PANalytical

DATA COLLECTOR

One consistent data acquisition tool for all your X-ray diffraction experiments

The Analytical X-ray Company

Pioneering measurement strategies throughout the years

From Debye-Scherrer film strips to fully digitized data acquisition and measurement strategies

2012 ***Data Collector*** continues to innovate and can now measure 0D, 1D, 2D diffraction data and even 3D computed tomography data

1997 Launch of ***X'Pert Data Collector,*** the first Windows-based data acquisition software, coupled with analytical software

1997 – 2012 Addition of multiple applications: non-ambient control, thin film measurement routines, PDF analysis, SAXS, etc.

1989 ***PC APD***, first form-based analytical suite

1983 ***APD1700,*** first complete analytical software suite

1980 ***APD10,*** first mainframe-based menu-controlled data acquisition software producing digital results

1979 ***PW1710,*** first programmable diffraction system

1945 First manually operated X-ray diffractometer with Geiger-Müller counter

PANalytical

DATA COLLECTOR

The ultimate central toolbox for data acquisition

Data Collector is the software program for the acquisition of all X-ray diffraction data from PANalytical's Empyrean, X'Pert PRO MRD (XL) and X'Pert Powder instruments. It offers one consistent workflow and user interface for all applications supported on our multi-purpose platforms, ranging from phase identification and quantification to thin film methods and area detector measurements.

Switching between point or line detector applications to area detector measurements does not require the execution of different data acquisition software packages; it can all be done within Data Collector.

Intuitive batch programming through the Graphical User Interface

One consistent workflow for 0D, 1D, 2D and 3D measurements

Easy experiment setup and execution

Open XML file formats

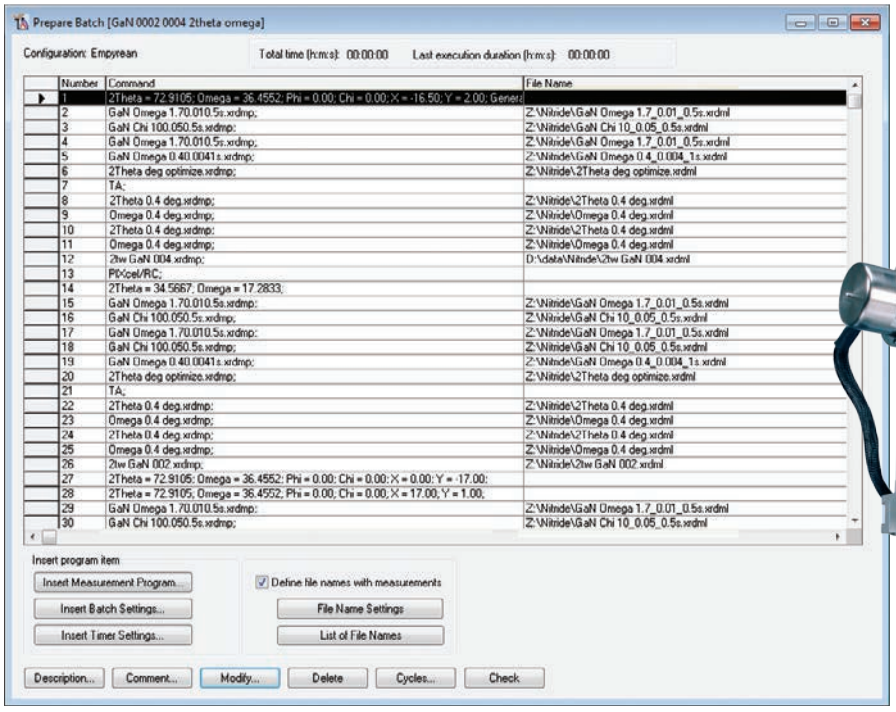
Operator Interface – simplifying complex measurements

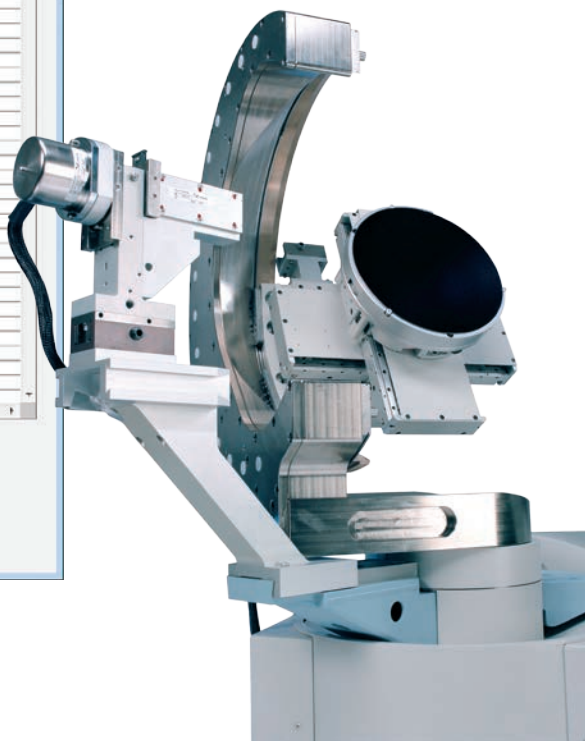
Easy previewing of data with Data Viewer and Area Director

Automatic processing program - easy automation of routine tasks

Batch programming

Data Collector's batch programming capabilities efficiently enable setup of measurement routines which contain various X-ray diffraction scans in combination with sample positioning and – optimization.

