PRESS

ISSUE **1/2018**

WELCOME TO MALVERN PANALYTICAL

Malvern Panalytical

WELCOME TO THE FIRST **MALVERN PANALYTICAL XPRESS MAGAZINE**

X'Press has been PANalytical's customer magazine for more than 20 years. Here, we have introduced our readers to other customers' labs and their applications and have informed you about new products and developments within our company. The latest development is reflected in this re-styled issue of XPress.

Pieter de Groot
Vice President Marketing,
Malvern Panalytical

"Malvern Panalytical is named after its two origins: both strong players in the world of materials analysis who have now been united."

Readers of X'Press issue 2/2017 were briefly informed about the merger of PANalytical and Malvern Instruments and its consequences. Such a merging of two companies brings not only organizational restructuring but a new name and house style have to be defined as well. Shortly after Malvern Panalytical's first anniversary we proudly present the results.

The new company Malvern Panalytical is named after its two origins: both strong players in the world of materials analysis who have now been united. Our new logo is representing this graphically: Malvern has contributed the green hills and PANalytical the incident and diffracted beams in two shades of blue. Like the two companies, both their components have been combined to form a unity. In the future, the restyled XPress will serve as a contact medium for all Malvern Panalytical customers.

During exciting events such as a merger you might want to look back at your origins. Where have the merging companies started and what technologies lie at their base? Which developments have formed their actual appearance? PANalytical's roots lie in the end of the 19th century when X-rays were discovered and when the company subsequently pioneered the development of the present equipment (see X'Press 2/2017). Malvern's very early roots can be found in 1917 when Einstein for the first time theoretically described the laser. From then it took almost 40 years until the founding of Malvern Instruments. In this XPress issue we take you to the period of 1917 to 1945 when the use of X-rays turned from a hazardous experiment into safe means of materials analysis.

We have interviewed Malvern Panalytical's president Paolo Carmassi, who introduces his vision for the new company; a company built on the strong pillars of two world-leading companies in the field of materials analysis. A new company, which is not just the sum of the two components but a new unity, reinforced by the expertise and knowledge of all our employees. Paolo will lead Malvern Panalytical into a future where our customers will see us as true partners and experts for their businesses.

In order to let this vision come true we are transforming Malvern Panalytical into a much more customer-focused organization, ensuring that you can discuss your business challenges with exactly the specialist you need. In this context my role has changed too and this is the last time that I am writing this XPress introduction. From January I serve you as leader of the business sector Raw and Bulk Materials and maybe we will meet soon in my new role.

I hope that you like the new style and content of XPress and welcome any feedback from you. You can always contact us at info@malvernpanalytical.com

With kind regards,
Pieter de Groot

IN THIS ISSUE

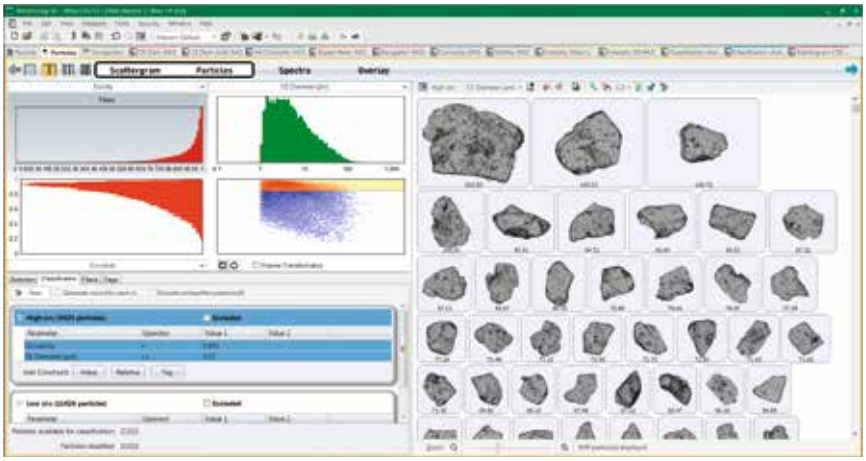
INVESTING IN MALVERN PANALYTICAL CREATED A **CLEAR COMMERCIAL ADVANTAGE** FOR KBI BIOPHARMA

Dr. Amber Fradkin manages the Particle Characterization Core Facility at KBI Biopharma in Boulder, Colorado (USA), where a team of experts provides particle analysis services for products ranging from parenteral biologics to small molecule topicals and inhalable powders. As our understanding and awareness of the importance and impact of particles in drug products increases, their characterization becomes ever more necessary, not only for ensuring drug stability, safety and efficacy, but also in order to meet regulatory expectations.

To support this requirement, analytical instrumentation has advanced significantly over the past decade. "The challenge has been what to do with all the data these new instruments produce, how to interpret it, how to store it, how to present it in regulatory filings, and so on. With the installation of routine Micro-Flow Imaging, we started to learn more about the particles in products, and what they look like", says Amber. "But with this additional information came more questions: 'Why do these particles look different to those ones? What are they?'

"The KBI Particle Core team needed a tool to help them complete their in-house characterization service by providing an answer to the question: "What is it?" for particles they detected in the subvisible and visible size range.

They also required a technology which was easy to use, with a range of options for analyzing the different samples they handle. Amber explains, "For instance, we wanted to analyze the particles in solution whenever possible,



"Our suite of Malvern Panalytical particle techniques has provided us with a unique advantage when clients are seeking help with particle characterization."

Dr. Amber Fradkin
Director Particle Characterization Core Facility at KBI Biopharma

to ensure that our analysis was as close as possible to *in situ* particle characterization. When you are forced to filter particles out of solution, it always leaves concerns such as, 'were the particles we found formed by the act of filtration itself?'. Malvern Panalytical was the first company to help us achieve a solution-state analysis for particle characterization by Morphologically-Directed Raman Spectroscopy (MDRS). They took our request and developed a solution for us with their wet cell for use with the Morphologi systems."

Following a thorough investigation of a range of systems, KBI's Particle Core team decided that Malvern Panalytical's Morphologi G3-ID best met their requirements. Amber states, "We found that the Morphologi G3-ID system had the best ease-of-use and also the most versatility, when compared with alternative solutions. We can now analyze such a diverse range of samples: powders, creams, oils, aqueous solutions, solids, and so on. But also, Malvern Panalytical's customer service is outstanding. The team is very responsive to our requirements. They continuously ask for our feedback and provide rapid solutions to our requests."

