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X'PRESS

HOW TO CONTROL?



PANalytical
get insight

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



Peter van Velzen
Managing Director

It is with great pleasure that I present the 'new' X'Press to you. We updated our house style in line with our newly defined vision and mission in which we commit ourselves 'to create a better world by helping people to analyze materials that matter to them and to the environment'. We aim at our customer magazine X'Press to be instrumental in realizing this mission.


We hope the new layout makes for an attractive magazine that keeps you informed about the latest developments in material analysis, its applications in daily life but also about the people behind those developments.

The theme of this issue is 'How to control' and we present interesting articles from the metals industry to illustrate how our solutions create more insight in your process and improve its outcomes. We also present a number of new products, which may help you controlling and improving your measurements.

With an article about the winner of the PANalytical Award we once more want to encourage young scientists from all over the world to apply for this award by submitting testimonies of their research. This program has now been launched for the third consecutive year. With this and other awards PANalytical strives to stimulate talents to achieve breakthroughs in the analytical science and application thereof.

I wish you a lot of reading pleasure.

PS You might already have noted that our PANalytical website now is available in 8 languages. I invite you to have a look at www.panalytical.com!



Kind regards,
Peter van Velzen

LATEST NEWS

Claisse becomes a member of the PANalytical family

In June 2014 it was announced that PANalytical acquired the business of the Canadian company La Corporation Scientifique Claisse Inc. ('Claisse'), a global market leader in sample preparation for atomic spectroscopy.

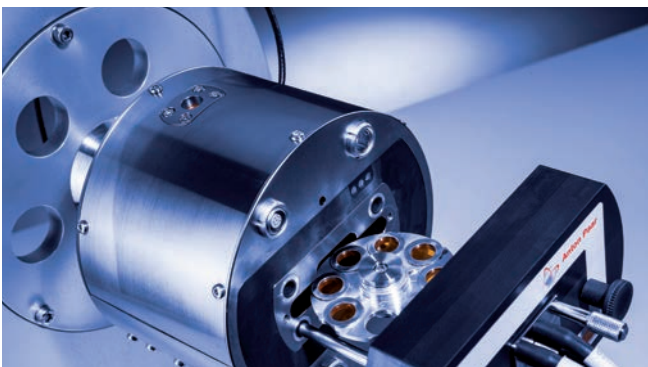
Claisse designs, manufactures and sells consumables and instruments used to prepare consistent and comparable samples for spectroscopic analysis in mining, pharma-ceutical, academic research and industrial applications. "We are confident that the market will benefit from PANalytical's support to Claisse's continued product and application (XRF & ICP) development plans, as Claisse becomes our center of expertise for fusion", says Peter van Velzen, CEO of PANalytical. And he continues: "We feel a strong cultural fit and are convinced that the combined capabilities and commercial networks will create significant value for our (potential) customers."

In the next issue of X'Press Claisse and its products will be presented in more detail.

In this issue



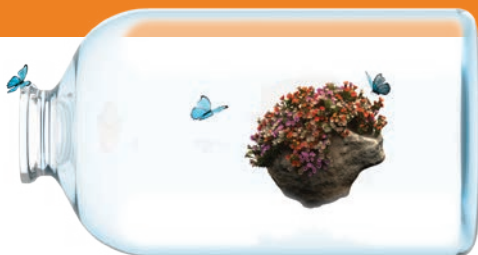
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Full control of ArcelorMittal's steelmaking process

ArcelorMittal Duisburg, situated in Duisburg (Germany), converts raw iron into high-quality long-carbon steel products for a large variety of applications. With about 1000 employees the steel plant runs 24/7, processing more than 1.15 million tons of raw steel per year. At the end of 2013 PANalytical delivered a new and fully automated laboratory for all steel analyses within the plant. This lab has successfully been up and running continuously since March 2014.

The properties of any steel are defined by the concentrations of iron, sulfur, carbon and various additives. It is crucial to determine the elemental concentrations to a very high precision. By analyzing these concentrations at the start of the production process and at intermediate steps, it is possible to steer the production process in the most cost-effective and efficient way. After 20 years of continuous and successful operation inside the production hall, ArcelorMittal's existing PANalytical lab was ready to be replaced by a new one which now complies with the latest requirements.

A team consisting of PANalytical specialists, together with ArcelorMittal lab crew designed a fully automated turn-key lab. For this an entire new building was set up at the side of the production hall and was connected via seven air tube lines to two factories. All incoming raw iron, slag and steel samples are treated fully automatically: they are unpacked, cooled, milled and the surface is inspected. Subsequently chips are produced and collected for combustion-based analysis. Samples are then analyzed by a PANalytical Axios FAST X-ray fluorescence spectrometer and/or an OBLF QSG 750-II optical emission spectrometer and finally screened for gamma-radiation. Data collection and storage, reporting and communications between all analyzers run via PANalytical's SPARCS LIMS system, which also communicates with the Level 2 production control system in the factory.

In order to avoid any interruptions of the continuous operation, two completely redundant laboratories have been created. They are cell-structured for optimal versatility, with automatic re-routing of samples when units in the primary lab are serviced or not available. The lab is now ready to process up to 500 samples per day. A few months of extensive testing have resulted in full confidence and successful commissioning of this unique new lab.

"PANalytical has been a perfect partner for this project. Their purposeful approach and their collegiality have made our cooperation not only pleasant but highly effective. Together we have found the best solutions for any upcoming question and have ended up with this unique turn-key lab which fully meets our expectations."

- Birgit Tenckhoff, lab manager at ArcelorMittal



The new automated lab at ArcelorMittal



ArcelorMittal

ArcelorMittal, the world's leading steel and mining company, employs about 245,000 people in 60 countries worldwide. The company covers all of the key steel markets, from emerging to mature and their top priority is to produce safe and sustainable steel.

