Empyrean

The intelligent diffractometer

With the 3rd generation Empyrean, Malvern Panalytical has now redefined the concept of a multipurpose diffractometer: our newly designed MultiCore Optics enable the largest variety of measurements **without any manual intervention**. Now central laboratories can benefit from more students having hands on use of the instrument as little or no operator training is required. More importantly, we do not need to worry about messing up optical paths.

Empyrean has the unique ability to measure all sample types - from powders to thin films, from nanomaterials to solid objects - on a single instrument. Different samples can be analysed in one automatic batch, allowing operators to step away from the instrument until all experiments are completed. Read more

X'Pert³ Powder

The next generation cost-effective, multipurpose X-ray diffraction platform

X'Pert³ Powder is the newest X-ray diffraction system based on the fully renewed X'Pert platform. With new on-board control electronics, compliance with the latest and most stringent X-ray and motion safety norms, advances in eco-friendliness and reliability the X'Pert³ Powder is ready for the future.

The system offers an affordable solution for high-throughput, high-quality phase identification and quantification, residual stress analysis, grazing incidence diffraction, X-ray reflectometry, small-angle X-ray scattering, pair distribution function analysis and non-ambient diffraction. Read more

Widest variety of detectors available

The X'Pert³ Powder can be equipped with either point or line detectors. A very cost-effective detector is our sealed Xe proportional detector, while our scintillation detector is very suited for hard radiation applications such as pair distribution function analysis.

As the world's first silicon-based position-sensitive line detector, the X'Celerator with 128 channels of 70 µm is the expression of PANalytical's pioneering work. With the R&D 100 Award winning X'Celerator detector you can measure up to 100 times faster than with a traditional point detector without compromising data quality. Without the need for cooling water, liquid nitrogen flow, counting gas or calibrations it is a very cost-effective solution.

One further step up is the PIXcel¹ᴰ detector. Developed together with CERN, the PIXcel¹ᴰ with 256 channels of 55 µm gives you superior resolution, an unmatched dynamic range and a high count rate linearity. Both, the X'Celerator and PIXcel¹ᴰ detectors come with no dead strips guaranteed. Interested in a quick and easy to use solution for your routine powder diffraction? Read more here.

SOFTWARE

What's new in HighScore (Plus)

Webinar - Recorded

HighScore (Plus) version 4.0 from Malvern Panalytical was released recently. This webinar will give you a guided tour along the most prominent new features of this powder diffraction analysis package. It will also explain important changes with respect to the previous versions. This webinar is, in the first place, for people who are already using HighScore. For those of you who have never worked with HighScore before, in the year 2014 we are planning a series of webinars that will give you an introduction to phase analysis.

Qualitative phase analysis with HighScore

Webinar - Recorded

This webinar explains how to perform a qualitative phase analysis with HighScore. Detecting the phases in a sample is often the first step of an X-ray powder analysis. .

Introduction to the HighScore (Plus) analysis software

Webinar - Recorded

This webinar will introduce you to the graphical user interface of HighScore and the basic ideas behind it. It will cover customization, the document model, editing and displaying of data and parameter sets. The webinar targets first-time and beginning users as well as all advanced users, who want to get the most out of the software. Mastering the graphical user interface is the basis for all analyses and applications possible with HighScore (Plus).

Quantitative analysis of blended cements using XRD in combination with Rietveld analysis

Webinar - Recorded

The production of blended cements with different additives is a significant contribution to the reduction of CO_2 emissions in the cement industry. A variety of completely or partly amorphous materials are used as additives, like slag, fly ash, silica, pozzolana and others. Controlling these additives quantitatively is essential in order to guarantee the cement norms. Of special interest is the quantification of amorphous content. X-ray diffraction in combination with *Rietveld analysis* allows a quantification of complex materials like blended cements.

XRD APPLICATIONS (POWDER)

Solving structure from powder XRD data: tutorial and best practice

Webinar - Recorded

The live webinar will show how to solve a crystal structure from powder data using the Empyrean diffractometer and the HighScore software suite [1]. We will discuss the requirements for solving a crystal structure from powder data and we will show recent examples of some vanadates among which a new larnite/belite structure [2]. Furthermore, as phase transitions may appear as function of temperature, the best practice for high-temperature measurements will be presented. The webinar targets researchers interested to learn how to solve a structure from powder X–ray data and in particular using Malvern Panalytical's HighScore suite. Additionally, people interested in the larnite and belite structures could learn how the chemistry stabilizing this structure type can be extended to open avenues for a better understanding of the crystal chemistry of this important crystal type in the cement industry and in mineralogy. This webinar will include a live question and answer session for our attendees

Mineralogical analysis of iron ore

Application Note

In this data sheet we show a typical example of the fast and precise analysis of mineralogical ore compositions. The exploitation of new iron ore deposits of lower ore grade requires accurate and frequent monitoring of the mined material during mine

planning and ore beneficiation. The presence of minerals such as clays, carbonates or silicates influence the properties and the grade of an iron ore. Resolving the mineralogical composition of the mined material by X-ray diffraction (XRD) is essential for optimizing operational efficiency of the mining and the beneficiation process of iron ore.

