Ultima IV

The Ultima IV represents the state-of-the-art in multipurpose X-ray diffraction (XRD) systems. Incorporating Rigaku's patented cross beam optics (CBO) technology for permanently mounted, permanently aligned and user-selectable parallel and focusing geometries, the Ultima IV X-ray diffractometer can perform many different measurements...fast.

Engineered for Performance

With a multipurpose diffractometer, performance is measured by not only how fast you perform an experiment but also how fast you can switch between different types of experiments. Individual experiments are optimized with accessories like the D/teX *Ultra* high-speed position sensitive detector system, but the speed between experiments is radically improved with the combination of the automated alignment and CBO.

Designed for Flexibility

The Ultima IV is the only XRD system on the market today that incorporates fully automatic alignment. When coupled with CBO and the in-plane arm, the automatic alignment capability makes the Ultima IV X-ray diffractometer the most flexible system available for multipurpose applications.

Functionality Redefined

In the Ultima IV XRD system, CBO technology eliminates time spent switching geometries, enables everyday users to run both sets of experiments without the need to reconfigure the system, and reduces wear and possible optic damage associated with

the recurrent switching process. CBO and automatic alignment combine for the ultimate in functionality for: micro-crystalline diffraction, thin-film diffraction, small angle scattering, and in-plane scattering.

Features:

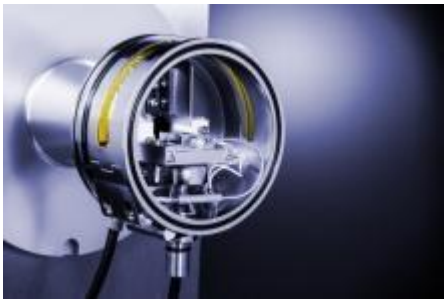
- Full automated alignment under computer control.
- Optional in-plane diffraction arm for in-plane measurements without reconfiguration.
- Focusing and parallel beam geometries without reconfiguration.
- SAXS capabilities.
- Optional D/teX *Ultra* high-speed, position-sensitive detector system.

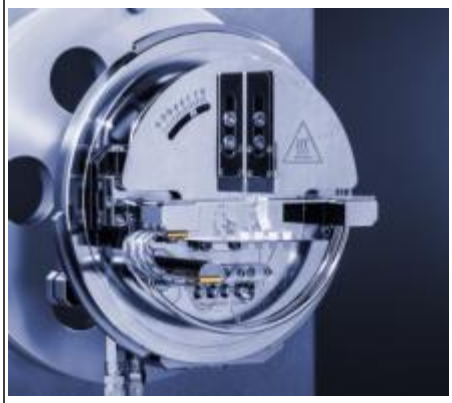
Ultima IV specifications

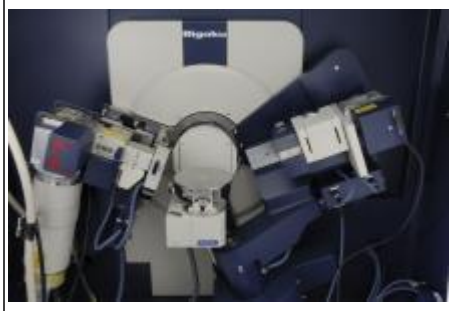
X-ray generator	Maximum rated output	3 kW
	Rated tube voltage	20 - 60 kV
	Rated tube current	2 - 60 mA
	Target	Cu (others: optional)
	Focus size	0.4 x 12 mm (others: optional)
Goniometer	Scanning mode	θs/θd coupled or θs, θd independent
	Goniometer radius	285 mm

	2θ measuring range	-3 to 162° (maximum)
	Minimum step size	0.0001°
Optics	Divergence slit	Fixed or automatic variable
	Scattering slit	Fixed or automatic variable
	Receiving slit	Fixed or automatic variable
	Optics alignment	Automatic alignment of tube height, goniometer, optics and detector
	Monochromator	Dual position graphite diffracted beam monochromator for Cu (others: optional)
Detector	Detector	Scintillation counter (others: optional)
Dimensions	H x W x D	1600 x 1100 x 800 mm
	Sample height	1050 mm

Ultima IV accessories

Anton Paar TTK 450 Low Temperature Chamber	Sample cooling and heating stage with liquid nitrogen cooling. Large temperature range and ease of use for a wide range of applications. With beam knife and optional zero background sample holder for investigation of organic materials at low 2θ angles. Temperature range: -193 °C to 450 °C Atmospheres: air, inert gas, vacuum(10^{-2} mbar)	
Anton Paar HTK 2000N High-Temperature Chamber	High-temperature sample heating stage with strip heater for powder XRD of refractory materials. The use of a tungsten strip offers extremely high temperature and fast heating and cooling, the strip pre-stressing mechanism ensures high sample position stability. Temperature range: with W-strip: 25 °C to 2300 °C in vacuum with Pt -strip: 25 °C to 1600 °C in air, vacuum Atmospheres: vacuum(10^{-4} mbar), inert gas, air	