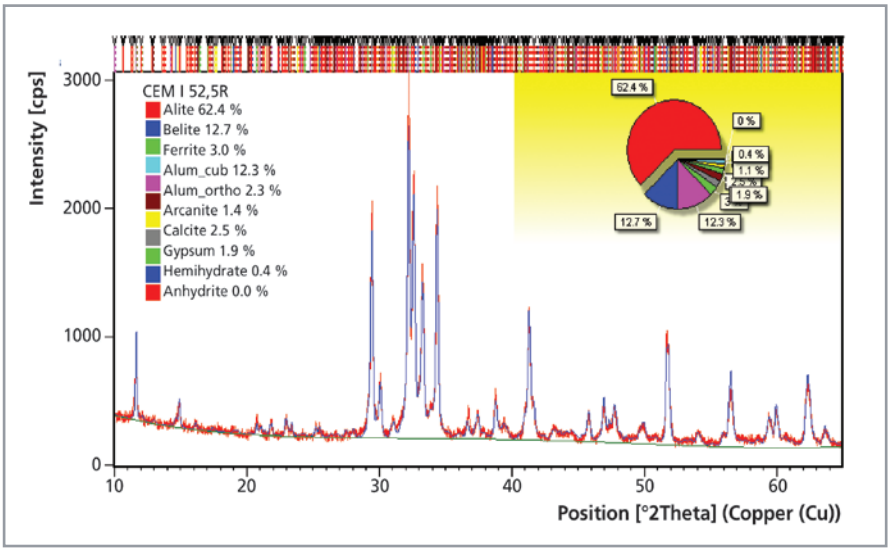




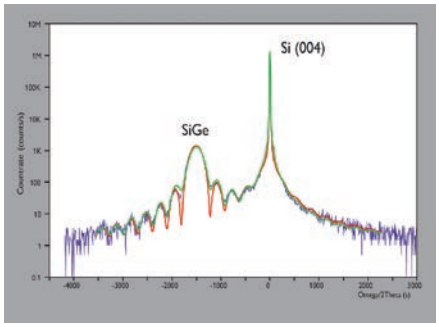
DATA COLLECTOR

The only software package for 0D, 1D, 2D and 3D

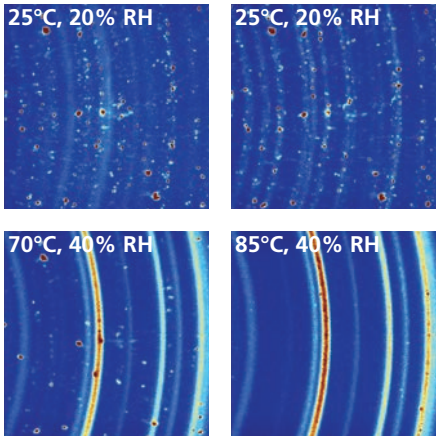
The PANalytical Empyrean, X'Pert PRO MRD (XL) and X'Pert Powder platforms provide a range of applications such as phase determination, Rietveld refinement, SAXS, pair distribution function, computed tomography, thin film analyses and many more.
Data Collector provides a logical, unambiguous, single workflow for all these applications. You can easily switch between applications.



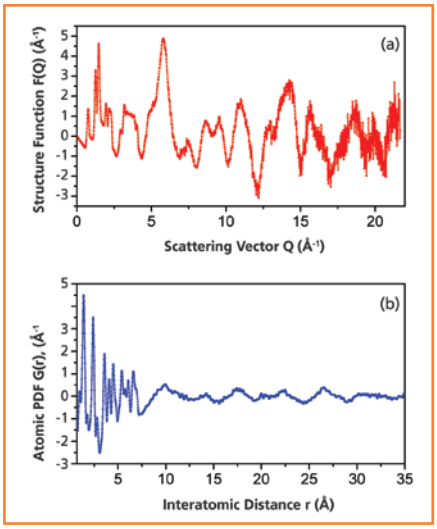
Example of data that is acquired in 0D or 1D mode. Phase identification and quantification is performed with HighScore Plus. Here an example of a quantitative analysis of a complex mixture.



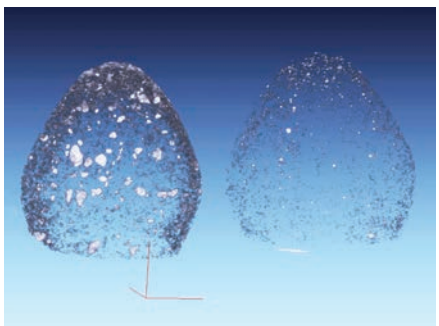
Acquiring data on epitaxial layers is typically done in 0D mode with a point detector. Here an example of SiGe on a Si (004) substrate.



