ISSUE 2/2015

X'PRESS

HOW TO ADVANCE?

PANalytical
get insight

Welcome to this issue of our **X'Press magazine**

Pieter de Groot
Corporate marketing director

Perhaps you are wondering what our cover photograph is displaying: it puts you 'eye to eye' with one of the most advanced X-ray diffraction detectors – the GaliPIX^{3D}. Accordingly 'How to advance' is the subject we want to discuss in this issue. In our interview, Martijn Fransen, product marketing manager X-ray diffraction, shares his opinion about the recent advances in X-ray diffraction (XRD).

One of Martijn's examples is the pair distribution function (PDF) analysis of amorphous solids and liquids, which has advanced considerably in the last years. In the past, without PDF analysis, only the crystalline phases of mixed phase materials could be successfully analyzed using XRD. During the last decades, however, PDF analysis has matured and is proving its usefulness for a considerable number of applications. Some of them are mentioned in the article about Dr. Alan Soper's research team at Rutherford Appleton laboratory in the UK. They use a combination of neutron and X-ray diffraction for their research on non-crystalline materials. You may remember that measurements at RAL were also used by the first winner of the PANalytical Award in 2012, Thomas Bennett, for his studies of an amorphous metal-organic framework (X'Press issue 1/2013).

We now proudly present the 2015 recipient of this award: Matteo Bianchini, a young Italian PhD student at the French Institut Laue Langevin (ILL). At the same time Matteo was also awarded the Graduate Student Silver Award at the 2015 MRS spring meeting, a truly worthy winner!

However, not only X-ray diffraction can take care of advanced materials analyses. In our article about the new Epsilon 1 Pharma, we explain how X-ray fluorescence has gradually been introduced as the alternative method for the advanced quantification of catalyst residues in pharmaceutical materials. Unlike 'classical' methods, such as ICP, only minimal sample preparation is needed here and results are extremely precise and reproducible.

X-ray analysis methods certainly don't stand still and we hope that these and the other articles inspire your interest in the latest advances.

With kind regards,
Pieter de Groot

LATEST NEWS

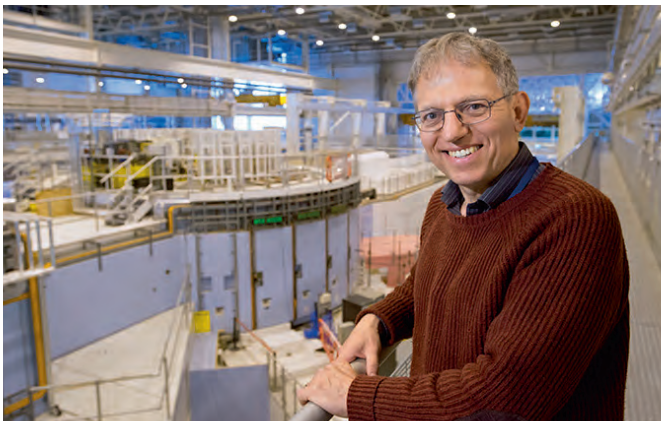
PANalytical's software is Windows 8.1 compatible

As of February 2015 all PANalytical X-ray systems are being delivered with personal computers running under the Windows 8.1 64-bits operating system.

Extended tests beforehand have confirmed that almost all available PANalytical software packages are compatible with Windows 8.1. For the few exceptions we provide PCs with Windows 7 Professional for the time being. PANalytical's software engineers are currently working to make the remaining packages compatible as well in the short term.
We will keep you updated.

www.panalytical.com/software.htm

In this issue



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A productive synergy between X-rays and neutrons

For a long time researchers in the Disordered Materials group at ISIS, the neutron facility at the Rutherford Appleton Laboratory (RAL) in the UK, have studied scattering from non-crystalline materials, specifically liquids and glasses. Prof. Alan Soper FRS, is a world expert on the structure of water and has studied structural transformations in amorphous ice and supercooled water. The understanding gained from these studies has relevance in many fields, for example in human biology where investigating water's structure can reveal the transfer of ions around the body's cells and how water clusters around proteins. In astrophysics, measuring the water-ice phase diagram aids the interpretation of spectral data from distant galaxies.

In Alan's work, instead of looking at the Bragg peaks in a diffraction pattern, as one would for a crystalline material, he studies the diffuse scattering using the 'total scattering' or pair distribution function analysis (PDF) technique. The diffuse scattering contains information about the atom-atom correlations in the liquid or glass and enables a model to be built detailing the preferred atomic interactions within that material. Having used this methodology with neutrons, Alan was keen to combine the neutron scattering data with data from X-ray scattering. He was interested in having a dedicated X-ray source close to his neutron scattering experiments.

