiht the XRD-6000, sample measurement condition can be set by easy operation.

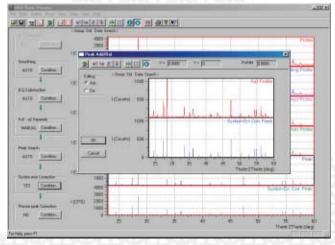
The scheduling and the progress condition of the measurement can be confirmed at one view by the analysis spooler.



Multitasking for enhanced analysis efficiency

Basic Data Processing

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

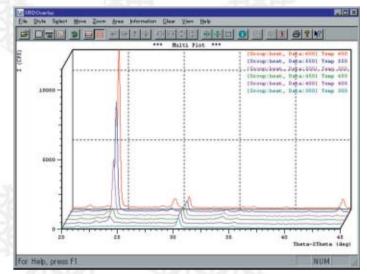


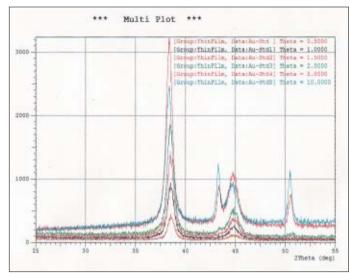
Basic Data Processing Screen

Pleasant 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 etc. is easily accamplished using combined 2-dimensional or 3-dimension-al 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, among others. Each type of data can be output to the color printer, so differences between samples can be recognized at a glance.



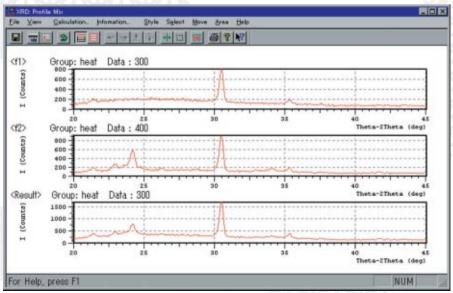


3-Dimensional Screen of Thin Film Sample

2-Dimensional Output of Thin Film Sample

Adding/Subtraction operations

Data manipulation functions such as deletion of unnecessary peak profiles and addition of re-analyzed data to obtain a summed profile are some of the invaluable tools available for conducting efficient data analysis. Spectral calculations are conducted in the window displayed at right.

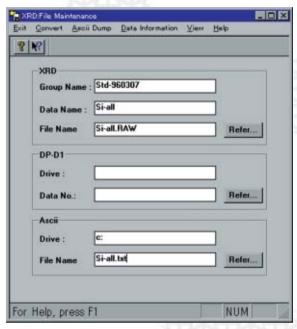


Spectral Calculation Window

File Maintenance ~Data Format Conversion~

Conversion between profile data and text data, conversion from Shimadzu X-ray Diffractometer

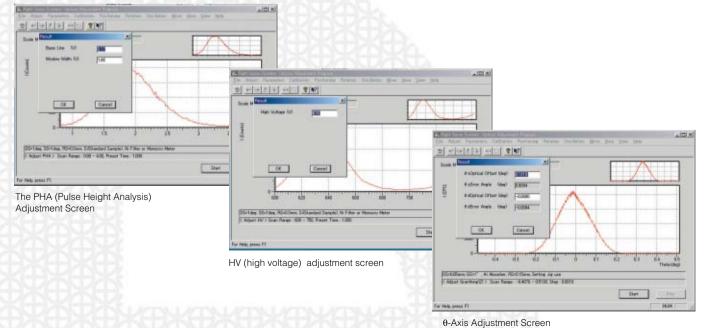
XD-D1(previous model) acquisition data to XRD-6000 format data, and re-analysis are all possible. File format conversion is conducted using the window displayed at right.



File Conversion Window

Optical Adjustments

The XRD-6000 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 θ and 2θ axes, the x-ray detector high voltage settings, the PHA baseline and window width settings, it also automatically saves the settings information. This feature can be utilized for routine maintenance.