Anton Paar HTK 16N High-Temperature Chamber	High-temperature sample heating stage with strip heater for powder diffraction. Allows for very fast heating and cooling and ensures high sample position stability with heating strip pre-stressing. Temperature range: with Pt-strip: 25 °C to 1600 °C in air, vacuum with Ta and C-strip: 25 °C to 1500 °C in vacuum Atmospheres: air, inert gas, vacuum(10^{-4} mbar)	
Anton Paar HTK 1200N High-Temperature Oven Chamber	High-temperature heating stage for powders and polycrystalline solid samples. Heating to 1200 °C in air and vacuum possible. Main features: furnace heater for good temperature uniformity sample spinning for good data quality capillary option for transmission XRD easy sample loading Temperature range: 25 °C to 1200 °C Atmospheres: air, inert gas, vacuum(10^{-4} mbar)	

Advanced thin film attachment	Multipurpose attachment for the precise alignment of thin film samples. Fully automated alignment provides extreme ease in the positioning of samples for X-ray reflectivity, in-plane diffraction, and orientation analysis. Utilizes the Rx/Ry design for the most flexible reciprocal space scanning options.	
Reactor X high temperature attachment for reactive gases	Reactor X allows measurements to be performed under high temperature (RT - 1000°C) in vacuum, inert gas, reactive gas, or mixture of these. Infrared heating enables rapid heating and cooling of the sample and use of wide variety of sample holders so that a suitable sample holder material can be selected according to the combination of the sample, gas, and applied temperature.	
Low & medium temperature attachment	Automated variable temperature stage for *in-situ X-ray diffraction measurements of materials at low and elevated temperatures (-180°C to 350°C). The stage may be operated in air, gas, vacuum, or under liquid nitrogen cooling conditions. The sample is heated radiantly for reduced heat gradients within the sample. Automated z*	

	translation within the stage assures precise sample positioning even in the presence of thermal expansion of the sample.	
HT 1500 high temperature attachment	Automated variable temperature stage for *in-situ* X-ray diffraction measurements of materials at ambient and elevated temperatures (up to 1500°C). The stage may be operated in air, gas, vacuum, or under inert gas such as helium or nitrogen. The sample is heated radiantly for reduced heat gradients within the sample. Automated z translation within the stage assures precise sample positioning even in the presence of thermal expansion of the sample.	

Software:

PDXL is a one-stop full-function powder diffraction analysis software suite. The modular design, advanced engine and user-friendly GUI have been satisfying both experienced and novice users since PDXL was released in 2007.

PDXL provides various analysis tools such as automatic phase identification, quantitative analysis, crystallite-size analysis, lattice constants refinement, Rietveld analysis, ab initio structure determination, etc.

Fundamental parameter method

The peak shape in a powder diffraction pattern would appear to be a delta function if measured under ideal conditions. In reality, the peak shape changes depending on a number of measurement conditions: wavelength distribution of the source, optical systems, slit conditions, crystallite size and strain, and so on. The peak shapes obtained

from measurements made under real-world conditions are described using an empirical function such as a split pseudo-Voigt function, or a split Pearson VII function which has a good agreement with the obtained peak shapes. The fundamental parameter method (FP method) is a method to calculate peak shape by convolution of the shapes caused by all the instrumental and sample conditions.

Phase identification using COD

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

Wizard for ab initio crystal structure analysis

Recently, there have been many published examples of ab initio crystal structure analysis performed on powder diffraction data. This development is attributed primarily to significant improvements in PC processing speed and in the efficiency of the algorithms used for structure determination.

PDXL has so far provided all of the functions required for ab initio crystal structure analysis, such as indexing, structure determination and structure refinement by the Rietveld method. Now the "Structure Analysis Wizard" is available in PDXL to provide support and guidance for users undertaking the complicated procedure of structure analysis, particularly of organic compounds. This wizard system will make it possible for even the beginner to achieve analytical success

Clustering function

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

Application:

Analysis of glazing chemicals, paints and a vermilion ink in arts and crafts

Arts and crafts use various coloring materials and dyes. X-ray diffraction can be used to obtain information concerning the crystallinities and the compounds present in the dyes. From the analysis of those dyes, it is possible to obtain information about how a picture was created, identify similar or related arts and crafts, and determine whether a particular item is real or a forgery.

Analysis of thin film materials

For thin film materials pole figure analysis can be used to determine orientation relationships between substrates and deposited materials. In this Ultima IV example in-plane pole figures were collected on both the Pt substrate and $(Pb,La)TiO_3$/Pt/MgO PLT thin layer. The epitaxial relationship between the substrate and layer material is clearly shown. Critical to this measurement is the in-plane geometry which allows full pole figures to be collected on both the substrate and thin layer.

Bentonite: A healing clay!

For centuries, bentonite clay has been used by natives and indigenous people to cure many diseases and promote internal healing.

An XRD pattern of the clay, shown in Figure 1, was collected on Rigaku's Ultima IV multipurpose diffraction system.

Contact printed Co/insulator/Co molecular junctions

Growing efforts are being dedicated to organic monolayer junctions that may afford a new generation of electronics devices of far smaller sizes and higher density. Contact printing is one of the most promising alternatives for depositing the top metal electrode without degradation of the underlying self-assembled monolayer (SAM). A large-area metal/SAM/metal junction based on magnetic metal cobalt, created by coupling the techniques of self-assembly and contact printing was reported recently[1].

Detailed observation of crystal phase transition of fats occurring over a narrow temperature range

Crystalline fat, which is raw material of cocoa butter, margarine, etc., has a number of crystal polymorphs and shows complex phase transitions around room temperature. Controlling crystal phase and phase transition process is important for manufacturing process management and quality assurance.