2-dimensional diffractograms, in this case measured with the PIXcel3D 2x2, yield not only phase information, but also yield information on texture and crystallization processes. Here an example of trehalose measured at various humidity levels and temperatures.

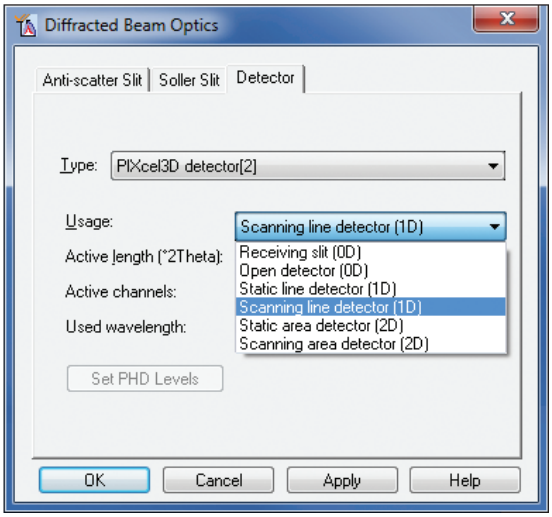


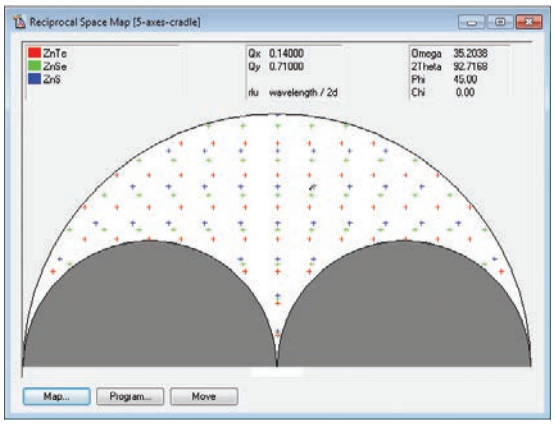
Example of a pair distribution function analysis of C_{60} fullerene (buckyball) to determine interatomic distances. The raw data can be acquired in either 0D or 1D mode using Mo or Ag radiation.



Going 3-dimensional: radiographs are collected at different sample orientations in area detection mode. Using computed tomography software 3-dimensional reconstructions of your sample can be made. Here a comparison of a counterfeit (left) and a genuine tablet (right).

From a phase identification in 1D mode to collecting 2D micro-diffraction scans: it's just a matter of a few clicks in Data Collector.





Reciprocal space map showing three structures: ZnTe, ZnSe and ZnS. The Ewald sphere construction is also shown.

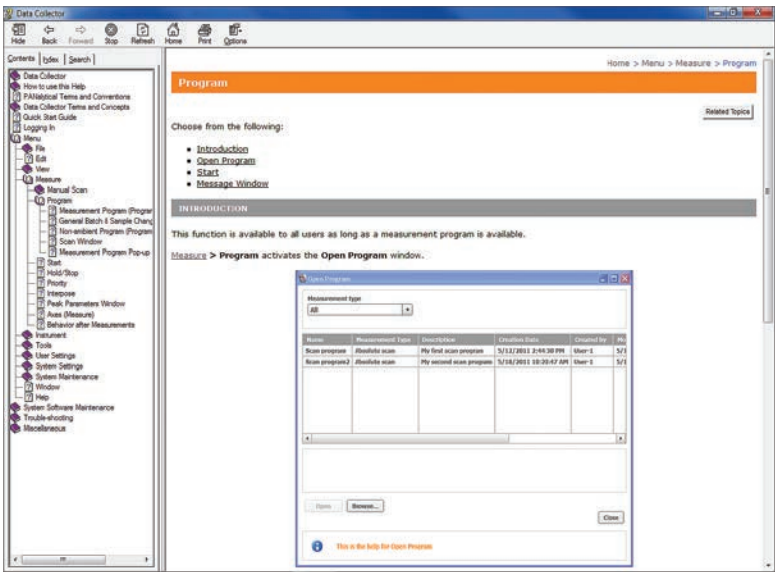
You can easily set up your measurements in reciprocal space with a graphical user interface.

Easily switch from one application to another

Always the same intuitive workflow independent of application

Extensive help and guidance

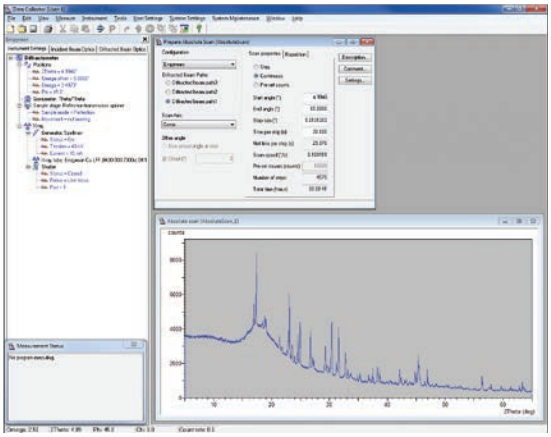
Data Collector and its modules have a powerful context-sensitive Help function to guide you through all aspects of the program's operation and to provide background information. In addition, where necessary, the theory behind a certain concept or function is explained. An easy to follow Quick Start Guide is provided with all modules.