Quick phase quantification of clinker and cement for environmentally friendly cement production

Application Note

In this data sheet we show that quantification results of the phases in clinker and cement are both accurate and precise, showing that Malvern Panalytical's XRD solution is a perfect tool for environmentally friendly cement production. A major aspect of environmentally friendly cement production is the use of alternative fuels. The change from fossil fuels to alternative fuels affects kiln control. With fossil fuels kiln control is done using the free lime information in combination with the alite, belite, aluminate and ferrite concentrations in the clinker. These are typically estimated assuming stoichiometry in the kiln. With alternative fuels, however, stoichiometry between alite, belite, aluminate and ferrite may no longer be valid and yield erroneous process control. In order to guarantee a correct kiln control direct probing of the clinker phases using X-ray diffraction is needed.

Mineralogical analysis of copper ore

Application Note

In this data sheet we show a typical example of the fast and precise analysis of mineralogical ore compositions. The exploitation of new copper deposits of lower ore grade or the expansion of existing copper mines towards ore zones with changing mineral composition require more accurate and more frequent monitoring during mine planning and ore beneficiation. The presence of minerals such as talc, clinochlore, vermiculite or muscovite influences the behavior of the ore during the flotation process. Clogging or total blocking of tubes in the processing plant can be the result of high amounts of such alteration minerals.

Redefining XRD: See how green and efficient cement production is made easy

Webinar - Recorded

Green production of cement is trending, but it comes with its challenges. From a chemistry point of view alternative fuels render stoichiometry in the kiln invalid and when producing blended cements many supplementary cementitious materials have a rather complex chemical composition. These are just two examples that can make process control and quality assurance of environmentally friendly cement production demanding. Full mineralogical analysis with X-ray diffraction (XRD) helps to draw the right conclusions about the process without any simplified assumptions. X-ray diffraction is an easy-to-use technology, which is not user-dependent. In this webinar, we will illustrate the benefits of Malvern Panalytical's newest XRD instrument and show how it can address the needs when producing cement in an environmentally friendly way. The webinar targets industrial as well as academic XRD users from the cement and related industries.

Redefining XRD: See how cost-effective and high-quality metals production is made easy

Webinar - Recorded

Traditionally, quality control of iron ore and iron ore sinter has relied on time-consuming wet-chemical analysis. The mineralogical composition that defines the physical properties such as hardness or reducibility is currently not monitored. X-ray diffraction (XRD) is capable of delivering rapid and accurate analysis of all incoming raw materials, intermediate products as well as finished products. It is ideal for monitoring and assuring the highest standards for process and quality control. However, the use of XRD is often considered a big step in terms of initial investment and operator training. To make XRD accessible to everyone, Malvern Panalytical introduces a novel XRD approach: a new diffractometer, which is cost-effective and designed for ease of use. In this webinar, we are going to illustrate the benefits of this instrument – the most innovative benchtop diffractometer available on the market – for the metals industry, and show how it can address the most stringent industry needs. The webinar targets industrial as well as academic XRD users from metals-related industries.

Redefining XRD: See how process monitoring in mining is made easy

Webinar - Recorded

Decreasing ore qualities and increasing prices for raw materials require a better control of ore processing and a more efficient use of energy. Traditionally, quality control in mining industries has relied on time- consuming wet-chemical analysis of the elemental composition. The mineralogy that defines the physical properties is often only monitored infrequently. Direct monitoring of minerals and process parameters does make the

difference in describing ore bodies and the efficiency of the beneficiation process. A full mineralogical analysis with X-ray diffraction (XRD) helps to increase mineral recoveries in the most effective and environmentally friendly way. X-ray diffraction is an easy-to-use technology, which is not user-dependent. In this webinar, we will illustrate the benefits of Malvern Panalytical's XRD instrument and show how it can address the needs of monitoring the processing of ores from the raw ore to the concentrate. The webinar targets industrial as well as academic XRD users from the mining and related industries.

ADVANCED APPLICATIONS

Computed tomography on alkaline batteries

Application Note

In this data sheet, we present CT results obtained on Zn – MnO_2 alkaline batteries using an advanced diffractometer in combination with hard X-radiation (Ag anode) and the GaliPIX^{3D} detector. The differences between the charged and the discharged state can be clearly observed and are in agreement with results obtained at synchrotron radiation facilities.