KBI now owns seven different Malvern Panalytical instruments, which together form a comprehensive analytical suite. Amber states, "All of our Malvern Panalytical instruments have been integral to the KBI Particle Core. Each instrument provides a unique dataset to characterize particles. However, the Morphologi G3-ID has truly been invaluable to our particle characterization core facility. This is the one instrument that provided the answer to 'what is it?' when characterizing particles. I have worked with this system for over 4 years now - **it is so versatile**, and whether we are using it to develop a method for determining particle size distributions of multi-API topical drug products or isolating subvisible particles from biologics for forensic identification, MDRS proves time and time again to be a powerful technique that gives us the answers we need."

Amber continues, "Applying the right combination of techniques allows us to characterize the full particle profile, spanning from nanometers to millimeters in diameter. Our suite of Malvern Panalytical particle techniques has provided us with a unique advantage when clients are seeking help with particle characterization. The KBI Particle Core loves to stay on the leading edge of the industry with our technology and Malvern Panalytical has helped us do that."

On February 14th, 2018, Malvern Panalytical launched the latest instruments in the Morphologi range – the Morphologi 4 and Morphologi 4-ID (see page 14).

KBI Biopharma is a biopharmaceutical contract development and manufacturing organization (CDMO) headquartered in Durham, North Carolina (USA), which specializes in accelerating the development of biological therapeutics to expand global access to life-changing medicines.

KBI's Particle Characterization Core Facility is located in Boulder, Colorado (USA), and provides specialist particle characterization for the (bio)pharmaceutical industry. Services offered by this facility include profiling of particles post IV-infusion, investigation of the kinetics of particle formation, particle identification for forensics applications, API characterization, profiling of particles in drug products for biosimilarity and biocomparability, and assessment of formulation stability.

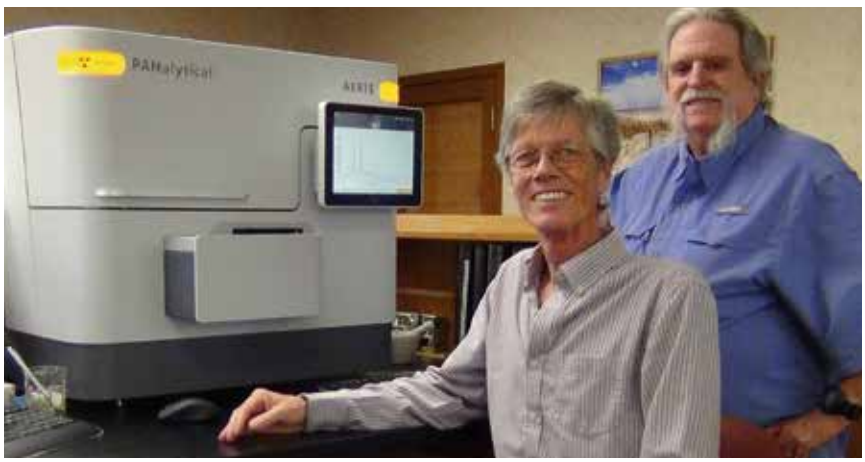
The Particle Characterization group at KBI Biopharma with Adam Lee, Aaron Krueger, PhD, Kevin Dahl, PhD, Amber Fradkin, PhD, Bradley Lara and Matt Baker, MSc (left to right)

GENERATIONS OF **BENCHTOP XRD SYSTEMS** AT LOUIS C. HERRING LABORATORY

Louis C. Herring Laboratory in Orlando, FL (USA) is specialized in the analysis of kidney stones, also known as urinary calculi and has been in business for over 60 years. In July 2017, they received Malvern Panalytical's Aeris benchtop X-ray diffraction (XRD) instrument; the second system to be installed in the United States.

Back in the early 1980s the lab received their previous system, a PW1840, the first benchtop produced by then Philips Analytical. This system ran for three decades, amassing over 41,000 hours of operating time and requiring little to no service through the years. But earlier this year it was decided to retire the system and look at modern XRD technology. The timing was impeccable, as the new Aeris benchtop XRD had just been launched in November of 2016.

Analysis of urinary calculi is an essential step in the examination and initial treatment of the patient with kidney stones (urolithiasis). Knowledge of the composition of calculi yields fundamental information on how the disease has developed, including metabolic abnormalities, presence of infection, possible artefacts, and even drug metabolism.



Glenn Austin and David Fletcher, of Louis C. Herring Laboratory

The lab's customers are medical and veterinary doctors and they have long regarded X-ray diffraction as a definitive technique in the identification of phases present in a kidney stone. "X-ray diffraction is key to our business. XRD is highly specific, and can distinguish between anhydrous, monohydrate and dihydrate forms of phases found in stones, for example, mixed urates and mixed oxalates" said company president Glenn Austin. "The average size of a kidney stone is 10 mg, but with the Aeris system we've been able to get a quality XRD pattern from as little as 1 mg of sample. Scan times are under 9 minutes for a 0 to 80 degree

scan on our small sample amounts." Glenn commented "the resolution is incredible, and the software is user-friendly – we have used the [Aeris] all day every day since it was installed."

"It's definitely easy to operate – we were all trained in a matter of hours to use the instrument, and it fits right into our workflow", said laboratory supervisor David Fletcher. He and his team of technicians analyze dozens of stones each day. According to their website, Louis C. Herring Laboratory has analyzed over 4 million calculi, more than all other stone laboratories in the United States combined.

Glenn stated "I would definitely recommend the Aeris to anyone considering a new XRD – it's very compact, with external sample loading, no doors to open. It's impressive to have PIXcel detector technology on a benchtop system, and the performance of the Aeris rivals any floor-standing, higher power laboratory system."

The results achieved with the PIXcel detector and the resolution of the Aeris system have led to more accuracy in identifying even trace phases in the typically mixed phase calculi. As their website cheekily states, they "leave no stone unturned".

"I would definitely recommend the Aeris to anyone considering a new XRD."