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-6000 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. Furthermore, the XRD-6000 comes with a standard function for element data, which takes up qualitative results (element analysis) from X-ray fluorescence spectrometers as files via LAN.

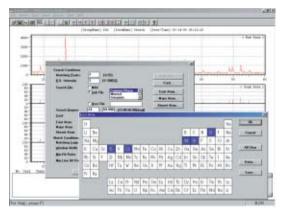
Replete with second search function for authoritative identification of small amount of components.

Identifying small amount of components with a primary search is difficult, a second search is needed after the maior components have been identified. The XRD-6000 comes replete with a second search function to provide an environment for easy identification of small amount of components.

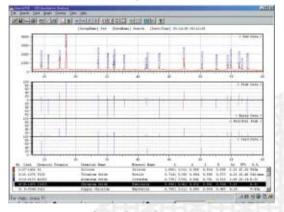
Various search result data can be displayed.

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 is included in the equipment.

If your system has a PDF2 or PDF4 database, PDF2 or PDF4 detailed data for candidate substances can be displayed on a separate window.



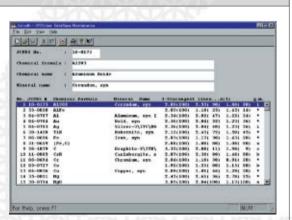
Search Parameter Setting Screen



Search Result Screen

Dedicated user database can be created.

The user's very own database file - separate from the sub-file sup-plied by ICDD (International Center for Diffraction Data) - can be created. Selected ICDD standard data and substance data not registered with ICDD can be input into this file. And data obtained through measurements by the XRD-6000 can be registered as they are 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

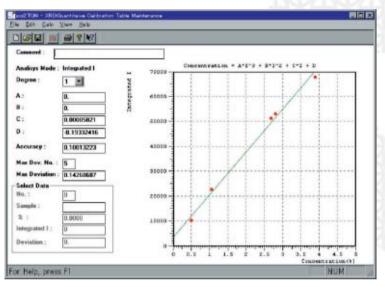
Polished Quantitation Software

[Satisfies your analysis objectives.]

Calibration Curves

Calibration curves can be generated for intensity, integrated intensity or intensity ratio.

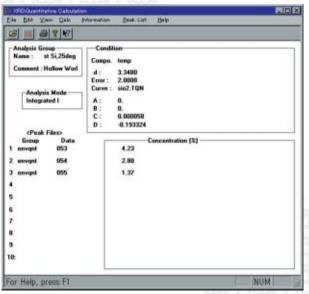
Intensity and integrated intensity calculations are used for the internal standard and standard addition methods.



Calibration Curve Screen for Integrated Intensity

Quantitative Analysis

The internal standard method and 2 intensity methods 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.



Integrated Intensity Quantitation Results Screen

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

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 ($K\alpha$ rays) to be detected. Exclusion of all other X-rays from the sample, including continuous rays and $K\beta$ 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



ICDD PDF2 / PDF4

This is the powder X-ray diffraction database provided by ICDD. PDF2 is provided on CD-ROM, and contains, in addition to substance name, chemical formula and d-I data, miller indices, lattice constants, space groups and other crystallographic information. Using the special PDF2 Automatic Search Software (option), unknown substances may be easily identified via the registered crystallographic information.

ICDD PDF2	P/N for Educational institutions	P/N for Other uses
Single license Note1)	239-50002-12	239-50002-11

In addition to the functions of PDF2, database PDF4 has the functions of data searching software (DDVIEW+), the display of 2D, 3D structural chart, various lattice parameters, and the simulation wave form by the calculation ,and the import of the measurement data. There are two kinds of databases of PDF4+ (for general) and PDF4/Organics (for organics).