High-pressure and high-temperature studies of hydrogen storage materials

Application Note

This application note shows the possibilities of the advanced XRD for the analysis of gas storage materials, illustrating two examples of interactions with hydrogen. Such studies are normally performed at large-scale facilities like synchrotrons and neutron sources, or by using dedicated instruments. In this application note we present the results obtained by in situ experiments on H2 storage materials performed on the multipurpose laboratory diffractometer Empyrean in combination with the high pressure heating stage Anton Paar HPC 900. Data presented in the application note were obtained using Si-based X'Celerator detector. The same experiment can be performed using GaliPIX^{3D} detector featuring 100% efficiency for hard radiation. Within the same measurement time GaliPIX^{3D} provides high quality data with higher intensity (compared to X'Celerator), therefore significantly improving the time resolution of in situ experiments with hard radiation.

XRD in transmission geometry with controlled temperature and relative humidity

Application Note

The use of advanced XRD in combination with the Anton Paar MHC-trans chamber enables us to characterize in situ the swelling of clay minerals at variable temperature and relative humidity conditions. By definition X-ray diffraction is the most comprehensive tool to study clay swelling. The measurements can be performed both ex situ and in situ, with the latter undoubtedly being a more accurate probe. Here we present an in situ comparative study of the swelling of montmorillonite and corrensite clays in a wide range of temperature and relative humidity.

In situ monitoring of the hydrothermal synthesis of nanoceria. Time-resolved small-angle X-ray scattering at variable temperature

Application Note

The use of the advanced diffractometer in combination with the Oxford Cryostream Plus compact enables us to evaluate the temperature effect on the synthesis process of nanoceria using the small-angle X-ray scattering (SAXS) technique at variable temperatures. We performed an extensive in situ study of hydrothermal synthesis of nanoceria by combination of X-ray diffraction and scattering techniques. Here we present the results of the in situ SAXS characterization of the nanoceria synthesis process in the temperature range from 5 to 90 °C.

In situ monitoring of the hydrothermal synthesis of nanoceria. Time-resolved total X-ray scattering for pair distribution function analysis

Application Note

The excellent hard radiation performance of the new GaliPIX^{3D} detector enabled us to monitor the 24-hour synthesis process of nanoceria using the pair distribution function (PDF) method on an X-ray diffractometer. We performed an extensive in situ study of hydrothermal synthesis of nanoceria by a combination of X-ray diffraction and scattering techniques. The results of time-resolved small- and wide-angle X-ray scattering (SAXS WAXS) at variable temperatures suggest that at room temperature the active nucleation and growth of particles is occurring within the first 24 hours.

THIN FILMS

Do you want to collect high-quality X-ray reflectometry data? Good practices that will help

Webinar - Recorded

X-ray reflectometry (XRR) is a well-established analytical method for the characterization of thin layered structures, surfaces and interfaces. It is used to determine layer thicknesses and densities and provides roughness-related information. The basics of XRR and the analysis of XRR data were discussed in one of our webinars last year. This time, the focus will be on a typical workflow, from setting up the X-ray optics of a diffractometer, the essential steps of the sample alignment procedures to the final XRR measurement.
Don't miss the useful practices and tips that we will share with you in this webinar. They will help you to collect high-quality XRR data from your layered samples.

X-ray diffraction techniques for characterization of thin film solar cells

Application Note

The present contribution is providing an overview of the X-ray scattering methods and geometries available on the Empyrean platform for the characterization of polycrystalline and epitaxial solar cell structures. High efficiency thin film photovoltaic solar cell devices are being created in a variety of crystallographic forms: epitaxial, polycrystalline, micro- or nanocrystalline or amorphous.

XRD characterization of highly oriented thin films

Webinar - Recorded

This webinar will focus on the X-ray diffraction (XRD) techniques applied in studying highly oriented (textured) thin film samples. Textured layers are often more challenging to analyze than polycrystalline or epitaxial thin films. For example, when the Perry method is used in the grazing incidence configuration, the uncertainty of residual stress determination can be rather large. This is mainly due to the fact that only a limited number of diffraction peaks can be measured in this configuration. In this webinar several practical examples (ZnO and PZT layers) will be presented and the possibilities to improve the accuracy in both data collection and analysis will be discussed.

Other characterization techniques such as X-ray reflectivity (XRR), grazing incidence X-ray diffraction (GIXRD) and texture determination will be covered as well. The corresponding instrument configurations and methods for data analysis will be illustrated.