Example of a help topic in the Help system. The topic provides background theory information, while the tree view pane on the left-hand side provides navigation information.

Focus on your diffraction experiment

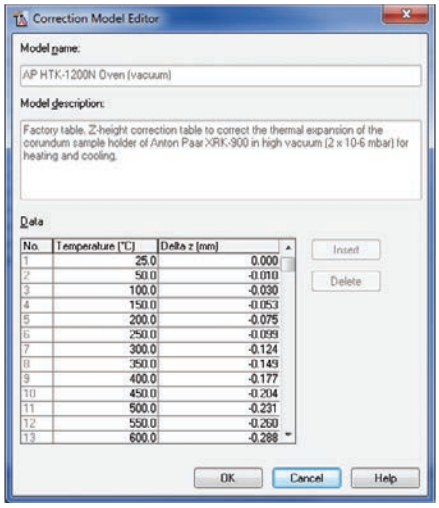
Intuitive system configuration



Data Collector's highly intuitive user interface provides you with access to a host of powerful functions that makes even the most complex and demanding analytical routine a relatively simple operation.

Typical example of a screen layout (customizable). The menu, toolbar and status bar are ready for direct instrument control, measurement status feedback, measurement control and resulting diffractograms.

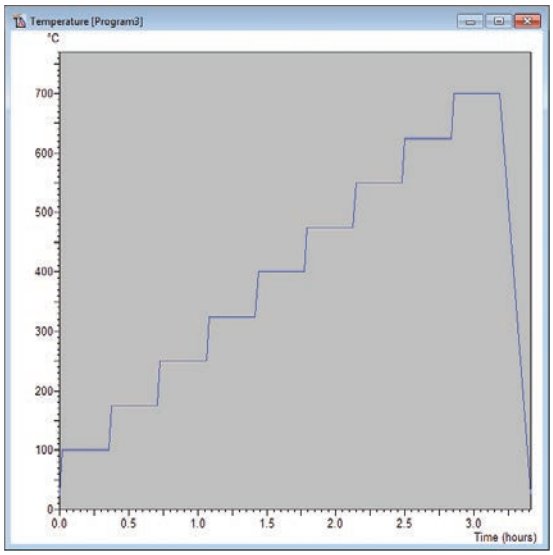
Data Collector supports a range of non-ambient data enabled by automatic sample height correction options. The correction tables of the most common non-ambient chambers are built in with Data Collector and can even be customized.



Easy setup and system configuration

Simple component interchange with software system validation

Batch approach for complete experiment control



Example of a non-ambient batch showing one cycle consisting of non-ambient settings, wait steps and measurements (yellow lines)

XML-based data and measurement strategy storage

The possibility to store both your raw data and your measurement parameters safely are of the utmost importance. XRDML files written by Data Collector make this possible by using the open XML format. XRDML files guarantee convenient data storage, accessibility and archiving. You have access to all parameters to repeat the measurement. Data storage, traceability, accessibility and archiving are all enhanced with XRDML software, guaranteeing the total experiment reproducibility.
The XML philosophy has recently been extended to measurement programs and batches, allowing the same advantages as with XRDML data. Measurement programs using the XRDML format can be easily shared, stored and backed up.
Both XRDML and XRDMP files are 21 CFR Part 11 compliant.