Glenn Austin
President Louis C. Herring Laboratory

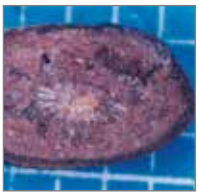
Micrographs of different types of kidney stones

Struvite

Struvite feline

Ca oxalate dihydrate

Uric acid dihydrate



Ca oxalate monohydrate

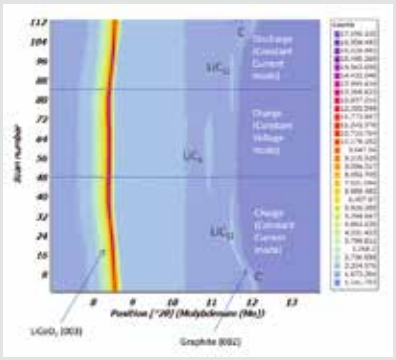
Cholesterol (biliary)

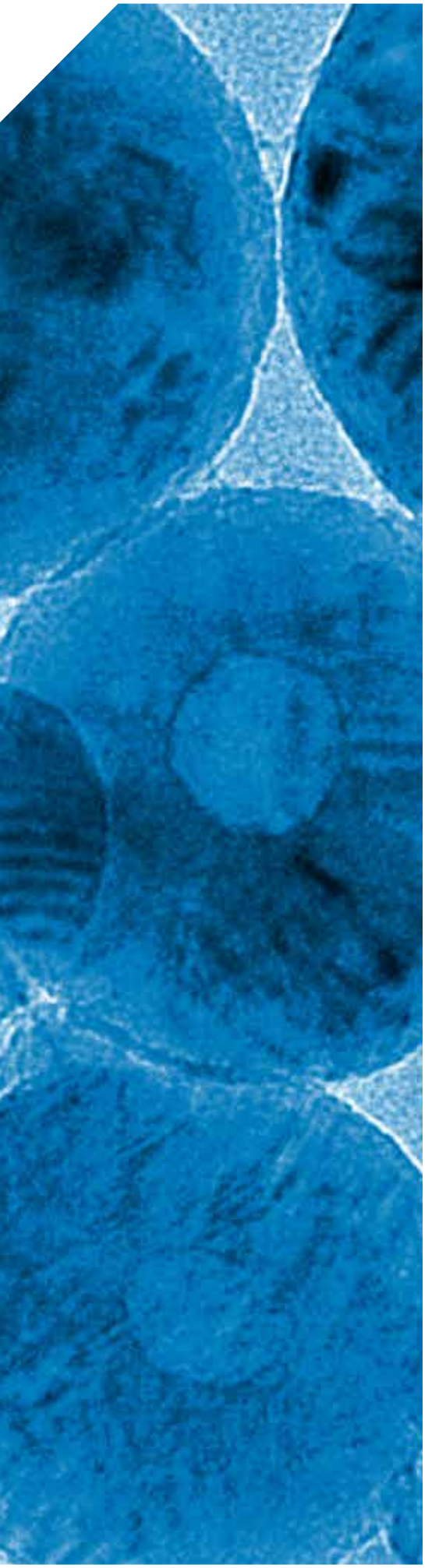
A SPECIAL SAMPLE HOLDER FOR YOUR **BATTERY RESEARCH**

The development of new batteries with improved properties is of major interest to industry as well as for the consumer. Researchers worldwide want to find out how battery quality is influenced by ageing processes during charge-discharge cycles. These ageing processes can be correlated to variations in crystallographic structure of the cell's components. Unlike electrical tests, which do not reveal what is really going on inside the battery, X-ray diffraction allows researchers to 'see inside' while operating the battery.

The commonly used reflection geometry and Cu radiation is not optimal for battery research, as only specially prepared cells can be measured. Not only do such cells have a limited lifetime but reflection geometry causes a change in information depth over the measurement range.
The method of choice works in transmission geometry with Mo or Ag radiation and using standard pouch cells, which do not suffer from leakage. A typical 2D graph (top) shows how charge-discharge cycles influence the phases inside a working battery.

Malvern Panalytical's sample holder for the Empyrean X-ray diffractometer is designed to clamp these pouch cells in a reproducible fashion. It can also be used for the analysis of other objects, like pharmaceutical tablets in blisters or thin metal or plastic sheets.





NEW **IN-HOUSE EXPERIMENTS** FOR VIRGINIA TECH RESEARCHERS

The Michel research group in the Department of Geosciences at Virginia Tech studies how the smallest minerals, known as nanoparticles, are formed, how they react with their surroundings and change with time and space in complex applied systems and the environment. Since the recent installation of an Empyrean Nano system at the Virginia Tech Crystallography Laboratory they are now able to perform experiments in-house, which previously had to be done at synchrotron facilities.

A primary area of the team's research focuses on understanding how different types of minerals crystallize from solution in environmentally-biologically-, or industrially-relevant conditions. Current projects are looking at the formation of iron hydroxide and aluminosilicate nanoparticles that are ubiquitous in the environment, and calcium phosphates and carbonates, like those present in bones and other skeletal features.

In order to understand the steps involved in mineral formation, the researchers use laboratory and synchrotron scattering spectroscopy, imaging, and synthesis to study mineral growth *in situ* and in real time. New discoveries in this area could very well unlock new ways to stimulate and innovate current technology and even the understanding of nature.

Founded in 1872, Virginia Tech offers programs to more than 33,000 students. The university has approximately 135 buildings on its 2,600-acre main campus, educational and research facilities across the state, a study-abroad site in Switzerland, and a 1,800-acre agriculture research farm near the main campus. The campus proper is located in the Town of Blacksburg in Virginia (USA).

Virginia Tech's Department of Geosciences focuses on research, education, and outreach dealing with the nature of the earth. Here, assistant professor Marc Michel's research group studies the formation and behavior of nanoparticles.

Marc Michel has more than 13 years experience performing X-ray scattering-based measurements at synchrotron facilities. He used X-ray total scattering and pair distribution function (PDF) analysis to understand the atomic structures of disordered and partially crystallized phases in solids, powders, dense slurries, and dilute suspensions.

"With the Empyrean system, we are now able to do many of these experiments in our own laboratory at Virginia Tech," says Dr. Michel. "Total scattering data can be collected up to ~22 $Å^{-1}$ using Ag radiation (λ = 0.56 Å) and the GaliPIX^{3D} detector. We only reserve synchrotron time now for *in situ* experiments on dilute aqueous samples that require extremely high flux and large 2D area detectors in order to reduce the data collection times to just a few minutes." Most experiments, however, can now be done at Virginia Tech's X-ray service lab, which is located only a short distance from the center of the campus.

This lab was also host for part of the latest NanoEarth Summer School, which introduced researchers from academia and industry to cutting-edge tools for conducting Earth and environmental nanoscience research. The school featured talks, demonstrations, and data analysis examples for three types of X-ray scattering measurements, scanning and transmission electron microscopy, and mass spectroscopy.

Students at work during the Summer School

Dr. Marc Michel demonstrating the capabilities of the Empyrean Nano

The X-ray scattering sessions were led by Dr. Marc Michel and Dr. Anasuya 'Anu' Adibhatla, Malvern Panalytical XRD applications specialist. Lectures and instrument and software demonstrations focused on practical applications of powder X-ray diffraction (pXRD), small-angle X-ray scattering (SAXS) of powder and liquid suspensions of nanosized solids, and total X-ray scattering of powders for PDF analysis.

After listening to basic theory, attendees headed to the laboratory to practice mounting samples, learn about the instrument configuration, and try out quick examples of data collection. Each session ended with a demonstration of software applications to examples of data collected from samples containing natural, synthetic and anthropogenic nanoparticles.