Alan was PANalytical's first customer to install an X'Pert^3 diffractometer using a silver (Ag) tube for PDF studies. Situated in a dedicated X-ray lab in the same building as the neutron beam lines, the X-ray diffractometer is conveniently at hand for users to easily transfer samples between instruments. Users from all over the world come to use ISIS; as part of their awarded beam time at ISIS they have the opportunity to also collect X-ray data on their sample using the XPert^3 diffractometer.

The Disordered Materials group at ISIS generally use the X-ray diffractometer in transmission mode with the sample contained in a quartz capillary. The data is processed by software written by Alan, and provides the interference function in reciprocal space, together with the radial distribution function. Subsequent incorporation into a combined neutron and X-ray modelling method allows the determination of the preferred interactions, atomic arrangements and molecular conformations in glasses and liquids. This approach can be applied to seemingly simple systems such as water, although the structure of water in both its solid and liquid forms still continues to produce surprises [1].

Other fundamental studies of solvents benefit from using both X-ray and neutron diffraction, for example the investigation of the stacking of molecules in liquid chloroform [2]. More complex liquid systems can also be investigated, such as the conformation and hydration of the neurotransmitter dopamine in aqueous solution. This provides further understanding of the interaction of the chemical in the body [3].

But the technique is not limited to liquid systems. The combination of X-ray and neutron measurements has proved highly beneficial for determining the local structure in glasses. Measurements made at ISIS have shed light on the structure directed divergence in physical properties of iron phosphate-based glasses, which are promising radioactive and toxic waste immobilization materials [4].

"It's a great credit that PANalytical can make this machine so reproducible and requiring so little maintenance."

- Prof. Alan Soper, STFC Senior Fellow and member of the Disordered Materials group at ISIS

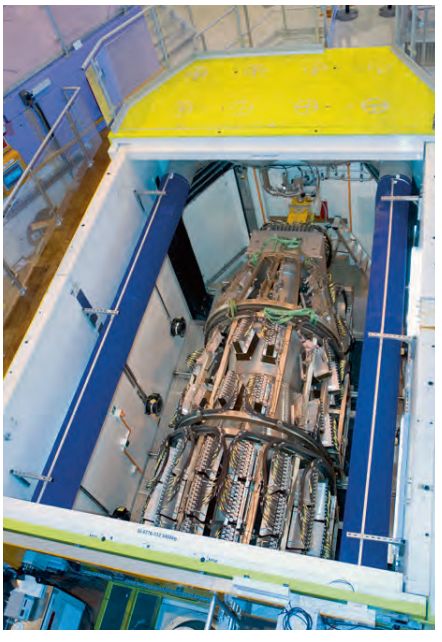
[1] A.K. Soper, ISRN Physical Chemistry 2013 (2013) 1-67
[2] J.J. Shephard, A.K. Soper, S.K. Callear, S. Imberti, J.S.O Evans, C. Salzmann Chem Commun., 51 (2014) 4770-4773
[3] S. K. Callear, A. Johnston, S.E. McLain, S. Imberti, J. Chem. Phys 142 (2015) 014502
[4] P.A. Bingham, E.R. Barney J. Phys.-Condens. Mat. 24 (2012) 175403

Prof. Alan Soper and Dr. Sam Callear at the neutron diffractometer, NIMROD

About Alan and NIMROD

Prof. Alan Soper FRS is a world leading experimentalist on the structure of water and aqueous solutions. He is a Senior Fellow of the UK's Science and Technology Facilities Council (STFC) and is a Fellow of The Royal Society (FRS). He is also the designer of NIMROD, the near and intermediate order neutron diffractometer, at the ISIS neutron spallation source, situated at the Rutherford Appleton Laboratory, UK.

NIMROD is the only diffractometer of its kind in the world as it bridges the gap between small-angle neutron scattering (SANS) and wide-angle neutron scattering, by using short and long wavelength neutrons together with a high detector coverage to encompass a wide range of Q space. This enables continuous access to length scales ranging from the interatomic (<1 Å) through to the mesoscopic (>300 Å). The Disordered Materials group at ISIS also operate two other neutron diffractometers, GEM and SANDALS, and generate novel computational techniques for interpreting diffraction data.