XML-based open data platform

Easy data sharing

Guarantees reproducibility

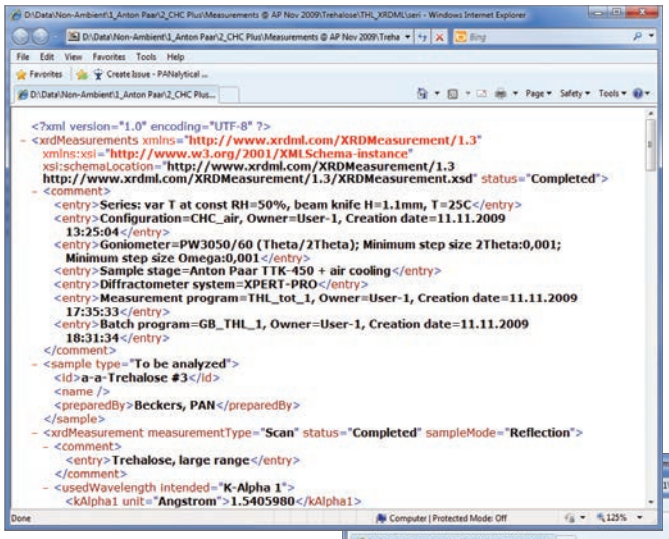
Complete traceability

Convenient file size

Efficient data management

Future-proof, open format

21 CFR Part 11 compliant



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- <xrdMeasurements xmlns="http://www.xrdml.com/XRDMeasurement/1.3"
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  xsi:schemaLocation="http://www.xrdml.com/XRDMeasurement/1.3
  http://www.xrdml.com/XRDMeasurement/1.3/XRDMeasurement.xsd" status="Completed">
  - <comment>
    <entry>Series: var T at const RH=50%, beam knife H=1.1mm, T=25C</entry>
    <entry>Configuration=CHC_air, Owner=User-1, Creation date=11.11.2009
      13:25:04</entry>
    <entry>Goniometer=PW3050/60 (Theta/2Theta); Minimum step size 2Theta:0,001;
      Minimum step size Omega:0,001</entry>
    <entry>Sample stage=Anton Paar TTK-450 + air cooling</entry>
    <entry>Diffractometer system=XPERT-PRO</entry>
    <entry>Measurement program=THL_tot_1, Owner=User-1, Creation date=11.11.2009
      17:35:33</entry>
    <entry>Batch program=GB_THL_1, Owner=User-1, Creation date=11.11.2009
      18:31:34</entry>
  </comment>
  - <sample type="To be analyzed">
    <id>a-a-Trehalose #3</id>
    <name />
    <preparedBy>Beckers, PAN</preparedBy>
  </sample>
  - <xrdMeasurement measurementType="Scan" status="Completed" sampleMode="Reflection">
    - <comment>
      <entry>Trehalose, large range</entry>
    </comment>
    - <usedWavelength intended="K-Alpha 1">
      <kAlpha1 unit="Angstrom">1.5405980</kAlpha1>
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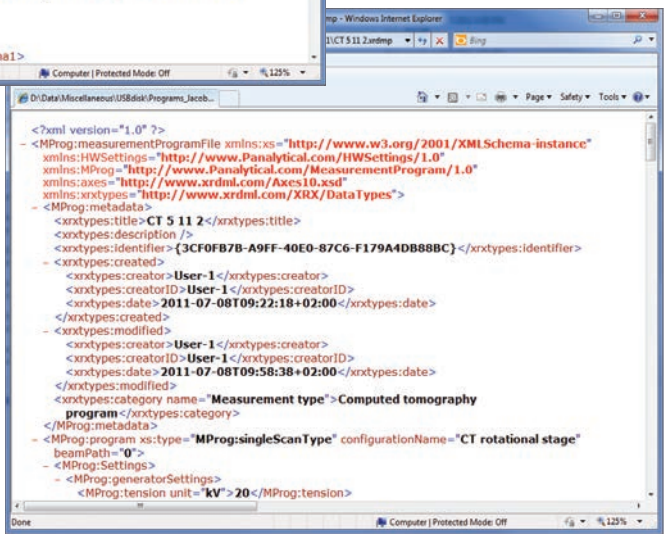
XML structured data including system settings that enable you to always repeat your measurement.



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  xmlns:HWSettings="http://www.Panalytical.com/HWSettings/1.0"
  xmlns:MProg="http://www.Panalytical.com/MeasurementProgram/1.0"
  xmlns:axes="http://www.xrdml.com/Axes10.xsd"
  xmlns:xrxtypes="http://www.xrdml.com/XRX/DataTypes">
  - <MProg:metadata>
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    <xrxtypes:description />
    <xrxtypes:identifier>{3CF0FB7B-A9FF-40E0-87C6-F179A4DB88BC}</xrxtypes:identifier>
    - <xrxtypes:created>
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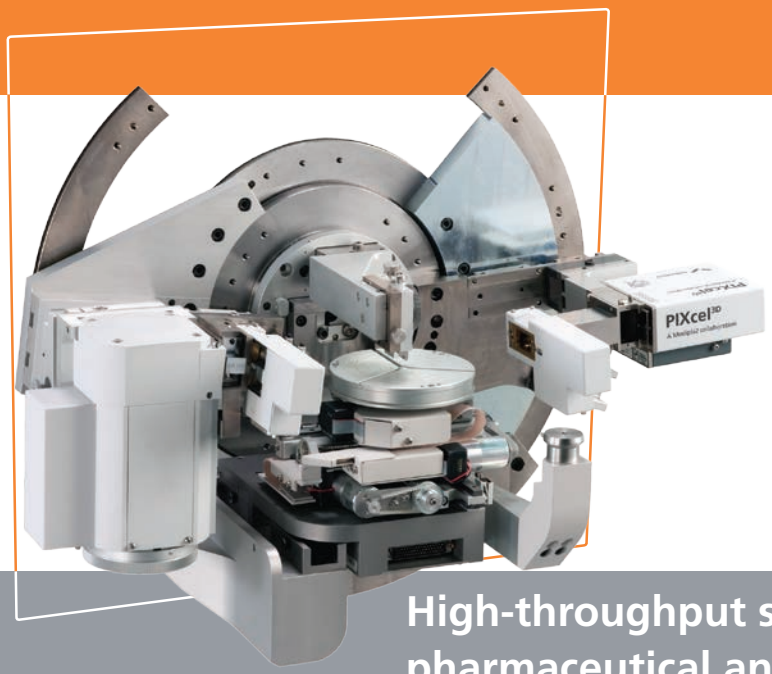
XRDMP files contain all the data you need for your measurement programs. You can easily share, store and access the programs centrally from your company server.