"It is something of a dream-come-true to have this suite of capabilities in house on a single platform. With Malvern Panalytical's Empyrean Nano, we do not have to apply for as much synchrotron time, which saves on travel expenses. It also provides the opportunity to train the next generation of scientists and engineers in the use of cutting-edge tools that are critical to advancing nanoscience and nanotechnology research. We gladly share our know-how and the possibilities of this instrument with other researchers", concludes Marc Michel.

INTERVIEW WITH **PAOLO CARMASSI**

Mr. Paolo Carmassi is the President of Malvern Panalytical, and the man who has been guiding us through our company integration since January 1st, 2017. Paolo has spent his first year in various airports, hotels, offices and laboratories worldwide, getting to know all the ins and outs of Malvern Panalytical. As we embark on our second year together as one organisation, we took the opportunity to get to know him a little better.

Paolo who?! Can you give us a flavor of who you are and where you're from?
"Of course! The best short description of me is that I am 'Mediterranean hardware, running on Anglo-Saxon software'. I spent 25 years of my professional career in corporate America, which is where the 'Anglo-Saxon software' comes in. But I'm Italian and I have a 'Mediterranean' way of doing things, which I think complements well the rigor and control typically associated with corporate American style.

"I've worked in a variety of industries, including automotive and aerospace, and recently in artificial intelligence. This has meant that over the years, I've moved my entire family to 6 locations across 3 continents: Italy, France, UK, Michigan, California and China, before we made our most recent move to Switzerland."

"My children are truly international - they have an Italian father and a British mother, but all four of them were born and have lived in most places except Italy and England. If you ask them where they're from, they have no idea how to answer you! We speak 3 languages as a family: English, Italian and French."

So, what makes you 'tick'?
"The single most important thing I've learned over the years, and all over the world, is that it's vital to ensure that your company, whether it is in the automotive, aerospace, or even the analytical instrumentation sector, has something special to differentiate it and deliver unique economic value to your customers. You need what I call a 'twist in the tale', or a 'secret recipe'. I like to challenge myself and those around me to think about what special touch they could add to their work to make it more fun, more difficult to copy, and more interesting and valuable to our customers. I try to do things a little differently, to do something that's never been done before, and then lock that down so that it's hard to duplicate.

"I love the idea of making something that will always be truly unique and one step ahead. I strongly believe that there's no 'silver bullet' that makes a business different to all the others, but you can formulate a combination of smaller things that together give you that killer secret recipe!"

"Our vision is to create an environment where customers talk to us about their real problems, where they see us as partners, collaborators, and experts in the detail of their business."

Paolo Carmassi
President of
Malvern Panalytical

What challenges or obstacles have you faced since arriving at Malvern Panalytical a year ago?

"Maybe 'challenges' isn't quite the right word, but I arrived to find a combination of 2 organisations which are both rightfully very proud of their heritage, their science, their innovation and their products. This is a PhD environment, and it's difficult to have a dull conversation at Malvern Panalytical!

"The challenge for me was to help this company of brilliant scientists, engineers and technologists realise that sometimes we are guilty of putting our products and our science, engineering and technology ahead of our customers. I had to figure out how to reconnect our fascination and hunger for technology to the prime principle of ensuring that our products deliver clear economic benefits."

What makes you proud of Malvern Panalytical? What makes it such a special company?

"Above all else, I'm very proud of the resilience with which our organisation responded to the merger, and to the arrival of a foreign object: me! A company merger always carries some element of risk and uncertainty – you can never quite tell what might happen. We braced ourselves for many different scenarios, but, as it happens, the process really couldn't have been more positive. I'm so proud of the entire team for taking a collective leap of faith and accepting that we're now all part of a bigger family and that we're creating something truly special by working together.

"We've managed to strike the balance between developing our new personality and finding exciting synergies, while continuing to deliver our trusted solutions and services. This combination has worked perfectly for us, as well as for our customers. Our resilience, enthusiasm and positivity about forming an exciting new partnership are the things that make me most proud of Malvern Panalytical."

What is your vision for Malvern Panalytical?

"Our customers can continue to depend on Malvern Panalytical for the highest quality technology and support – that's a given and won't be changing. But now we're starting to think bigger than we ever have before, as we really align as one organisation, with all our collective talent and know-how.

"I think that this industry suffers from a common problem, in that it can be hard for us to get to the root of the specific issues our customers are facing. We don't usually know the underlying problem that they're trying to solve – the question behind the question, if you like. Our vision is to create an environment where customers talk to us about their real problems, where they see us as partners, collaborators, and experts in the detail of their business.

"Our customers can expect us to know exactly what value we can deliver, and what economic impact our solutions will have. We'll provide knowledge that leverages facts and data across our different technologies. This will give them answers that are just not possible with one instrument, and that enable vital decisions to be made much more quickly and painlessly.

"What really makes Malvern Panalytical so special is that we don't limit ourselves to thinking in a simple, linear way. We're not intending to just extrapolate the future from what's happened in the past – this is far more radical and exciting! The achievements we are aiming for will bring an order of magnitude more value than our customers are currently experiencing, far beyond what they currently see."

THE HISTORY OF **X-RAY TECHNOLOGY**

1917 - 1945

A SIX-PART SERIES

Twenty years after their discovery in 1895, X-rays were widely used not only in hospitals and medical institutes but also in analytical chemistry and materials science. As more applications for the investigation of elemental composition and crystalline structure of materials were developed, the need for safer and more reliable X-ray equipment increased.

1895 - 1917

1917 - 1945

1945 - 1972

1975 - 2002

2002 - 2017

Malvern Panalytical

2017 - ...

TOWARDS SAFE X-RAY TECHNOLOGY

Philips enters the X-ray market

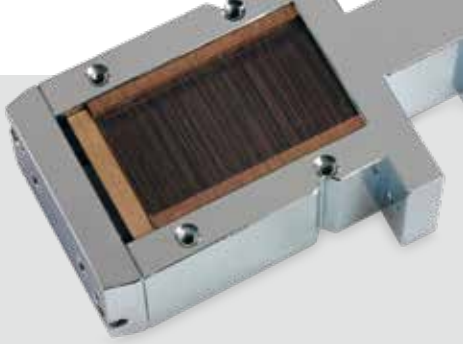
In 1899 neurologist and technical physician Johan Wertheim Salomonson became Europe's first professor in radiology at the University of Amsterdam where he built his own X-ray tubes for his medical investigations.
For the expansion of his research, he was, however, concerned about the fact that there was no X-ray tube manufacturer in the Netherlands. This became a serious problem during World War I, when no X-ray tubes could be supplied to the Netherlands from abroad.