X-rays vs. neutrons

Data from neutron and X-ray scattering are very complementary because neutrons scatter from the atomic nuclei whereas X-rays scatter from the electrons around the nuclei. As a result the two techniques respond differently to the same materials; for example, they have different sensitivities to different elements in the periodic table. X-rays scatter particularly well from high atomic number elements. Neutron scattering, on the other hand, can be particularly informative for investigations of lighter atoms such as hydrogen, which is an especially important element in aqueous processes.

More information can be found on their website **http://www.isis.stfc.ac.uk/groups/disordered-materials/disordered-materials-6252.html**

XRD applications now and in the future

Martijn Fransen, product marketing manager X-ray diffraction, about 'How to advance'

'How to advance?' is the theme of this issue of X'Press. A quick consult of a dictionary brings up 'to move forward, to make progress' as synonyms for 'to advance'. The editors of X'Press asked Martijn Fransen, PANalytical's product marketing manager for X-ray diffraction (XRD), about his view on advancements in the XRD world.

Martijn, can you tell our readers whether the world of X-ray diffraction has advanced during the last years?
Oh yes, it has. It is amazing to see how many advances have been made in this technique, that has been around for almost a century. Especially the new advances in data analysis software and X-ray detection have changed this world considerably.

Can you give us a few examples?
One example that I would particularly like to mention is the ease of use in analyzing X-ray diffraction data. With the latest release of the HighScore software, the integration of the whole data analysis process from identification to quantification has been further improved with the new full pattern refinement kernel and the addition of new methods like partial least squares regression. We see that many of our customers don't want to spend their time anymore on learning every detail of the diffraction analysis; thanks to new algorithms we can make things easy that used to be difficult in the past.

"During the last years advances in data analysis software and X-ray detection have changed the world of X-ray diffraction considerably."
- Martijn Fransen, product marketing manager X-ray diffraction

On the other hand, we see that our experienced customers increasingly make use of synchrotron beam time for their most difficult data collection questions. We see it as a challenge to reproduce such results on laboratory instruments. The data collection time is of course much longer, but there is the obvious advantage of not having to wait for available beam time.

In the last years, we have been able to show that new applications like small-angle X-ray scattering (SAXS) for nanoparticle size distribution and shape analysis, grazing incidence small-angle X-ray scattering (GI-SAXS) for nanostructures on surfaces, and pair distribution function analysis (PDF) for amorphous and nanocrystalline materials, can be done on our laboratory instruments.

Not all of us are familiar with PDF analysis; can you explain that in short? And why is this interesting and for whom?
With PDF analysis one determines the presence of specific atom-atom distances in a material. Even in amorphous solids and liquids, some inter-atomic distances can still be recognized and thus a unique fingerprint can be obtained, also of amorphous materials. For readers interested in more details I refer to our article on page 4.

Isn't this something for very specialized labs only? Or can PANalytical contribute to PDF analysis?
PDF measurements can be obtained on any recent PANalytical diffractometer that is equipped with Mo or Ag X-ray sources, preferably run at 60 kV, and appropriate shielded optics. We have upgraded many of our instruments in the field to be able to perform PDF experiments in addition to the normal powder diffraction work.

Our first diffractometer sold with this functionality is at ISIS, the neutron facility at the Rutherford Appleton Laboratory in the UK. It is used by neutron beam line customers interested in collecting also X-ray data at the same time. A few of the research projects at ISIS are described in our article.

The PDF technique has now become quite popular and we have therefore recently added a new detector to our portfolio, optimized for collecting data at high energy. With GaliPIX^{3D}, the time needed for the recording of a meaningful PDF data set is reduced to a few hours instead of a few days!

Where do you see XRD applications in the future?
New materials and technologies are required for dealing with challenges such as the limited availability of energy, clean water, food and medicines for the world population. X-ray diffraction is an important tool for the characterization of these new materials. Our challenge is to develop new XRD applications for our instruments to help our customers to stay at the forefront of these developments.

The use of Mo or Ag radiation in combination with the GaliPIX^{3D} detector also boosts other applications. An interesting development, for instance is the possibility of computed tomography (CT) on our systems. The CT addition allows a direct inspection of 3D printed objects, which recently have become of great interest. With the same source and detector, transmission diffraction studies can be done on reaction cells, such as Li-ion batteries. PANalytical's team of scientists and developers is frequently participating in conferences across the globe in order to present our latest advances and at the same time stay in touch with the experts in the field.

Martijn Fransen studied Experimental Physics at the Technical University of Delft, the Netherlands. In his PhD work, carried out in collaboration with the Philips Research Laboratory in Eindhoven, the Netherlands, he investigated novel electron sources for electron microscopes based on carbon nanotubes using custom-built characterization equipment.