ICDD PDF4+	P/N for Educational institutions	P/N for Other uses
Single license (New, 1years license)	239-50015-02	239-50015-01
Single license (Renewal, 1years license)	239-50015-04	239-50015-03
Single license (Renewal, 3years license)	239-50015-06	239-50015-05
Single license (Renewal, 5years license)	239-50015-08	239-50015-07

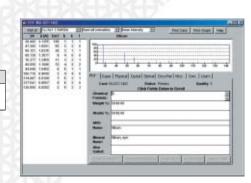
ICDD PDF4 / Organics	P/N for Educational institutions	P/N for Other uses
Single license (New, 1years license)	239-50015-22	239-50015-21
Single license (Renewal, 1years license)	239-50015-24	239-50015-23
Single license (Renewal, 3years license)	239-50015-26	239-50015-25
Single license (Renewal, 5years license)	239-50015-28	239-50015-27

PDF2 Search Software (P/N 215-00272)

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

PDF2 Search Software (DDVIEW)	P/N for Educational institutions	P/N for Other uses
Single license Note1)	239-50002-22	239-50002-21

Note 1: After 5 years, this license will need to be re-affirmed in order to make it perpetual.



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 (θ) to minimize the scatter in diffraction pattern intensities attributable to the sample crystalline orientation, and thereby enhance the precision in most types of quantitative analysis.

Main specifications

Rotation
 ß axis (sample in-plane)

Rotation speed 1~60rpmMinimum step width 0.1 degree

Operation modes
 Constant speed rotation, oscillation sample in-plane rotation scan (continuous, step)

Measuring angle range 20 7°~163°

Part Description	P/N
Rotational sample stage (with option driver)	215-21766
Rotational sample stage (without option driver)	215-21766-01



Environmental Measurement Stage RS-2001

A complete environmental analysis system, this comprises a special environmental quantitative analysis stage, filter holder and quantitation software. A special filter holder is provided which allows measurement using an asbestos-imbedded filter just as it 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 sample holder (optional) is also available.

The sample stage option driver can also be used with the rotational sample stage.

Main specifications

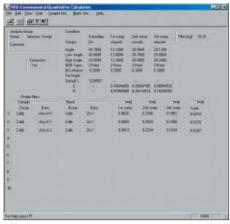
Measuring angle range 20 7°~163°

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Part Description	P/N	
Environmental Analysis Stage (with option driver, S/W)	215-21767-02	
Environmental Analysis Stage (with S/W)	215-21767-03	
Al filter holder (ø25)	215-22775-02	
Aluminum sample holder (5PC)	215-22507-06	
Aluminum sample holder (with through hole) (5PC)	215-22507-10	



Environmental Quantitation Software (P/N 215-00271-02)

Environment samples as suspended dust particles, in very small quantity, collected on filter present an analytical challenge. XRD-7000 allows a reliable analysis. The software eliminates the effect X-ray absorption by the filter, providing a calibration curve having good linearity and high accuracy. The software associated with the use of a special sample holder allows the application of a very efficient filter absorption correction.



Quantitation Results Screen

Automatic Analysis

Auto 5 Position Sample Changer (ASC-1001)

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

Main specifications

Sample position

Sample Size
 Powder:25mm ø
 Filter:25mm or 47mm ø (option)

Rotation speed 1~60rpm
 Measuring angle range 20 7°~163°

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Part Description	P/N
Auto 5 position sample changer (with 2 option driver units)	215-23175
Auto 5 position sample changer (with a option driver unit)	215-23175-01
Zn filter holder (25mm ø)	215-22775-01
Al filter holder (25mm ø)	215-22775-02



Sample plates for RS-2001 and ASC

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-refltctive sample holder (2pc)	215-22507-09

Thin Film Analysis using Attachment THA-1101

This is a specialized thin film analysis system, including 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. Specimens 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

Rotation
 B axis (sample in-plane)

Rotation speed 1~60rpm
 Minimum incidence angle 0.1degree

Sample suction pump AC100V, 10W (1 pump)

Operation modes
 Constant speed rotation, oscillation, sample in-plane rotation scan,

(continuous, step)

Part Description	P/N
Thin film analysis attachment (with option driver)	215-21765
Thin film analysis attachment (without option driver)	215-21765-01



Fiber Sample Attachment

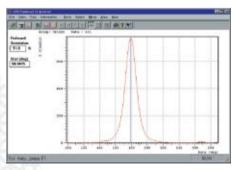
Used in combination with the Rotational Sample Stage (RS-1001), this system measures the degree of orientation for fibers. The acquired data is then processed using the provided fiber sample attachment software to calculate degree of orientation.

