PANalytical

X'PERT QUANTIFY

Quantitative phase analysis software for X-ray diffraction applications

The Analytical X-ray Company

X'PERT QUANTIFY

Bringing automated quantitative analysis to XRD

Extending PANalytical's range of innovative software for XRD, X'Pert Quantify provides users of PANalytical X-ray diffractometers with a powerful tool for quantitative phase analysis. X'Pert Quantify is a complete quantitative analysis package that includes measurement, extraction and correction routines.

X'Pert Quantify controls a broad range of PANalytical systems comprising X'Pert-MPD, X'Pert PRO MPD, CubiX XRD, CubiX PRO, PW1800 as well as PW3710 and PW1710 microprocessor controlled systems.

The package provides a large selection of currently accepted analytical models, including as many as 10 calibration models and a wealth of intensity-correction methods to give you the broadest spectrum of analytical solutions meeting all your needs. The accuracy of all results is estimated using the counting statistical errors in all related measured intensities.

Capable of working independently or in conjunction with other X'Pert Software such as X'Pert Data Collector, X'Pert Quantify accepts input from peak-intensity measurements, integrated-area measurements and scans in PANalytical's open XRDML data format, and stores quantitative results in an MS Access database. What's more, as measurement and analysis are independent of each other, it is also able to evaluate data off-line, allowing you to extract relevant intensities from previously-acquired scan files and/or analyze previous measurements.

PANalytical

- User Batches allow fully-automated quantitative phase analysis
- 10 quantification models
- Complete set of intensity correction methods
- Off-line extraction of relevant intensities from existing scans
- Standard deviations in results estimated from counting statistics
- Fully integrated in X'Pert Software range

No need for crystal structure data

In contrast with the Rietveld method of quantification, X'Pert Quantify doesn't require crystal structure data for the analysis.

The methods used by X'Pert Quantify are based on direct measurement of intensities of individual reflections rather than the interpretation of a complete scan.

X'PERT QUANTIFY

Powerful algorithms… Proven methods… Ease of use

Quantification models

To provide optimum power and flexibility, X'Pert Quantify offers the most complete range of quantification models of any package currently available.

General model
This model makes use of the fact that the intensities of observed reflections are a function of both the concentrations of the corresponding compounds and the mass absorption coefficient of the sample. You can therefore use it if the mass absorption coefficients of all samples are known.

Straight Line model
This model assumes a linear relation between the concentrations of the compounds in a sample and the corresponding observed intensities. Use when the mass absorption coefficients can be assumed constant for all samples.

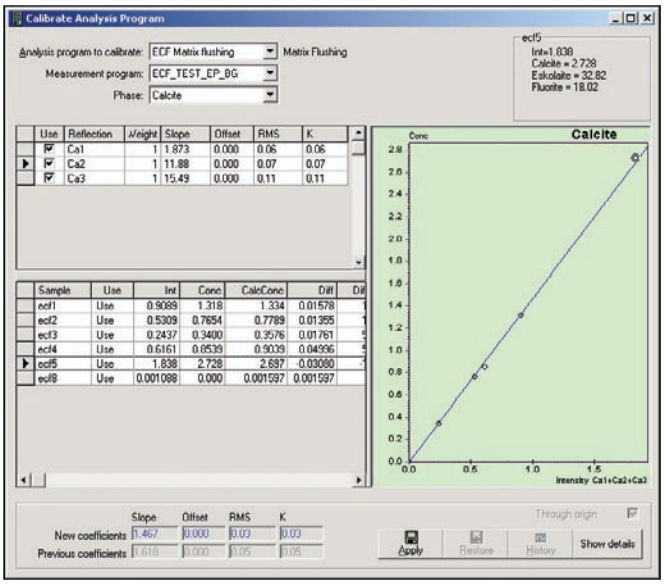
Linear Multi-Variate Regression model
This is an extension of the Straight Line model in which the concentration of a compound in a sample is determined from measurements of the intensities of various independent reflections.

Matrix Flushing model
The Matrix Flushing model is also known as the Normalization, Chung or Adiabatic model.
Use when the sum of the concentrations of all phases is known. The Matrix Flushing model is especially popular, because it was the first that enabled mineralogists to perform quantitative phase analysis without the need to know, or make assumptions about, the mass absorption coefficients of each of their samples. This model determines the relative abundances of all compounds and normalizes the sum to the known sum of all concentrations.