He started within Philips/ PANalytical in 1998 and has been involved in the creation and marketing of several key elements of the X-ray diffraction product line, such as X'Pert PRO, Empyrean, X'Celerator, the PIXcel detector family and many more. Since 2007, he is the product marketing manager for the X-ray diffraction line of business.

Epsilon 1 Pharma –
Advanced quantification of catalyst residues in pharmaceutical materials

The Annual Meeting of the American Association of Pharmaceutical Scientists (AAPS) in November 2014 served as stage for the launch of PANalytical's new Epsilon 1 Pharma. The instrument comes pre-calibrated for quantifying catalyst residues (Ru, Rh, Pd, Ir, Pt) and is tailored for the pharmaceutical industry including 21 CFR Part 11 software together with Installation Qualification (IQ) and Operation Qualification (OQ) documentation. The Epsilon 1 Pharma release coincides with changes in the United States Pharmacopeia (USP) and International Conference on Harmonization (ICH) requirements for elemental impurity analysis.

A key source of impurities in pharmaceutical products are catalysts used in their production process. As these may be harmful to users, regulatory guidelines have been developed which define reproducible and precise monitoring methods. Chapter <231> of the United States Pharmacopeia had been in use since 1905 as the industry standard for the control of elemental impurities. However, this approach lacks both selectivity and sensitivity, and can fail to detect key elements at toxicologically relevant levels.

Since 2005, the USP has been working to develop new regulations. A process of consultation with the industry, chemists and toxicologists has produced two recently published chapters: USP <232> (changes to the concentration limits for elemental impurities) and USP <233> (changes to the testing methods). These requirements will affect products newly released onto the market as well as legacy products, which will need to be retested for compliance.

USP <233> allows manufacturers a choice in the analytical method used for the determination of elemental impurities, providing two example procedures based on ICP (inductively coupled plasma) methods. These techniques are already in use in parts of the industry. As there is dilution required during sample preparation errors in analysis cannot be excluded, while the cost of the instruments may be prohibitively expensive.

Alternative methods for elemental impurity testing are permitted, where the technique has been validated in line with the requirements in USP <233>. X-ray fluorescence (XRF) is one of the new options and has recently been added to the USP as chapter <735> X-ray fluorescence spectrometry. XRF is well-established in other industries and may be used for both product development and process control. It follows similar principles to X-ray diffraction, which is widely used in the pharmaceutical industry for many applications, including studying polymorphism.

Although it is not yet established in the pharmaceutical sector, XRF offers several significant advantages over ICP:

- XRF is non-destructive, which is important during drug development when samples may be in short supply.
- XRF involves minimal sample preparation, avoiding the dilution errors which can occur with ICP-based methods.
- No solvents are needed, reducing the cost of ownership.

Epsilon 1 Pharma is the latest in PANalytical's range of Epsilon 1 systems dedicated to key applications, including mining, lubrication oils, sulfur in fuels, research and education and milk powder - as already presented in previous issues of X'Press (issues 4/2013 and 1/2014).

"The Epsilon 1 Pharma is a push-button solution enabling non-expert users to utilize XRF to quantify catalyst residues at concentration levels required by USP <232> and ICH Q3D."

- Lieven Kempenaers, product marketing manager XRF

44 Ru 101.1 Ruthenium, a hard white metal, is an extremely rare element with a wide range of uses including as a catalyst for reactions in organic and pharmaceutical chemistry.

45 Rh 102.9 Rhodium, a silvery-white inert metal, is used as an automotive catalyst and used for chiral synthesis.

46 Pd 106.4 Palladium, a silver-white, ductile metallic element, is used in the pharmaceutical industry as a catalyst in a number of hydrogenation reactions.

77 Ir 192.2 Iridium, a brittle silvery-white metal, is the most corrosion-resistant metal and is commonly used as part of organo-metallic compounds used for catalysis.

78 Pt 195.09 Platinum, a grey-white precious metal, is the heaviest of the platinum group metals and has been shown to catalyze numerous oxidation-reduction reactions in a wide range of industries.

PharmaCAT setup samples

The PharmaCAT setup samples are the latest addition to our range of application solutions. They are designed to allow pharmaceutical companies to quantify catalyst residues for catalysts commonly used in the production of pharmaceuticals. Catalyst residues which can be quantified at pharmaceutically relevant levels include ruthenium (Ru), rhodium (Rh), palladium (Pd), iridium (Ir), and platinum (Pt).