Part Description	P/N
Fiber sample attachment (with S/W)	215-22624

Fiber orientation software

• 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

AVS-1101 Automatic Variable Slit System

Environment samples as suspended dust particles, in very small quantity, collected on filter present an analytical challenge. XRD-7000 allows a reliable analysis. The software eliminates the effect X-ray absorption by the filter, providing a calibration curve having good linearity and high accuracy. The software associated with the use of a special sample holder allows the application of a very efficient filter absorption correction.

This mechanism automatically sets the DS, SS and RS slit widths according to the measurement mode selected on the screen.

- Fixed Irradiation Width Mode:
 The emission slit is adjusted so that all sample surfaces are irradiated with the x-ray of the same width. The detector slits (SS and RS) are also adjusted in accordance with the irradiation width
- Fixed Irradiation Width Mode:
 The DS, SS and RS slit widths are fixed at the set values.

The data obtained using this software can be converted to the conventional fixed-slit-width data by performing irradiation width compensation (patent pending).

Part Description	P/N
AVS-1101 Automatic Variable Slit System	215-23950



Degree of Orientation Evaluation Screen

MDA-1101/1201 Micro Area Measurement Attachment

The Micro Area Measurement Attachment uses a pinhole slit for emission, allowing the measurement of micro regions. Measured surfaces are observed via a CCD camera, so observation images can be loaded onto a computer, saved and edited. The product line includes two models: the MDA-1101 that uses an optical microscope and the MDA-1201 that uses a zoom (8 - 80 mm) camera lens.

Key Specifications

Pinhole Emitter Slit 0.1, 0.2, 0.3, 0.5, 1, or 2 mm diameters

XYZ Movement ±7.5 mn

Sample Surface Observation Method CCD camera image viewed on computer screen

Part Description	P/N
Micro Area Measurement Attachment (MDA-1101)	215-23180
Micro Area Measurement Attachment (MDA-1201)	215-23180-01



Stress Analysis Attachment SA-1101

This specialized stress analysis system using the side-inclination method include 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 following functions, as measurement, width at half height, peak position calculation and stress calculation. Depending the type of sample and reflective plane, either the Cr X-ray tube or Co tube is necessary. The sample stand option driver can also be used with the rotational sample stage.

Main specifications

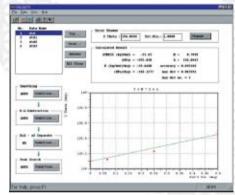
Inclined axis α axis Inclined angle range 0~50 degrees Operation modes Oscillating, fixed

Part Description	P/N
Stress analysis attachment (with Cr tube, option driver, S/W)	215-21769
Stress analysis attachment (with Co tube, option driver, S/W)	215-21769-02
Stress analysis attachment (with Cr tube, S/W)	215-21769-01
Stress analysis attachment (with Co tube, S/W)	215-21769-03

Stress Analysis Software

 This software can analyze data obtained using either a parallel-beam (fixed ψ or fixed ψ 0) or orthogonal-beam method.





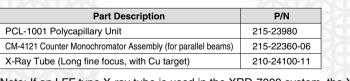
Residual Stress Analysis Result Screen

PCL-1001 Polycapillary Unit

The polycapillary unit is a new optical X-ray element that splits a single X-ray beam emitted from a point light source into multiple X-ray beams using three-dimensionally arranged capillary optics to create 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.