It was then that Wertheim Salomonson approached incandescent lamp manufacturer Philips to repair broken X-ray tubes. The visit of Philips' research director Gilles Holst to the Van Leeuwenhoekhuis (an institute for cancer research and treatment in Amsterdam) in December 1917 marks the start of X-ray tube manufacturing and development at Philips. Just one year later, Philips started to sell X-ray tubes.


PHILIPS
RÖNTGENBUIZEN
NEDERLANDSCH FABRIKAAT.
VOOR DIAGNOSTIEK, OPNAMEN, DIEPTETHERAPIE ENZ.
PROSPECTUS WORDT OP AANVRAGE GAARNE VERSTREKT.
LEVERING UITSLUITEND DOOR BEMIDDELING VAN RÖNTGEN-INSTALLATIE-BUREAUX.
N.V. Philips' Gloeilampenfabrieken.
AFD. RÖNTGENBUIZEN.

Advertisement of Philips X-ray tubes (from Nieuwe Rotterdamse Courant of 4 September 1918)

Metalix tube from a German brochure



Soller slits

Metalix X-ray tubes

The early X-ray tubes were far from safe with the continuous risk of being exposed to high radiation doses or to high voltages. At the Philips X-ray department, physicist Albert Bouwers developed an X-ray tube comprising a grounded metal canister and a glass window. This construction ensured that X-rays were only emitted through the glass window. Introduced in 1923, this tube later became known as the Metalix X-ray tube. In order to handle the success of the Metalix tube, Philips started to work with the tube manufacturer Müller from Hamburg (Germany) in 1923. On April 17, 1927, C.H.F. Müller became an integral part of the Philips company.

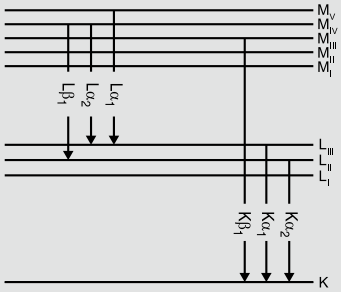
In 1928 Bouwers developed a complete X-ray diffraction system that he described as 'a simple, easily portable device ... with which any risk that parts being under a high tension are touched, is excluded...The device perfectly prevents undesired X-rays from emerging therefrom while it can function without the use of a pumping installation'.
This system was Philips' first 'apparatus for fine structure research'.

X-ray fluorescence spectroscopy

At the University of Lund (Sweden), physicist Karl Manne Siegbahn proved in a series of publications that Moseley's characteristic X-ray lines could be used for the determination of the elemental composition of substances.

Karl Manne Siegbahn

For this purpose, he developed a number of high-precision X-ray spectrometers with a wavelength resolution up to a factor 1000 higher than Moseley had used. In this way, he discovered that Kα lines actually consist of two closely separated lines: Kα_1 and Kα_2. In 1923, he published his standard work 'Spektroskopie der Röntgenstrahlen', in which he introduced the nomenclature for X-ray lines, now known as the Siegbahn notation. Siegbahn received the Nobel Prize in Physics in 1924 for his discoveries and research in X-ray spectroscopy.



Representation of the characteristic lines

X-ray diffractometry

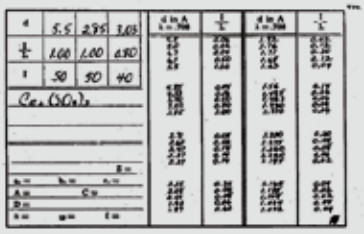
The Debye-Scherrer camera, developed for powder diffraction, uses a glass capillary for the sample. Although this has many advantages, it is less suited for heavily absorbing materials. After moving to Lawrence Bragg's lab in Manchester (UK) in 1920, German scientist Johann Brentano developed a diffractometer for flat powder samples. This setup is now known as the Bragg-Brentano geometry.

Schematic of the Bragg-Brentano geometry

In 1924, Walter Soller from the University of Cincinnati (USA) published his newly created high-precision diffractometer[1], in which he used a set of parallel plates to increase the resolution of the diffracted X-ray beam. Nowadays, Soller slits are used to limit the axial divergence of X-ray beams in Bragg-Brentano geometry.

The Powder Diffraction File

Although it had been known for many years that crystalline substances produce a unique diffraction pattern, a useful identification method was not available in the early days.
In the early 1930s, Donald Hanawalt, X-ray diffraction specialist at the Dow Chemical Company in Midland, Michigan (USA), started to collect diffraction patterns of a thousand pure crystalline materials. From these patterns, he created a database of 1054 patterns, which he organized according to the three strongest lines in their diffraction patterns. Unknown substances could now be identified by a manual search through an index, a method now known as Hanawalt Search.



Example of a card from Hanawalt's database

Hanawalt published his results in 1938 in an article titled 'Chemical analysis by X-ray diffraction: classification and use of X-ray diffraction patterns[2]'. This article was so well regarded that it was reprinted in a second edition of more than 5000 copies.
Based on this success, the American Society for Testing and Materials (ASTM) established the Joint Committee on Chemical Analysis by X-ray Diffraction Methods in 1941, nowadays known as the International Centre for Diffraction Data (ICDD). Hanawalt's database was included as Set 1 of the Powder Diffraction File.

(1) Physical Review, 24, 158 (1924)
(2) Ind. Eng. Chem. Anal. Ed., 1938, 10 (9), 457-512

NEW TO THE MARKET

Morphologi 4-ID

Automated imaging for advanced particle characterization

Morphological imaging is fast becoming an essential technology in the laboratory toolkit for particle characterization. Analytical environments where a deeper understanding of a process or a sample is required will profit from the new Morphologi 4 - a fully automated static image analysis system which provides a complete detailed description of the morphological properties of particulate materials. The Morphologi 4-ID combines the same automated static image analysis with Raman spectroscopy in a single, integrated platform, providing component-specific morphological descriptions of chemical species within a blend. The seamless combination of precise particle size and shape data with the chemical identification delivered by Morphologically-Directed Raman Spectroscopy (MDRS) helps unlock complex particle characterization problems.

Providing automated, rapid, and component-specific morphological information, Morphologi instruments are employed to solve formulation and deformulation challenges, optimize material properties, and create confidence throughout development and manufacturing. The systems enable process control and optimization and provide quick identification of the cause of process deviations.
www.malvernpanalyticalcom/morphologi

Superior at-line elemental analysis

Industries which are obliged to comply with international regulations and test methods can profit from Epsilon 4, Malvern Panalytical's new benchtop XRF spectrometer. Built on the experience of the proven Epsilon 3 range and equipped with the latest excitation and detection technologies and mature software, the performance of this new benchtop instrument approaches that of more powerful and floor-standing spectrometers.