Epsilon 1 Pharma

The Epsilon 1 X-ray fluorescence (XRF) spectrometer is the ideal analytical solution for quantification of palladium, platinum, rhodium, ruthenium and iridium in pharmaceutical materials. Considerable savings in time and cost are two of the many benefits XRF can bring to the pharmaceutical industry.

Supporting compliance for the pharmaceutical industry

Installation Qualification (IQ) and Operational Qualification (OQ) are verification and validation procedures which cover the whole PANalytical system including the instrument and the software. IQ and OQ are available for customers that are required to meet good laboratory practice (GLP), and good manufacturing practice (GMP) regulations, for example pharmaceutical and food manufacturers.

In addition to the IQ and OQ procedures we also offer enhanced data security features in our software to support customers abiding by the FDA 21 CFR Part 11 regulation. The FDA 21 CFR Part 11 regulation concerns electronic records and electronic signatures and requires full data traceability to ensure complete analytical integrity. PANalytical's enhanced data security software tracks authorized and unauthorized attempts for application login/logoff, starting and stopping of instrument sessions and any changes to electronic records.

The IQ and OQ documentation, and enhanced data security features are included in the Epsilon 1 Pharma package and are also available as optional extras on all PANalytical systems.

Reliable automated quality check at Teijin Aramid

The production process of aramids consists of three steps, starting with the polymerization of the monomers into a firm fine-grained polymer powder. This polymer is then dissolved in sulfuric acid and spun into fine filament yarn, which is subsequently crimped and treated with a finishing agent. As each of Teijin Aramid's products has to meet special requirements of the customers, strict monitoring of the product quality is necessary. Teijin Aramid's lab in Delfzijl checks all products for elemental impurities which could influence the properties of the produced fibers.

One indicator for the product quality is its color. Teijin Aramid had already used a specialized color-checking camera for a while. They wanted this to be combined efficiently with an X-ray fluorescence (XRF) system for elemental analysis. PANalytical was able to design a very compact automated solution consisting of a Herzog sample press and an industrial XRF analyzer. The color-checking camera has been included in this automated setup and a 30-position sample carousel allows the automated analysis of a whole batch of samples.

The sample is pressed and then transported on a specially adapted conveyor belt. It incorporates a small platform which can lift the sample towards the color-checking camera. After this initial check the sample is forwarded to the CubiX XRF analyzer for elemental analysis. The SamTracs system takes care of the entire sample tracking and control including the camera. This small but effective automated system has reliably been taking care of Teijin Aramid's analytical needs for years now on a daily basis.

TEIJIN

Human Chemistry, Human Solutions

Teijin Aramid, a subsidiary of the Teijin Group, is a global leader in aramids and is well-known for its five high performance products, Twaron®, Sulfron®, Teijinconex®, Technora® and Endumax®.

Delfzijl is one of the company's three locations in the Netherlands and employs about 250 people. The Japanese mother company Teijin Ltd operates worldwide in more than 150 companies and employs more than 15,000 people.

"We are very satisfied with the reliability of this system, which was designed in close cooperation with us. It's great how the PANalytical people took all our needs and requirements into account."

- Ing. Armant Reitsema, Method Development at Teijin Aramid

Aramid (short for 'aromatic polyamide') fibers are synthetic high-performance fibers where polymer chains are linked by strong hydrogen bonds that transfer mechanical stress very efficiently. Due to their high strength, good resistance to abrasion and organic solvents and their low flammability they are for example used for firefighters and military applications. Other applications include helmets, elastomer reinforcements, heat-protection products, optical fiber cables, tires and sails, to name only a few.

Twaron yarn, fiber and pulp

Twaron in all sails at the Volvo Ocean Race

The CNA family growing up

PANalytical's CNA analyzers, featuring proven Sodern neutron technology, are providing fast on-line elemental analysis for industries in need of real-time process control. In April 2015 the fifth generation of the world's most advanced on-line elemental analyzer, the CNA Pentos, was introduced to the public at the IEEE Cement Conference (Toronto, Canada) and at PANalytical's Workshop in Dubai.

The CNA Pentos is the latest release of the CNA family. Like its predecessors, it is based on pulsed fast and thermal neutron activation (PFTNA) technology. The heart of the system is the Sodern neutron tube, which provides a controlled neutron stream with unmatched safety. Entire batches of material, moving on a conveyor belt, can be analyzed in real time, making the technique ideal for high-speed process control. These analyses can provide guidance for quarry development, stockpile construction and raw mix proportioning.