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Part Description	P/N
PCL-1001 Polycapillary Unit	215-23980
CM-4121 Counter Monochromator Assembly (for parallel beams)	215-22360-06
X-Ray Tube (Long fine focus, with Cu target)	210-24100-11





Note: If an LFF type X-ray tube is used in the XRD-7000 system, the X-ray tube listed above is not required.

Sample Heating Attachment HA-1001

This system, consisting of a special sample heating furnace and temperature controller, is used to heat the sample during X-ray diffractometry to study the influence of heat on the crystalline structure. The atomosphere 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 format 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 (N2)

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



HA-1001

Heating or cooling attachment TTK-450

This system, consisting of a special sample heating furnace and temperature controller, is used to heat the sample during X-ray diffractometry to study the influence of heat on the crystal structure. The atmosphere in the furnace, consisting of air, an inert gas or vacuum, may be heated to 450°C during measurement at TTK-450.

With vacuum kit and cooling kit, the atmosphere may be cooled to -180°C.at TTK-450

The measurement results are output in multiple data format to enable comparison of

X-ray diffraction patterns obtained at various temperature.

Main Specifications

	TTK-450
Thermocouple	PT100 resister
Power supply	RT~300°C (in the air,or an inert gas)
Temperature	RT~450°C (in vacuum)
	-180~450°C (With cooling kit in vacuum)
Control	PID value setting fixed temperature control
functions	(increase, decrease, hold, stop)
Power supply	single phase 200/220V±10% 5A

Part name	P/N
Heating attachment TTK-450	215-24030-91
Vacuum kit for TTK-450	215-24034-92
Cooling kit for TTK-450	215-24033-92



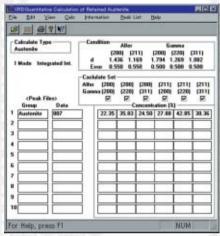
TTK-450

Quantitative Analysis

Residual Austenite Quantitation (P/N 215-00270-02)

Common method to quantify the residual austenite is to apply the method for samples consisting of 2 components such as tempered copper α -iron and γ -iron. The special software allows the determination without the need of standard sample.

The software directly uses the intensity ratio of the measured X-ray peaks of the α -iron and γ -iron components to theoretically perform the calculation. The five-peak average method is use to make the determination, so scattering due to the matrix effect is reduced to enhance the reliability of the results. Using the rotational sample stage (P/N 215-21766) for measurement even further helps to overcome data scattering.



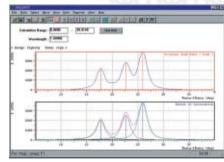
Quantitation Results Screen

Peak Processing

Overlapping Peak Separation Software (P/N 215-00273-02)

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.



Peak Separation Screen

Crystalline Structural Analysis

Precise lattice constant determination software (P/N 215-00274-02)

In X-ray diffractometry, a 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 content. 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 even further minimize error in diffraction angles. In addition, the miller index is applied to each peak.

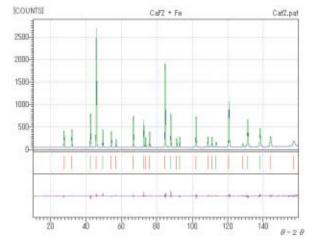


Precise lattice constant determination calculation Result Screen

Rietveld Analysis Software (P/N 215-00283-02)

The Rietveld method analyzes the crystalline structure by directly refining structural parameters and lattice constants over the entire powder X-ray or neutron diffraction pattern. It compares the diffraction pattern calculated from a presumed structural model with the actually measured pattern, and refines each parameter using the nonlinear least square method developed by the National Institute for Materials Science (formerly the Institute for Research in Inorganic Materials). This Rietveld Analysis Software utilizes the RIETAN program created by Mr. Fujio Izumi at the National Institute for Materials Science.