Option to simplify complex measurements

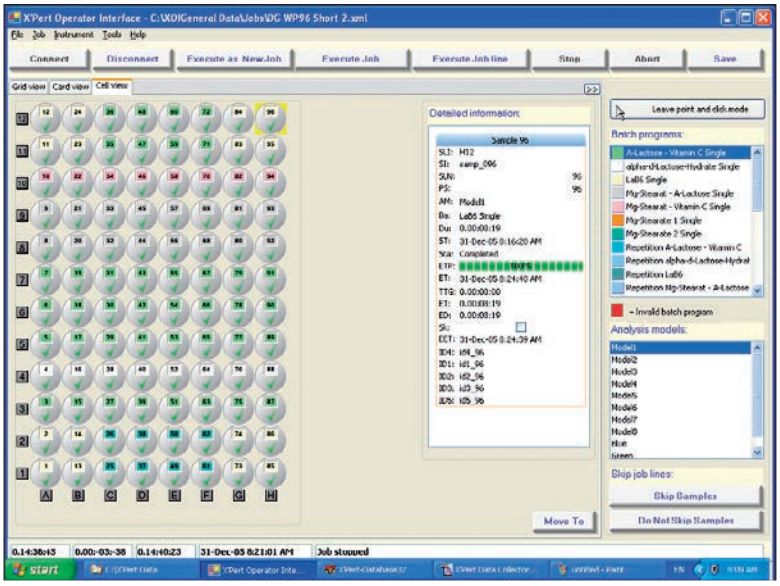


- Adaptive user interface
- Use both on- and off-line
- More automatic analysis options
- Flexible job control
- Status overview at a glance

High-throughput screening for pharmaceutical and biochemical research

The special Operator Interface module, using Data Collector in the background, provides you with the ideal solution for your high-throughput screening needs. Measurements on complete well plates can be programmed in a second, while cluster analysis with HighScore Plus commences automatically afterwards. Well plates of different numbers of wells and well spacings can be accomodated. Graphical feedback provides you with status and progress information.

The customizable user interface allows you to use local well plate numbering and terminology, creating a conveniently arranged work environment.



Operator Interface gives status and progress feedback about the well plate being measured and detailed information of any selected individual well.

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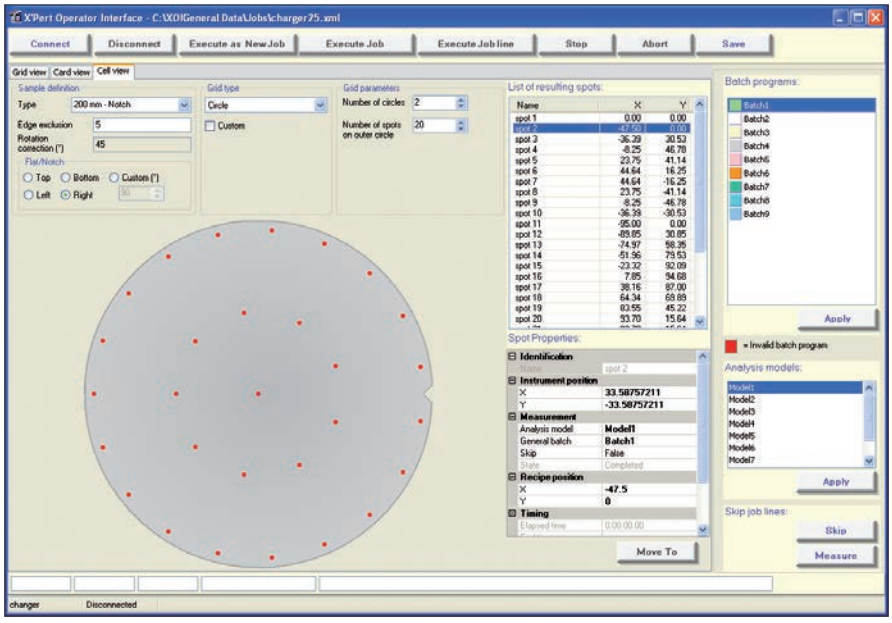
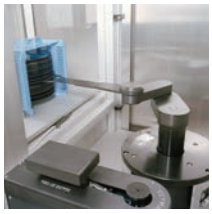
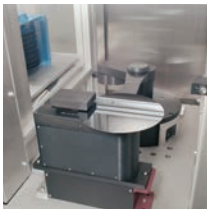
Cassette-to-cassette and mapping solution for wafer analysis

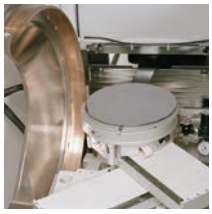
Production control for the semiconductor industry is also enabled by Operator Interface, allowing cassette-to-cassette operation and flexible wafer mapping that puts complex high-resolution XRD analysis in the hands of operators. Jobs can be prepared on- or off-line, with integrated use of bar code reader and label printer. Specific analysis model information can be transferred via the resulting XRDML data file names. The local situation can be reflected in the terminology you wish to use in the customizable user interface. Ample status and progress information is provided to the operator.