The new CNA Pentos includes upgrades to most key components to improve its reliability and performance. A new user interface and improved maintenance tools facilitate access to the system's features. Increased calibration flexibility enables the unit to operate over a wide range of materials and compositions. In addition to improvements in electronics design and detector stability, the neutron regulation has been enhanced, making the CNA Pentos an extremely reliable and safe member of the CNA family.

The CNA family

CNA Pentos - fifth generation of the traditional CNA and used primarily in the cement and related industries. It is a closed analyzer that encloses the conveyor belt with the neutron source below the belt and detector above the belt.

CNA^3 - designed for minerals applications that feature wide conveyor belts with deep loads and large material size. It is an open analyzer that is installed below the belt with both the neutron source and the detectors below.

"The CNA Pentos is designed for the cement industry and similar applications, while the CNA^3 configuration of the analyzer focuses on mining and other applications where large material size and belt width occur."

- Jeffrey Kemmerer, global product manager CNA, PANalytical.

Matteo Bianchini – Winner of the third PANalytical Award

The PANalytical Award, founded in 2012, aims at supporting young scientists at the beginning of their career. Each year they are encouraged to submit their articles describing groundbreaking research that required the use of a laboratory X-ray diffraction, X-ray fluorescence or any X-ray scattering instrument as the primary analytical technique. The winner of the 2014 competition is Mr. Matteo Bianchini, a young Italian scientist, affiliated to three French institutions. He is currently finalizing his PhD about research on Li-ion batteries.

Matteo Bianchini's article 'Multiple phases in the ϵ-VPO_4O-$LiVPO_4O$-Li_2VPO_4O system: a combined solid state electrochemistry and diffraction structural study' (published in J. Mater. Chem. A, 2(26) (2014), 10182) was listed by all 5 jurors as their number one. They were impressed by the comprehensive investigation, which was carried out with a masterful understanding of crystallography.

Mr. Bianchini is affiliated to the Laboratoire de Réactivité et de Chimie de Solides in Amiens (awarding his PhD), the Institut de Chimie de la Matière Condensée in Bordeaux (co-supervision and laboratory X-ray experiments) and the Institut Laue-Langevin in Grenoble who is funding the project.

The Award will be presented to Matteo at this year's European Crystallography Meeting in Rovinj, Croatia on 26 August where he will present his research to the professional community during a talk.

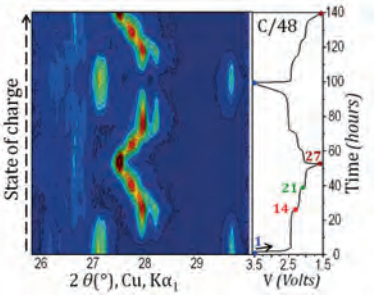
"Mobility and exchange of ideas are fundamental in today's scientific research. This award will be helpful while looking for a post-doctoral position abroad and it will facilitate the transition to a new life and to new scientific challenges."

- Matteo Bianchini, winner of the 3rd PANalytical Award

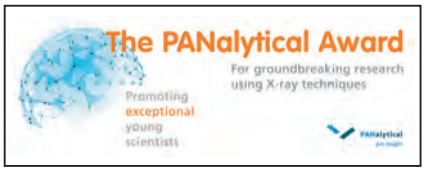
In his winning article Matteo describes in detail the properties of a promising new Li-ion system, a Tavorite-type vanadium oxy-phosphate $LiVPO_4O$. The electro-chemical behavior and the various three-dimensional structures of the redox system were thoroughly investigated by using *in situ* and *ex situ* X-ray and neutron diffraction.

The combination of *in situ* studies performed using an electrochem-ical cell developed at ICMCB and an Empyrean PANalytical diffrac-tometer equipped with Cu $K\alpha_1$ radiation, enabled the monitoring of complex structural changes in the Li_xVPO_4O ($0<x<2$) system at various voltages.

With the resulting detailed data a phase diagram of the material could be plotted and a deeper under-standing of the properties of this new redox system was achieved.



In situ *X-ray diffraction measurement of $LiVPO_4O$ cycled at C/48 rate; first cycle and a second discharge are recorded.*



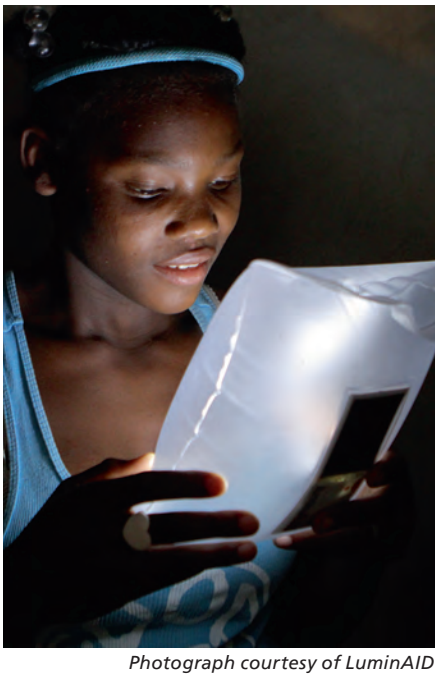
Applications for the PANalytical Award 2015 can be submitted on www.panalytical.com/award with a deadline of 1 December 2015.