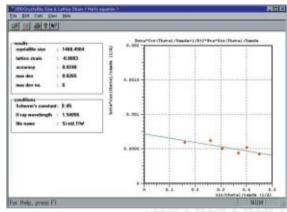
	Part Description	P/N
Γ	Rietveld analysis software RIETAN	215-00283-02



State Analysis

Crystallite Size & Lattice Strain Software (P/N 215-00276-02)

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 that 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)

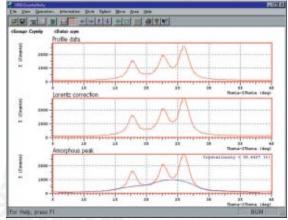


Hall's Equation Calculation Result Screen

Crystallinity Calculation Software (P/N 215-00277-02)

The degree of crystallization of a mixture of crystalline and amorphous substance, such as found in high polymer samples, is an important parameter of substance characterization.

This software automatically or manually separate the measured diffraction patterns into those of crystalline components and those of amorphous components. Then, it calculate the integrated intensity of the two types of substance, called degree of crystallization using the peak area ratio of the two classes of components.



Crystallinity Calculation Result Screen



Sample Holders

The following sample holders are available to allow different application, including the aluminum sample holder.



1 30 1 37 1 30 1				
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	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

X-ray Tubes and X-ray Filters

Focus Type	Type NF	Type BF	Type LFF
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/I		N
Cu	2.0kW (062-40003-03)	2.7kW (210-24016-21)	2.2kW (210-24100-11)
Co	1.8kW (062-40003-04)	2.7kW (210-24016-24)	1.8kW (210-24100-14)
Fe	1.5kW (062-40003-05)	2.7kW (210-24016-25)	1.0kW (210-24100-15)
Cr	1.8kW (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)	(215-22500-04)	
V filter (for Cr)	(215-22500-05)	

Cooling Water Circulator

HYCOOL HYW2023C-S15 (for 2kW X-ray tube)

HYCOOL HYW2045C-S36 (for 3kW X-ray tube)

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



Main specifications

Power supply
 Single phase 200V ±10% 20A (HYW2023C-S15)
 Single phase 200V ±10% 30A (HYW2045C-S36)

Ambient temperature 5~40°0

Cooling capacity 1750/2000kcal/h (50/60Hz) (HYW2023C-S15) 3600/3900kcal/h (50/60Hz) (HYW2045C-S36)

Part Description	P/N
HYCOOL HYW2023C-S15	044-01807-11
HYCOOL HYW2045C-S36	044-01807-12

Cooling Water Pump CW-1

This water pump supplies cooling water to the X-ray tube and high voltage tank.

It is recommended when the available tap water has a pressure below 3kgf/cm2 or when the water pressure fluctuates excessively.

Main specifications

Power supply AC100/200V 5/2.5A

Output pressure 0~5kgf/cm²(continuously variable)

1	Part Description	P/N
	Cooling water pump CW-1	239-15023



System Configuration and Accessories

Following is the standard system configuration and the various accessories listed according to application.

1 Standard configuration

		2kW	type		3kW type	
	XRD-6000	1 unit P/N 2	15-21750-10	1 u	nit P/N 215-21750-12	
•	Goniometer		1	•	X-ray tube	1
•	Data processo	r	1	•	Scintillation detector	1
	High voltage to	ansformer			Standard accessories	1set

3 Convenient sample holders

Glass Sample Holder
 Glass Micro Sample Holder
 Ø25 x 1.0 5pc/set
 Ø15 x 0.5 5pc/set
 P/N 215-22507-02
 P/N 215-22507-03

Non-reflective Sample Holder 2pc/set P/N 215-22507-05

2 Special setup accessories

Tap water pressure low
Cooling water pump CW-1 P/N 239-15023

Un-available tap water or low quality tap water
 Cooling water circulator HYCOOL HYW2023C-S15
 Cooling water circulator HYCOOL HYW2045C-S36
 P/N 044-01807-12