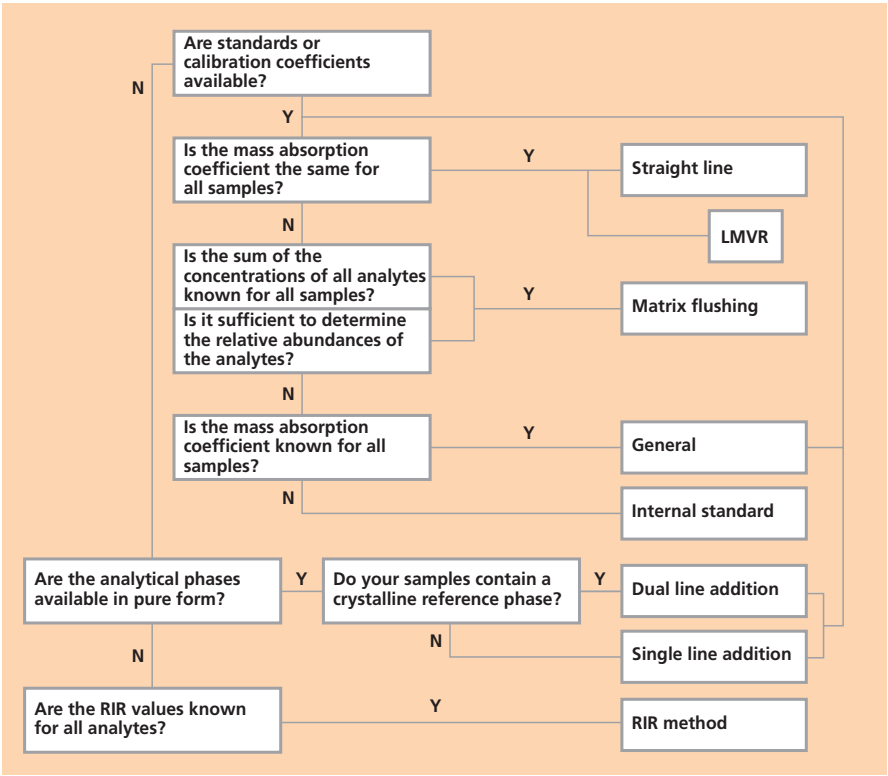
RIR (Relative Intensity Ratio Method)
If none of the previous models is applicable, this model may still provide the required information. Here a known concentration of a standard compound is mixed with the sample and from the ratio of the net intensities of the peaks produced by the standard and unknown components, the concentrations of the components of the original sample are determined.

This model uses RIR data documented for 50/50 mixtures of corundum and crystalline phases of known compounds in the ICDD (International Centre for Diffraction Data) PDF database.
In its primitive form a known mix of corundum and sample is made and from the measured Relative Intensity Ratio of the phases of interest to that of corundum, X'Pert Quantify derives the concentration of the phases using the reported RIR values.

Alternatively, corundum can be substituted for any other compound and the RIR value of that compound is used to recalculate a new RIR for the phase of interest.



Example of a calibration with multiple reflections per phase



Decision schematic to select the appropriate calculation/ quantification model for infinitely thick samples

Addition models

Addition models in which after the initial measurement on a sample, the sample is measured again with the concentration of the component of interest enriched by a known amount. X'Pert Quantify provides two Addition models

Single Line Addition
For use when the sample contains just one crystalline phase plus an amorphous phase.

Dual Line Addition
For use when the sample contains a 'reference phase' available in fairly high concentration with a line that preferably does not overlap the lines of other components.

X'PERT QUANTIFY

Powerful algorithms… Proven methods… Ease of use

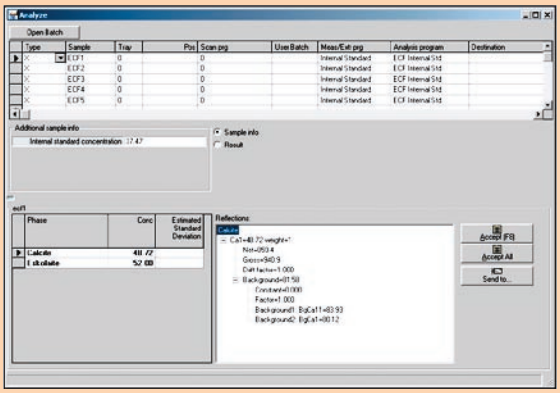
Models for thin samples

Thin layer with base-plate correction
Used for thin samples, defined as samples that are sufficiently thin to be transparent to X-rays. This affects the relative intensities in the diffraction pattern.
Measurements are taken with a clean support plate and with support plate plus sample. From the relative intensities of the peak produced by the support plate alone to that produced by support plate plus sample, X'Pert Quantify determines the transmission factor, which is a key element for determining the concentration of the phase of interest. Because of the finite thickness, one can even determine the total mass of the phase of interest.