There are no restrictions on the manufacturer of the equipment used for the published research.

The International **Year of Light 2015** (IYL 2015)

Proud to be in the LED and photovoltaics supply chain

After the International Year of Crystallography in 2014 UNESCO has declared 2015 as the International Year of Light. While for many of us electric lighting is normal there are still more than a billion people worldwide who do not have access to it. That's why the UK National Committee for IYL has started the 'Study after Sunset' initiative to bring safe off-grid lighting to school-age children in particular. The modern light emitting diodes (LEDs) together with solar powered batteries are our safest and most effective methods for generating light off grid [1]).



Photograph courtesy of LuminAID

Currently many LEDs are fabricated using gallium nitride compounds and solar cells are often based on silicon technologies. Generally opto-electronics, employing semiconductor materials, have revolutionized our lives, in many areas, from lighting and solar power to telecommunications and computing to name a few.

A key fabrication process, early in the semiconductor device supply chain, involves the growth of high-purity single crystal epitaxial layers on polished single crystal substrates. Those layers need to be analyzed and checked for their quality. X-rays play a unique role in the non-destructive evaluation of semiconductors because only X-rays can provide the necessary resolution to measure epitaxial layer thicknesses, strains and alloy compositions. This is why an X-ray diffractometer has become one of the primary metrology tools for crystal growers in epi-layer foundries.

PANalytical is proud to have been at the forefront of semiconductor materials analysis for nearly 3 decades now. We have developed analysis methods for semiconductor single crystal epitaxial layer structures that are employed in all kinds of devices ranging from simple LEDs to photovoltaic cells and lasers. Our diffractometers, X'Pert³ MRD (XL) and Empyrean can be configured for the necessary high-resolution measurements. As these systems have been built with the future in mind, they will continue to serve the semiconductor supply chain.

Epitaxial layers: An historical synergy between XRD and semiconductors

Many semiconductor devices make use of epitaxial strained-layer growth, a concept that was pioneered in the 1970s when crystal growth methods and purification methods were sufficiently advanced to fabricate the first single-crystal epitaxial layers.

Measurement of these layer structures using existing diffractometers was challenging. The crystals required precise alignment and peaks from the epitaxial layers were too close to be distinguished using slit-based optics. Analysis was initially performed using electron microscopy.

At that same time, as a result of the commercial availability of near-perfect and highly polished single-crystal silicon and germanium, researchers in X-ray diffraction were using the Si and Ge single crystals as collimating monochromators. This led to the development of high-resolution X-ray diffraction methods in which X-ray beams were extremely well defined and diffraction patterns from the epitaxial layers were achieved with unprecedented resolutions.

By the 1990s, the synergy of crystal optics, together with innovations in XRD methodology and instrumentation resulted in the high-resolution diffractometers that we see today. What had started out as a niche research area became a mainstream method for the analysis of semiconductors, facilitating mass production of the much-needed solar-powered LED lamps.

[1]) http://www.light2015.org/Home/LightForDevelopment/Study-after-Sunset.html

Events calendar 2015

The list shows a selection of events during the next half year where you will find us. Please come by and visit us when you attend any of these events.

3 - 7 August	Denver Conference 2015	Westminster, CO, USA
4 - 6 August	LAB Africa	Johannesburg, South Africa
9 - 14 August	Geoanalysis 2015	Leoben, Austria
23 - 28 August	The 29th European Crystallographic Meeting	Rovinj, Croatia
1 - 4 September	Asia Pacific International Mining Exhibition	Sydney, Australia
2 - 4 September	JASIS 2015	Messe, Japan
25 - 29 October	AAPS Annual meeting and exposition	Orlando, FL, USA
27 - 30 October	BCEIA	Beijing, China

www.panalytical.com/events

PANalytical webinars

27 August	XRF solutions to support your QAQC program
17 September	XRF applications in the steel industry using SumXcore technology and Zetium
6 October	XRD characterization of highly oriented thin films

www.panalytical.com/webinars

Ore and Minerals Analysis (OMA) Workshop

On 24 August the University of Minas Gerais (UFMG) in Belo Horizonte (Brazil) will be the host of this year's PANalytical Ore and Minerals Analysis Workshop.