4 Main maintenance / consumable items

X-ray tube 2.0kW, NF
 X-ray tube 2.7kW, BF
 Si standard sample, 20g 325 mesh 1
 P/N 215-21723

Special Accessories

Special Accessories		○ :Absolutely req	uired	<u> </u>	:Red	quire	d (:Re	quire	d dep	pendi	ng or	n obje	ctive
Analysis Objective	Part Description	Part Number	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	Environment, industrial waste
1 BG reduction, especially iron samples	Counter Monochromator CM-3121	P/N 215-22360-02	0	0	0	0	0	0	0	0	0	0	0	0
O Ovelitetive coelusis DDFO Oceans	ICDD PDF2 file (CD-ROM)	P/N 239-50002-11,12												
2 Qualitative analysis PDF2 Search	PDF2 Search S/W (DDVIEW)	P/N 239-50002-21,22					0			0		0	0	0
3 Qualitative analysis PDF4 Search	ICDD PDF4 + (CD-ROM)	P/N 239-50015-01,02	0	0	0	0	0	0	0	0	0	0	0	0
	Rotational Sample Stage RS-1001	P/N 215-21766												
4 General purpose quantitative analysis	Auto 5 position sample changer ASC-1001	P/N 215-23175								0		0	0	0
	Residual austenite quantitation S/W	P/N 215-00270-02	0		0									
5 Residual austenite quantitation	Rotational Sample Stage RS-1001	P/N 215-21766	0		0			. 10						
Environmental quantitative	Environmental Quantitative Analysis Stage RS-2001 (Filter holders Zn, with S/W)	P/N 215-21767				vă	d	K	1	4	H		Š	0
analysis system	Filter holder AI (ø 25mm)	P/N 215-22775-02			A	Q.				7				0
7 Multiple peak separation	Peak separation S/W	P/N 215-00273-02	•	•		•		•			•	•	•	
8 Precise lattice constant determination	Precise lattice constant determination S/W	P/N 215-00274-02	•	•	•	•		•		•		7		
9 Crystal structure analysis	Rietveld analysis, Software RIETAN	P/N 215-00283-02	•	•	•	•	•	•		•				
10 Crystallite size / lattice stress	Crystallite Size / Lattice Stress S/W	P/N 215-00276-02	M					1.4	0	0	0			
11 Degree of crystallization	Degree of Crystallization S/W	P/N 215-00277-02	•						0	0	0			
12 Heating analysis	Sample Heating Attachment HA-1001	P/N 215-23000-01	•	•	•	•		•						
13 Thin film analysis	Thin Film Analysis Attachment THA-1101 (stage, monochromator, suction pump)	P/N 215-21765	•	•	•	•	•	•						
NAME OF THE PROPERTY OF THE PR	Rotational Sample Stage RS-1001*	P/N 215-21766	•	•	•	•	•		0					
14 Fiber degree of orientation analysis	Fiber Sample Attachment (with S/W)	P/N 215-22624	•					•	0					
15 Residual stress analysis	Stress Analysis Attachment SA-1101 (with Cr X-ray tube, S/W)	P/N 215-21769	0	0	0	•	•	•						
16 Micro Measurement	Micro-Measuring Attachment MDA-1101	P/N 215-23180	•	•	•	•		•						
17 Fixed irradiation width analysis	Automatic Variable Slit System AVS-1101	P/N 215-23950	•	•	•	•		•				•	•	•
18 Powerful parallel X-ray beam / Bumpy samples	Polycapillary Unit PCL-1001	P/N 215-23980	•	•	•	•				•	•	•	•	•