Most applications can now be operated at ambient conditions, reducing the costs for helium or vacuum maintenance. Due to its low infrastructural requirements Epsilon 4 can be placed close to the production line anywhere in the process where it delivers compliant results for years without the need for costly calibrations.

Industry segments such as mining, pharma or oils & fuels can profit from investing in this compact high-performance spectrometer, which takes care of compliant elemental analyses. www.panalytical.com/epsilon4

Epsilon 4

Le Doser-12

A new benchmark for the weighing step in sample preparation

Have you always believed that performing the weighing step manually was a very tedious and time-consuming task in the laboratory? Because we agree, we have developed the solution for you!

The new Claisse® LeDoser-12 automatically weighs samples and dispenses flux with high precision so you get the accurate and precise XRF analytical results you need. You are free to perform other tasks in your lab while LeDoser-12 works for you. In fact, this 12-position dispensing balance can save up to 90% of weighing-related labor time.

Are you interested in increasing the repeatability of your analytical results and in avoiding sample inversion, misidentification, or mistakes in data transfer? And do you want to get your samples ready just in time for the subsequent fusion and analysis steps?
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SAVE COSTS WITH SAMPLE PREPARATION BY FUSION

Knowing the exact concentrations of all ingredients in your final products helps you to avoid waste and can save significant costs. This holds for many businesses, from animal feed products to raw materials. A prerequisite for obtaining reliable results is the good and reproducible sample preparation for your XRF analysis. Claisse experts discuss new applications in two publications.

Even highly volatile and organic samples like dog food can be prepared for XRF analysis. This is described in detail in the application note ***Elemental Determination of Dog Food Samples Using Lithium Borate Fusion and XRF Analysis.***

Here, Claisse chemists show that the combination of **TheOx® Advanced** with adequate thermal pre-treatment and a proper oxidizer is well-suited to prepare dog food for XRF analysis. This way you will obtain the best analytical results and avoid legal and financial consequences related to misbranding.

Borate fusion using **LeNeo®** and **LeDoser™** instruments is the best technique to obtain very precise and accurate XRF results of major elements in sand and aluminosilicate matrices. Our application note ***Determination of the Composition of Sand and Aluminosilicates Using Borate Fusion for XRF Analysis*** explains the procedure, which results in a constant quality of final products and may lead to a major financial gain.

Both publications can be accessed via our website for free. Don't hesitate to contact Claisse fusion specialists to discover how they can help you to find the perfect fusion method for your tricky samples.

LeNeo

Claisse experts are "[…] very dedicated to ensure the optimal use of my fusion instrument and the achievement of the objectives related to my fusion application method."

Minna Jokinen
Experimental Development Chemist at the Outotec Research Center in Finland

NETWORKING FOR **BETTER ANALYSIS** OF PETROCHEMICALS AND POWDERS

Just like any other analytical technique, good X-ray diffraction (XRD) analysis starts with proper sample preparation, observes Dr. Liu Weiling, research scientist at the Nanyang Technological University's Facility for Analysis Characterization, Testing and Systems (FACTS). She was an invited speaker, alongside fellow research scientist, Dr. John Pio. Together, they shared their experiences on better XRD powder analysis during the Malvern Panalytical networking event held in Singapore last August. The FACTS facility has an X'Pert PRO X-ray diffractometer.

Interested in improving your application or analytical knowledge? Check our upcoming training courses and user days in your region at www.malvernpanalytical.com

The Malvern Panalytical networking event was tailored for the petrochemicals and powders analysis market in Singapore. "We have created a platform for people to learn and to improve their analysis, work processes and consequently product," explains Vijay Sethi, country manager for Malvern Panalytical Singapore.

Mastersizer laser diffraction end user, Mr. Lim Chee Wee, technical development manager for Intertek Singapore was another invited speaker. He shared his knowledge about the importance of particle size distribution analysis for industries like aerospace, oil refineries and chemicals. Particularly how consistent particle size could affect chemical reactions, potential to dissolve as well as product appearance. Intertek Singapore has a Malvern Panalytical Mastersizer 3000.

It was the first time that the Singapore team has organized an event involving external speakers. "We want to shift from organizing events that talk only about products towards addressing our customers' business challenges," comments Gjalt Kuiperes, Regional Director for Malvern Panalytical Asia Pacific.

He specially flew in from the Shanghai regional headquarter and had the exciting role of unveiling the company's newest benchtop XRD instrument, Aeris. Without the need for an external chiller, Aeris has a compact footprint. Dr. Umesh Tiwari, Malvern Panalytical's Asia Pacific XRD product manager, demonstrated how easy it is to operate the instrument, which only requires a single-phase power outlet. Customers gathering around the Aeris saw superior phase quantification and identification results, comparable to those of floor-standing systems.

After a morning of discussions, attendees were treated to an afternoon of hands-on demonstrations. The team showcased Malvern Panalytical's holistic range of analytical solutions from crystallographic analysis and fusion sample preparation to quality control and process efficiency with X-ray fluorescence and particle size distribution analysis.

Dr. Umesh Tiwari, Malvern Panalytical's regional XRD product manager (second from left) demonstrates Aeris' ease of use.

"What better way to learn than through networking and picking up best practices from each other."

Gjalt Kuiperes
Regional Director for
Malvern Panalytical Asia Pacific

FOCUS ON THE **DETAILS** TO CAPTURE THE **BIGGER PICTURE**

Is the composition of your products regulated by global directives like RoHS-2/WEEE/ELV regulations? Do you want to analyze every detail of your sample while complying with the ASTM 2617 test method? Or do you need to analyze very small objects, inclusions or inhomogeneities in rocks, toys, jewelry or any other final product? Is your space limited or do you need a mobile unit for your analyses? Then it's time to meet the Epsilon 1 for small spot analysis, our latest addition to the Epsilon 1 family.

This benchtop X-ray fluorescence spectrometer is ideal for the fast and precise analysis of small objects or inclusions in a large variety of samples, regularly as well as irregularly shaped. Just place your sample inside the spectrometer and use the incorporated camera together with the straightforward positioning procedure to focus on the points of interest in your sample. The elemental analysis of the spot in question takes only a few minutes and delivers a detailed report with the picture included.