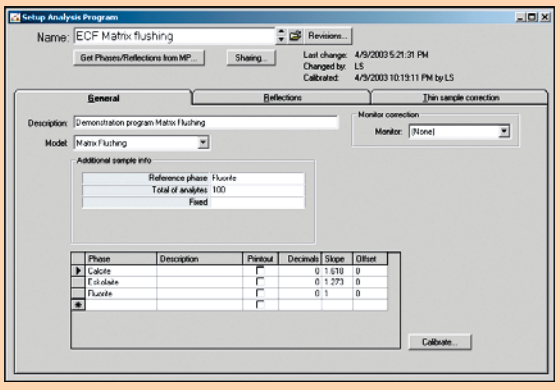
Thin layer dual reflection model
Used for thin samples where a clean support plate is unavailable or the support plate doesn't have usable reflections. To use this model, two reflections from one selected phase must be measured. Using the intensity ratio of these reflections for an infinitely thick sample (either measured or derived from the ICDD PDF database) X'Pert Quantify then calculates the transmission factor and subsequently the concentration, or mass of the phase of interest.
What's more, for all models, you can use either one, or the weighted sum of several reflections corresponding to the phases of interest. This feature often helps you cope with the detrimental effects of preferred orientation.

Advanced intensity corrections for optimum analytical integrity

X'Pert Quantify also provides a broad range of correction algorithms to obtain the net intensity of a peak with the highest degree of accuracy. These include: overlap correction using either a fixed correction factor or calibration with a linear multivariate regression formula, monitor drift correction and background corrections using a range of correction techniques including interpolation between measured points in the background, averaging the background over the area of interest, subtraction of a constant pre-determined background level and the multiplication by a background factor that takes account of the real intensity profile.



Analyze screen with detailed tree-view of all contributing reflections



Definition of a quantitative analysis program

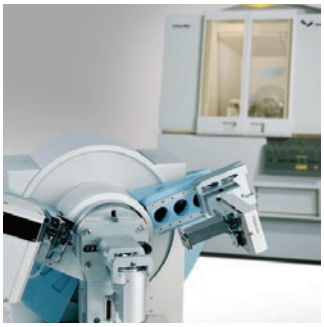
Operational ease

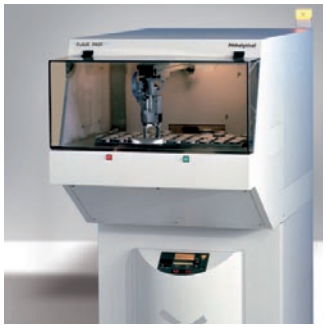
The program's intuitive Windows®-based user interface allows for easy setting up for quantitative measurements and analysis. It also provides full reporting facilities ranging from result reports for a single sample or batch, to complete daily, weekly or monthly reports and control graphs of, for example, your intensity monitor. X'Pert Quantify also features comprehensive on-line Help and a Quick Start Guide.

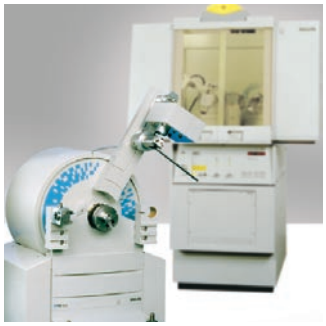
Graphical interface for setting up peak areas - simply use the mouse to set the start and end points of a peak area measurement.

Systems supported by X'Pert Quantify

X'Pert Quantify supports many generations of PANalytical and Philips Analytical diffractometers. For older systems in particular, X'Pert Quantify enables an upgrade to modern software running on today's computer hardware.