The entire range of PANalytical's mining solutions, based on a variety of technologies, will be discussed during the workshop. Participants will not only be introduced to the latest applications of X-ray diffraction and fluorescence but also to the on-line analysis (CNA family, see page 12), NIR (near-infrared) and sample preparation.

http://www.panalytical.com/pt/Eventos/reserve-essa-data.htm

Colophon

Please send your contributions, suggestions and comments to the following address.

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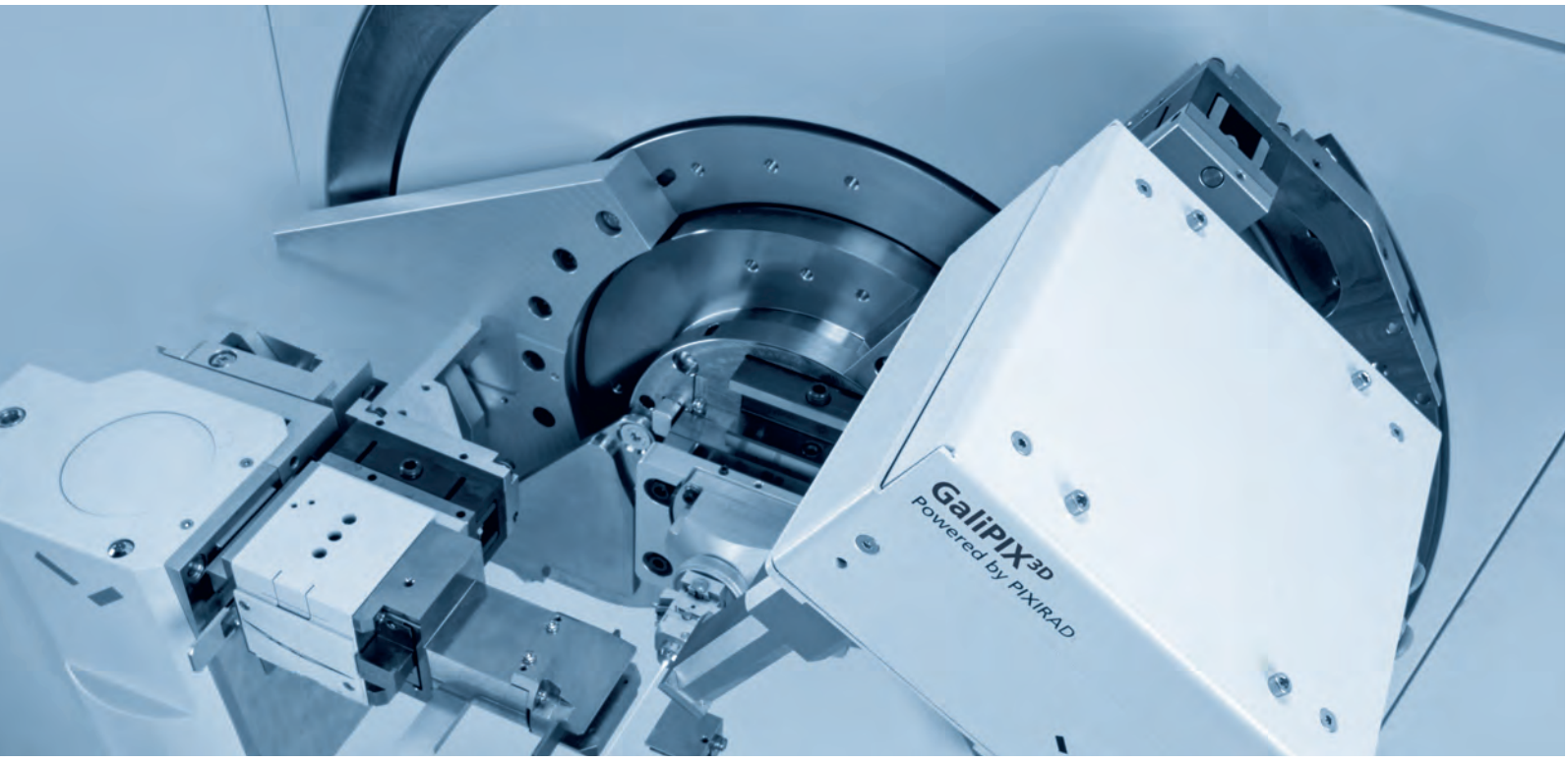

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