The small footprint and self-contained design of Epsilon 1 allow placement close to the sample location and make it the ideal tool for quick and easy small spot elemental analysis. Using Malvern Panalytical's standardless analysis solution package Omnian the spectrometer is ready for a wide range of samples. "The Epsilon 1 for small spot analysis system is very easy to operate and requires no sample preparation", says Michel Zoontjes, product manager at Malvern Panalytical. "It enables the flexible and fast screening of small objects or inclusions and is the ideal tool for failure analysis and troubleshooting of finished products".

www.malvernpanalytical.com/epsilon4

TOWARDS A **MEASURABLE SOLUTION**

ASD is a brand of Malvern Panalytical, and a manufacturer of top-grade, high-class, well-cited near-infrared (NIR) scientific spectrometer instruments. Our customers - true adventurers and discoverers out in the field - utilize this instrument line for a multitude of different applications and they often get back to us via feedback, testimonials and use cases. We are inspired by this creativity and together we are moving towards bettering our product range – all with the same goal in mind: collecting the most accurate data in the form of spectral signatures.

This quest can often lead to innovative and creative 'solutions' involving the pairing of materials and technologies alongside an ASD instrument in order to create a data collection solution capable of achieving results. From ideas as simple as attaching an ASD contact probe to a broomstick or metal pole to accomplish above-ground measurement results, to mounting an ASD FieldSpec® instrument on a tower system in the sky above a corn field and paired with a hyperspectral camera, the following images offer some creative examples of our customers' innovations.

Figure 1. Innovative use of an ASD pistol grip to measure light being reflected off snow (left, with fiber optic cable accessory) and sand (right, with fore optic accessory)[1]

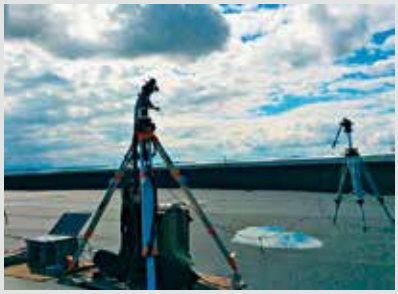


Figure 2. An example creating more accurate simulated skies using a custom sky scanner, paired with an ASD FieldSpec instrument

Figure 3. An ASD instrument on a UAS / mini-helicopter for the purpose of collecting airborne remote sensing measurements[2]

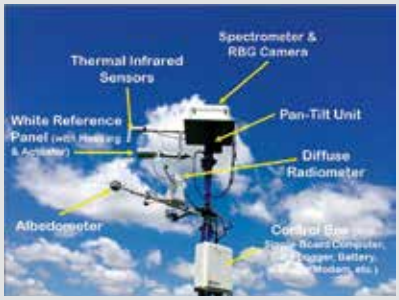


Figure 4. Components of the EcoSpec system (collecting white reference data before every data collection from the land surface, at each position around the tower, so that hyperspectral data is accurately converted to reflectance values). The spectrometer in this setup is an ASD FieldSpec 4.[3]

The EcoSpec system, as shown in Figure 4, was the main topic of discussion for ASD's webinar presentation in April 2017. This system, developed by a team of Argonne National Laboratory (Illinois, USA) scientists and engineers, was created for the purpose of conducting a, 'study on how plants and ecosystems respond and contribute to environments'. [4]

It is exciting to see our customers continue to invent and pair technologies, all for the cause of creating their own solutions, helping them to even better analyze materials that matter to them and the environment.

(1) kwsn.com/news/articles/2015/jun/23/sdsu-engineer-receives-first-google-earth-research-award
(2) www.asdi.com/solutions/image-classification-analysis/airborne-remote-sensing-measurements
(3) www.evs.anl.gov/research-areas/highlights/ecospec.cfm
(4) ecospec.evs.anl.gov

NEW PREMISES AROUND THE WORLD

Bringing two companies together to form a brand-new business requires building partnerships, knowledge, and sometimes even new spaces to work together within! XPress invites you to take a first look at some of Malvern Panalytical's new premises. Not only are parts of our headquarter buildings under renovation, but a number of our worldwide offices and supply centers have moved to better serve our customers and accommodate our employees and technologies.

The applications lab at our Dutch headquarters in Almelo has undergone a radical refurbishment. Here, we welcome our customers from across the globe for training or demonstrations of Malvern Panalytical's applications and product portfolio. The new lab was opened on 6 July 2017 by our President, Paolo Carmassi, and we hope to see you there sometime soon!

Our US offices in Westborough will soon follow this example with a renovation of their laboratory space, creating a spacious new facility which will accommodate Malvern Panalytical's entire product portfolio. We'll keep you posted on our progress.

The UK headquarters in Malvern are also currently undergoing a major renovation. Phases 1 and 2 of this project have focused on our production and support areas, as well as the hub area for all employees. Work on the next phase is now in progress!

Malvern Panalytical Germany – South Office – has recently moved to a new facility, just 500 m from the old office in Herrenberg. The new building houses an advanced applications lab and a service lab, together with well-equipped conference and work spaces.

Several other local offices have moved in order to share facilities and strengthen customer support, with one of our UK offices now sharing space with another Spectris subsidiary, Bruel and Kjaer, and some of our regional European offices moving into our Dutch headquarters in Almelo. Outside Europe, our Malvern Panalytical ASD office in Boulder, Colorado, made the short move to their new Longmont office.

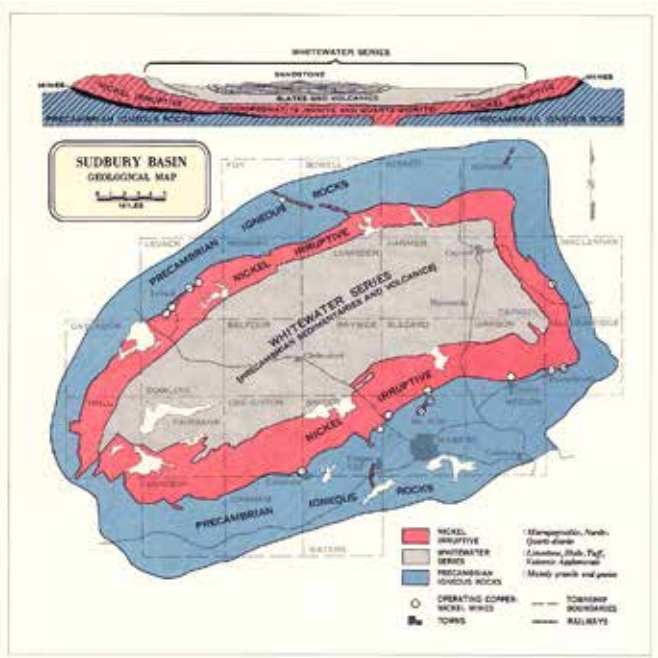
As always, all our colleagues across the business have been patient and supportive during these exciting changes, which are designed to create happier and more collaborative work spaces tailored to better serve our customers. We look forward to showing you around soon!