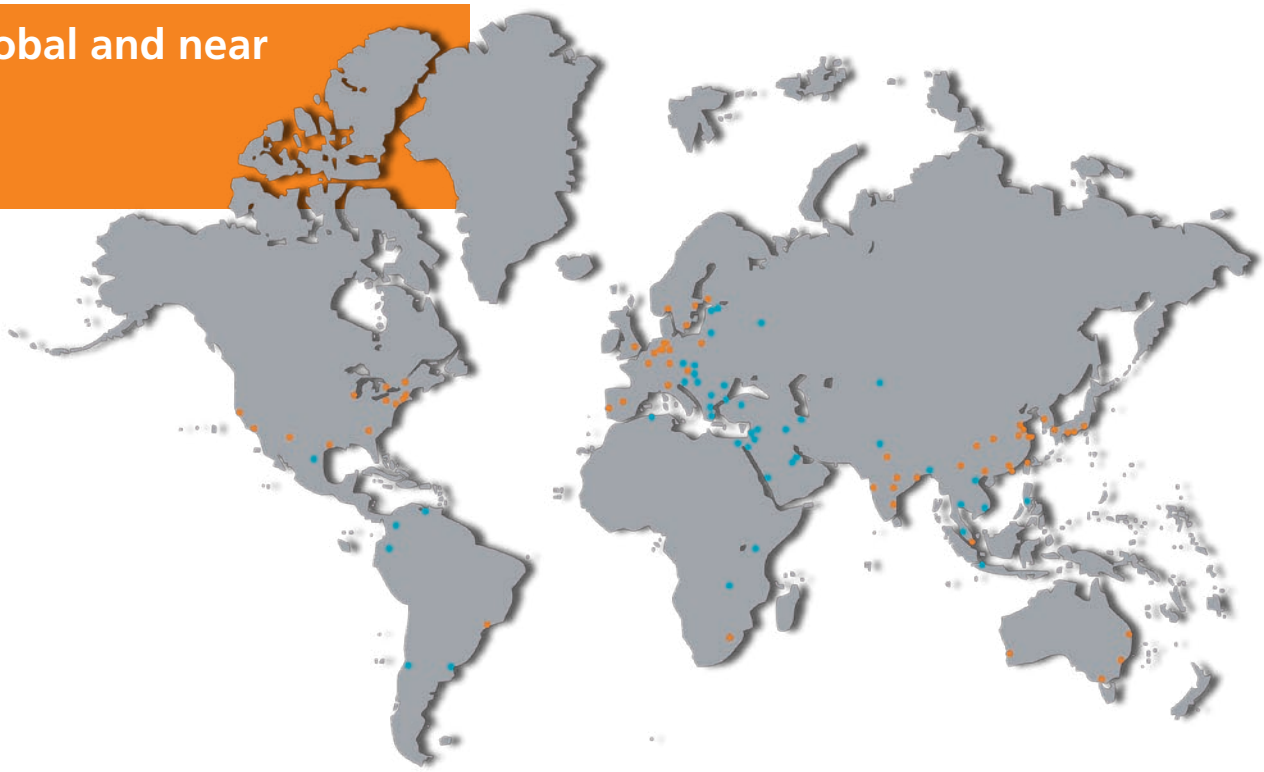






PANalytical

Global and near



PANalytical
PANalytical is the world's leading supplier of analytical instrumentation and software for X-ray diffraction (XRD) and X-ray fluorescence spectrometry (XRF), with more than half a century of experience. The materials characterization equipment is used for scientific research and development, for industrial process control applications and for semiconductor metrology.
PANalytical, founded in 1948 as part of Philips, employs around 850 people worldwide. Its headquarters are in Almelo, the Netherlands. Fully equipped application laboratories are established in Japan, China, the USA, and the Netherlands. PANalytical's research activities are based in Almelo (NL) and on the campus of the University of Sussex in Brighton (UK). Competence and supply centers are located on two sites in the Netherlands: Almelo (development and production of X-ray instruments) and Eindhoven (development and production of X-ray tubes). A sales and service network in more than 60 countries ensures unrivalled levels of customer support.
The company is certified in accordance with ISO 9001:2000 and ISO 14001.

The product portfolio includes a broad range of XRD and XRF systems and software widely used for the analysis and materials characterization of products such as cement, metals and steel, nanomaterials, plastics, polymers and petrochemicals, industrial minerals, glass, catalysts, semiconductors, thin films and advanced materials, pharmaceutical solids, recycled materials and environmental samples.

Visit our website at www.panalytical.com for more information about our activities.
PANalytical is part of Spectris plc, the precision instrumentation and controls company.

PANalytical B.V.
Lelyweg 1, 7602 EA Almelo
The Netherlands
T +31 (0) 546 534 444
F +31 (0) 546 534 598
info@panalytical.com
www.panalytical.com

Regional sales offices

Americas
T +1 508 647 1100
F +1 508 647 1115

Europe, Middle East, Africa
T +31 (0) 546 834 444
F +31 (0) 546 834 499

Asia Pacific
T +65 6741 2868
F +65 6741 2166

Printed in The Netherlands on 50% recycled, chlorine free paper. Data subject to alteration without notice. For reference purposes only. 9498 702 10512 PN5226