^{*}Can be used together with general purpose rotational sample stage

^{*}For application, refer to information on Sample Holders





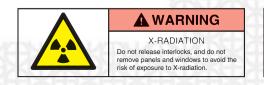
XRD-6000

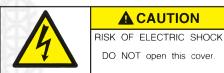
Item		XRD-6000 2kW type	XRD-6000 3kW Type						
		(1) (1)	41:						
	Туре	Cu, NF type	Cu, BF type						
X-ray tube	Focus	1.0 x 10mm	2.0 x 12mm						
	Max. output	2kW	2.7kW						
	Max. output	3kW							
	Output stability	±0.01% (for 10% power fluctuations)							
	Max. tube voltage	60kV							
	Max. tube current	80mA							
X-ray generator	Voltage step width	1kV							
	Current step width	1mA	1mA						
	Overload limit setting	Setting changeable with tube type	Setting changeable with tube type						
	X-ray tube protection	Against undervoltage, overload, overvoltage, o	Against undervoltage, overload, overvoltage, overcurrent and/or failure of water supp						
	Safety mechanisms	Door interlock mechanism (X-ray can be generate	ed only afterdoor is closed) Emergency sto						
	Туре	Vertical typ							
	Scanning radius	185mm	185mm						
	Min. step angle	0.002°(2θ) 0.001°(θ)							
	Angle reproducibility	±0.001° (2θ)	不						
	Scanning angle range	-6°~163° (2θ), -180°~180°(θ)							
0	Scanning system	$\theta/2\theta$ linkage mode, θ , 2θ independent mode							
Goniometer	Operation mode	Continuous scan measurement, step scan n θ axis oscillation (when using 2θ continuous							
	Slewing speed	1000°/minute (2θ)	PATRICIA PATRICIA						
	Scanning speed	0.1°~50°/min (2θ), 0.05°~25°/min (θ)							
	Divergence slit (DS)	0.5°, 1°, 2°, 0.05mm	X(H)X(H)X						
	Scattering (SS)	0.5°, 1°, 2°							
	Receiving slit (RS)	0.15mm, 0.3mm							
本中本中本年	Detector	Scintillation counter							
Detector/country	Scintillator	Na I	Na I						
Detector/counter	Scaler	Preset time $0.1 \sim 1000~{ m sec}$ No. of colu	umns 7 columns						
	HV/PHA	High voltage supply 500 - 1200V, baseline a	High voltage supply 500 - 1200V, baseline and window auto-control						
Cooling	Dimensions	W900 x D700 x H1600							
Casing	Leakage X-rays	Less than 2.5μSv/h (at maxium out put)	t)						

Data Processing Unit

Computer type	IBM PC/AT compatible
os	WindowsXP
Display	17-inch color monitor
Printer	Color printer (A4)
Items controlled	Goniometer, X-ray generation, tube voltage, tube current, detector high voltage, PHA, 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 PDF2/PDF4 options) calibration curve generation, quantitation calculation
Quantitative analysis	Calibration curve generation, quantitative analysis

^{*}Windows is a registered trademark of Microsoft Corporation





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 Ω resistance			

Installation site environment

The following ambient temperature and humidity are required.

Temperature	23°C ± 5°C
Humidity	60% ± 5%

Heat generated from the instrument is approximately 860cal/h. When the cooling water circulator is installed in the same room, this is increased by 2,720cal/h and 4,580cal/h for the 2kW and 3kW types, respectively.

Cooling water supplied to instrument

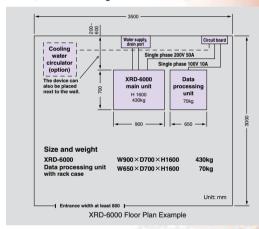
When cooling water supplied to the instrument becomes dirty due to piping corrosion, etc., this causes clogging of the X-ray tube filters. Cooling water should be supplied using the following conditions.

Temperature	23°C ± 5°C
Humidity	60% ± 5%

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 860cal/h. When the cooling water circulator is installed in the same room, this is increased by 2,720cal/h for the 2kW X-ray tube and 4,580cal/h for the 3kW X-ray tube.

Flow rate	at least 4.0L/min
Water pressure	3~5kgf/cm ²
Water quality	pH6~8, 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 flow-rate could not be fulfilled, use the cooling water circulator, available as an option.





JQA-0376

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