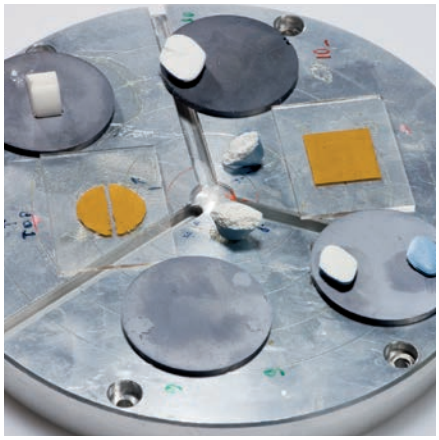


Operator Interface in mapping mode, allowing any grid of measurement spots to be defined using grid type and corresponding parameters





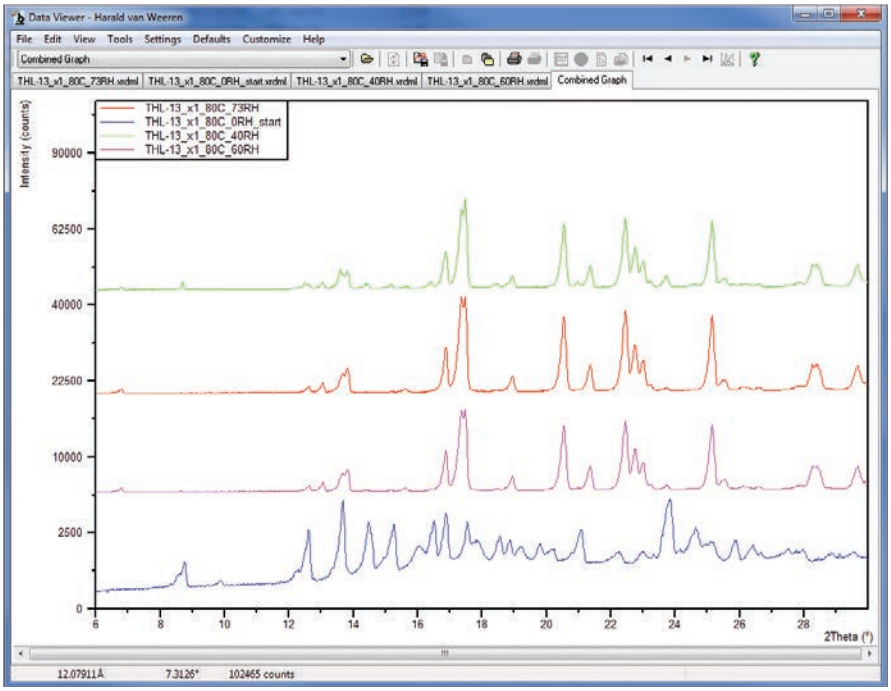




Operator Interface works just as easy with the wafer loader as with a sample table with any number of samples with different shapes and measurement grids.

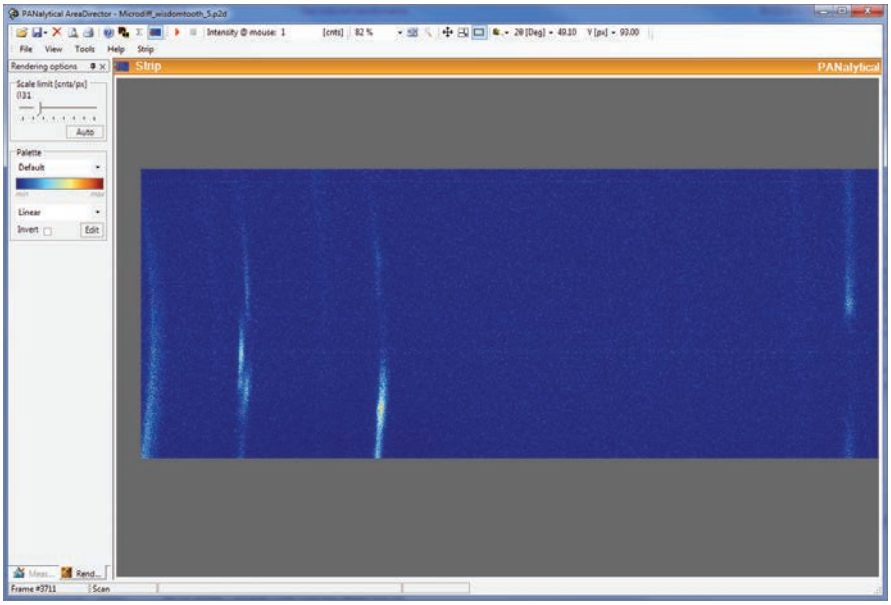
Previewing your data using Data Viewer and Area Director

With Data Viewer you can easily preview data; you can scale, shift and compare different data sets. Data Viewer allows you to make quick analyses. It is also possible to export to other commonly used file formats with Data Viewer.



Data Viewer showing diffractograms of trehalose at different humidity levels

2D or CT measurements performed with PIXcel^{3D} or PIXcel^{3D} 2x2 area detectors, can be quickly previewed with Area Director.