THE RESURGENCE OF **CANADIAN MINING**

Blessed with an abundance of natural resources, Canada is the world's top producer of potash and uranium, the world's third-largest producer of diamonds and ranks in the top five in output of nickel, cobalt, cadmium, zinc, salt and molybdenum. Additionally, the Labrador Trough, a geological belt straddling the Quebec-Newfoundland-Labrador border, is one of the world's most promising regions for clean high-quality iron ore (Mark Morabito, Vancouver Sun, 13th April 2017[1])**.**

As commodity prices rise and even more potential sources of growth emerge on the horizon, Canada's mining industry is ideally situated as a secure, sufficient and stable base of supply to help meet demand. They do, however, need to deal with the present challenges for any industry: to produce in the most efficient and environmentally friendly way. To help meeting these targets, Malvern Panalytical organized Ore and Mineral Analysis (OMA) workshops in Sudbury and Quebec where information about the latest innovations for elemental and mineralogical monitoring, particle size analysis and sample preparation could be exchanged.

The Sudbury Basin, also known as Sudbury Structure or the Sudbury Nickel Irruptive, is a major geological structure in Ontario, Canada[2]. It is the second-largest and one of the oldest known impact craters on Earth. The crater formed 1.849 billion years ago in the Paleoproterozoic era. Deposits of nickel, copper, platinum, palladium, gold, and other metals are bound on the geological impact structures.
Because of these metal deposits, the Sudbury area is one of the world's major mining communities and the region is one of the world's largest suppliers of nickel and copper ores.



OMA workshop Sudbury - September 26, 2017

The 6th OMA workshop was hosted by the Goodman School of Mines / Laurentian University in Sudbury. 47 participants from nine different companies and research institutions discussed topics and trends for process monitoring in the mining industry.

Glenna Keating (Geoscience Laboratories) and Dr. Bruce C. Jago (Goodman School of Mines) shared their experiences with the audience and Malvern Panalytical presented solutions for ore and mineral analysis. The workshop ended with practical demonstrations at the Geoscience laboratory.

OMA workshop Quebec - September 28, 2017

The 7th OMA workshop was hosted by Claisse in Quebec. Quebec is one of Canada's largest provinces and is renowned for the natural resources of its vast territory. It has about 30 mines, 158 exploration companies and fifteen primary processing industries. Many metallic minerals are exploited, mainly gold, iron, copper and zinc. Many other commodities are extracted including titanium, asbestos, silver, magnesium, nickel and many other metals and industrial minerals. However, only 40% of the mineral potential of Quebec is currently known.

More than 55 participants from 25 mining, metals and cement companies made the workshop in Quebec a very interactive event. A wide spectrum of topics from mining and metals industries gave a perfect overview of current and future needs to increase the efficiency during ore processing.

Our thanks go not only to presenters Dominique Huot (Reflex), Michel Chabot (Ciment Québec), Marc Gravel (ArcelorMittal), Maxime Larouche (COREM), Julie Salesse (Aluminerie Alouette) and Harris Bujold (IOC) but to all participants. They turned both workshops into exciting and interactive meetings, which will certainly be repeated.

References:
(1) vancouversun.com/opinion/op-ed/opinion-the-coming-resurgence-of-canadian-mining
(2) https://commons.wikimedia.org/wiki/File:Sudbury_Basin_Non-Ferrous_Metals_-_Eastern_Canada_map.png

YUE DENG, **WINNER** OF THE 5TH **PANALYTICAL AWARD**

Promoting exceptional young scientists

The PANalytical Award, founded in 2012, aimed at supporting young scientists at the beginning of their career. Each year they were encouraged to submit their articles describing groundbreaking research requiring 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 2016 competition is Dr. Yue Deng, a young Chinese scientist, who did his PhD at the University of Bath (UK) and the University of Picardie (Amiens, France).

Dr. Deng's article 'Structural and Mechanistic Insights into Fast Lithium-Ion Conduction in Li_4SiO_4-Li_3PO_4 Solid Electrolytes' was published in the Journal of the American Chemical Society, (2015) 137, 9136-9145, and was chosen from more than 100 entries submitted from around the globe. The judges were especially impressed by the original results of Dr. Deng's comprehensive work. He investigated the Li_4SiO_4-Li_3PO_4 solid electrolyte system using a powerful multi-technique approach of diffraction, AC impedance, NMR spectroscopy and atomistic modeling to obtain new information about the crystal structures and lithium-ion conduction mechanisms. The results open the way to new solid electrolytes with enhanced conductivity. Yue Deng is delighted by PANalytical's recognition of his research and says:

"Diffraction has been a key technique connecting our experimental findings and results from computer simulation. This award is a great acknowledgement for the value of our work, and a great encouragement for me to apply my knowledge of diffraction and crystallography in my career. I am very grateful for it." He received the trophy and €5,000 prize money in late October at the Malvern Panalytical offices in Shanghai (China) where he is currently working.

Dr. Yue Deng (center), with his PhD supervisors Prof. Christian Masquelier (left) and Prof. M. Saiful Islam

In the strong field of candidates the jury identified two close runners-up: Dr. Nathan Bossa for his publication in Cement and Concrete Research 67 (2015) 138-147, 'Micro- and nano-X-ray computed-tomography: A step forward in the characterization of the pore network of a leached cement paste' and Dr. Clément Falaise for his article in Chemistry – A European Journal (2016), 22, 14678-14687, 'The Key Role of U28 in the Aqueous Self-Assembly of Uranyl Peroxide Nanocages'.

In light of the merger of PANalytical with Malvern Instruments, the PANalytical Award has been discontinued. We very much appreciated receiving so many high-quality scientific articles during the past 5 years and hope to continue our support for promising young scientists in another way in the future.

ASTM **AWARD OF MERIT** FOR BRUNO VREBOS

In July 2017 ASTM International's Committee on Declarable Substances in Materials (F40) presented its top annual award (the Award of Merit) to Dr. Bruno Vrebos, internationally renowned X-ray scientist at Malvern Panalytical. The prestigious award includes the accompanying title of Fellow and is ASTM's highest recognition for individual contributions to developing standards.

Bruno, a member of ASTM International since 2005, was honored for meritorious and dedicated service, with a strong commitment to the pursuit of scientific depth and accuracy in testing through standards development, especially in the area of elemental analysis using X-ray fluorescence.

Read more about PANalytical's award-winning scientist on www.panalytical.com/ASTMaward.

COLOPHON

Please send your contributions, suggestions and comments to **info@malvernpanalytical.com**

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Want to visit us at an event? **malvernpanalytical.com/events** shows a list of events where you will find us. We are happy to welcome you!

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