Area Director showing 2D XRD micro-measurement of a wisdom tooth

Quick overview of your data

Immediate feedback on data quality

Fast comparisons

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AUTOMATIC PROCESSING PROGRAM

Automatic processing eases routine tasks

Automatic processing allows tasks to run unattended

Operates with any command-line interface-enabled software package

Allows working in 21 CFR Part 11 Support mode

Suitable for both low- and high-level programming

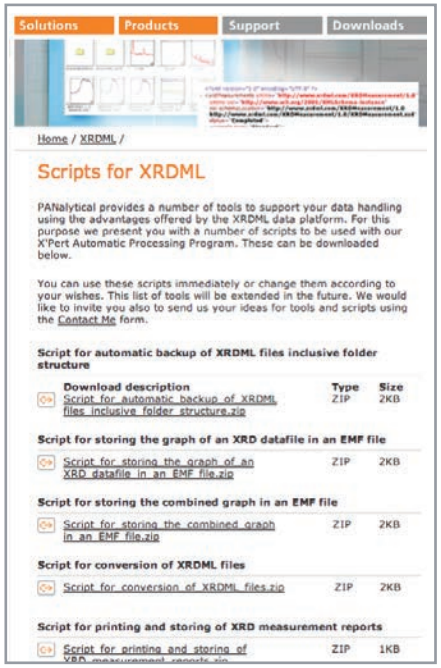
Open XRDML data platform allows for high degree of customization

Automatic processing eases routine tasks

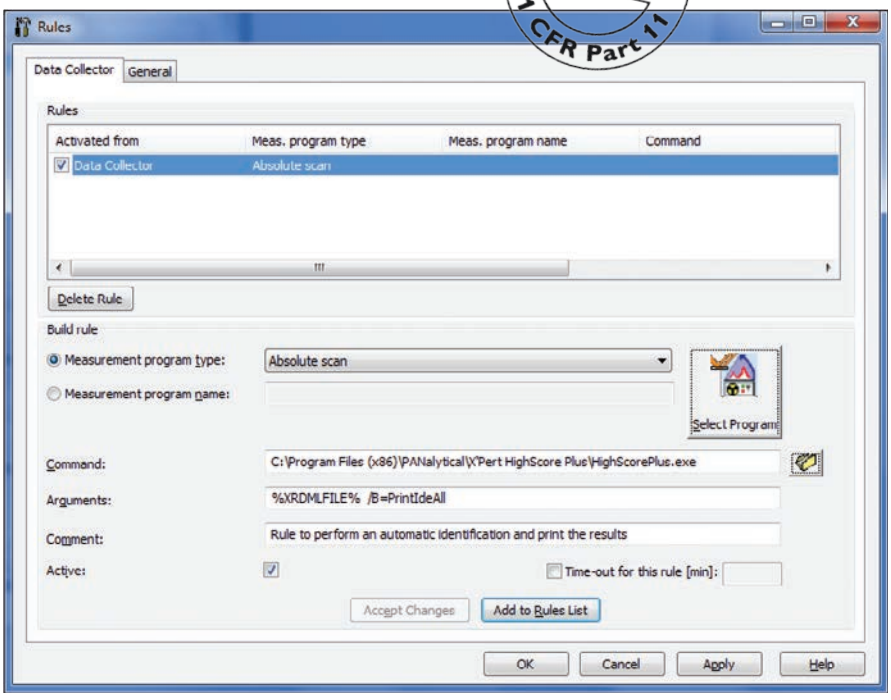
Data Collector comes with an additional Automatic Processing Program to allow small or large everyday tasks to be set up and run unattended.

The program issues command lines containing executables, scripts like Java scripts or Visual Basic scripts, and DOS command files. Just starting a measurement initiates a whole chain of operations, which run without operator intervention, even in 21 CFR Part 11 Support mode.

For example, you can automatically print a graph after your measurement or perform a complete phase identification including preparing and printing the report.
Several standard scripts are included in the software package but you can customize these or write your own programs. In this way you can even connect to your own routines, influence other software-controlled devices or integrate routines from third-party packages.



Scripts for use with Automatic Processing Program are published on www.xrdml.com.



Automatic Processing Program uses rules which contain flexible conditions, command lines, additional parameters and, if required, comments. Activation of a rule is under user control.

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Software Product Identification

Data Collector is a software program for the acquisition of data using PANalytical's Empyrean, X'Pert Powder and X'Pert PRO MRD (XL) systems. Any scan in reciprocal space can be performed as well as radiographs for computed tomography measurements. Users can be assigned with various access levels, defining the level of permission. Data Collector supports you as user in defining your diffraction system and organizing your daily work.

The Data Collector software allows for direct diffractometer control, manual scans, programmed measurements and checking and modifying the status of the instrument. The results and measurement programs are stored in XML-based files. Results are stored in the XRDML data platform; measurement programs are stored in the XRDMP files.

The included Automatic Processing Program allows automation of your data handling and/or analysis. In addition, Data Viewer, which is also included, provides data file handling, viewing, reporting and conversion.

Finally, handling and previewing 2D diffraction data and radiographs for computed tomography are provided in the optional Area Director software.

When the optional PANalytical Audit Trail Software is installed on the same computer, Data Collector automatically switches to the 21 CFR Part 11 Support mode enabling electronic signatures and audit trail functionality.

A connection can be established between Data Collector and the optional Operator Interface.

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 1000 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). Supply and competence 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 ISO9001-2008 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 productivity-enhancing instrumentation and controls company.

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