1400 researchers in 11 laboratories worldwide are developing cleaner processes and greener products to help to reduce ArcelorMittal's and their customers' environmental impact.





Expertise for Jewometaal Stainless Processing B.V.

Jewometaal Stainless Processing B.V. (Jewo), situated in the port of Rotterdam (the Netherlands), is part of the ELG group. Per year Jewo processes about 350,000 t of stainless steel scrap in various forms (for example chippings, foils, spongy material, sheets and rods up to e.g. solid distillation columns weighing 20 tons) and consisting of different alloys. Delivered by truck or ship, one batch of material may easily weigh hundreds to thousands of tons. Precise knowledge of the composition of the incoming material is important for the control of the subsequent processes. For these analyses Jewometaal acquired a PANalytical Axios^mAX X-ray fluorescence spectrometer in 2005. A few years later PANalytical was asked for their expertise to improve the analysis results by optimizing the calibration.

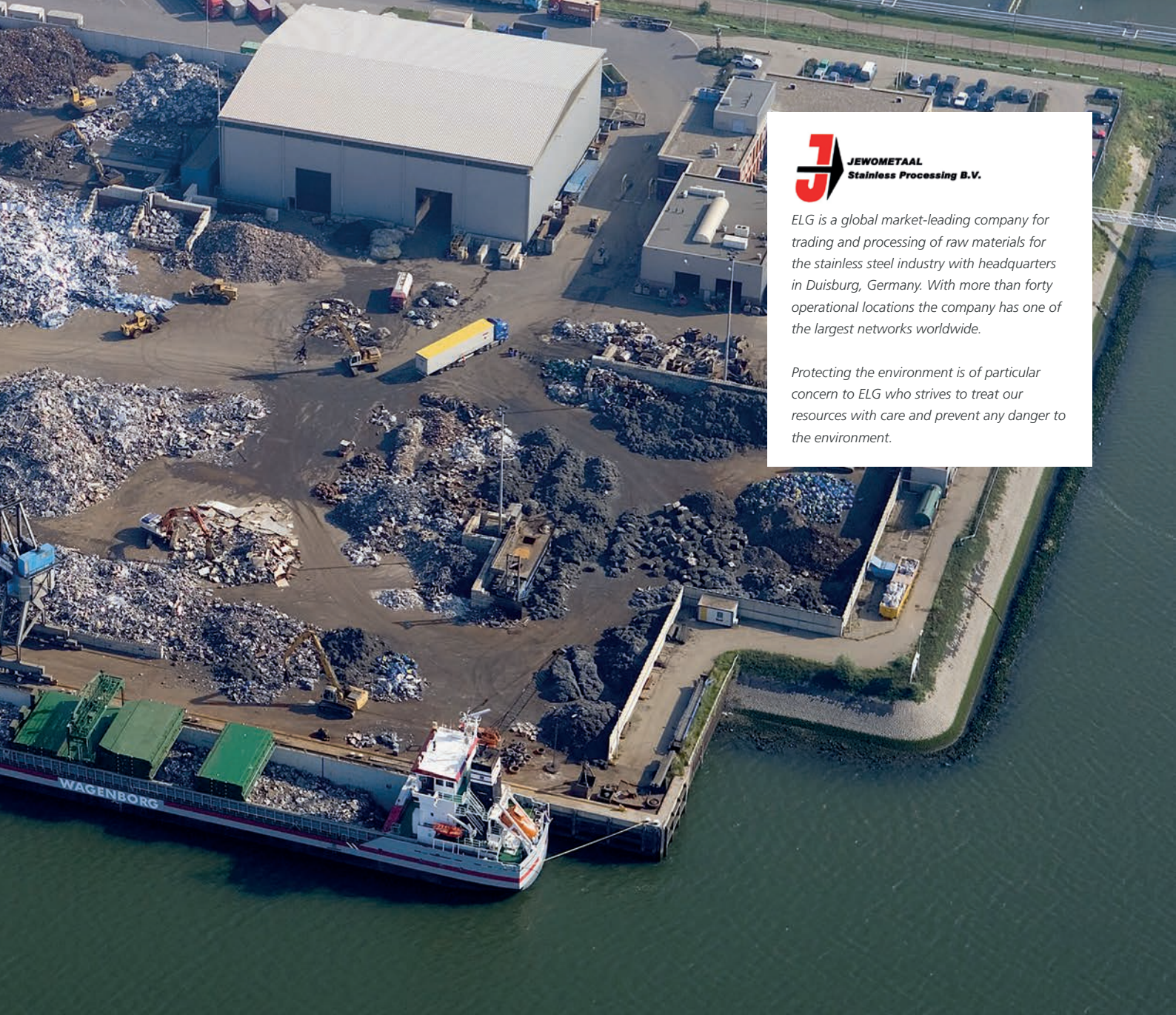
Starting with the collection of scrap samples at the beginning of the process, PANalytical's application specialist was able to standardize and optimize the sample preparation. Representative pieces are cut out of incoming material and any lead and copper components are removed, in order to avoid excessive concentrations of these metals in the process. Subsequently the material is melted in an induction furnace and a

"I am very satisfied with this long-lasting and beneficial partnership which has resulted in better and more cost-effective analyses of our incoming material."

- Eric Oosterom, manager operations at Jewometaal

sample is cast, ground and polished. The procedure has now been taken over by a routine operator who also performs the measurements, assisted by (remote) expertise from PANalytical.

At first, the calibrations each covered very wide concentration ranges, using a combination of certified and secondary standards. Acquisition of additional standards enabled the setup of a parallel



ELG is a global market-leading company for trading and processing of raw materials for the stainless steel industry with headquarters in Duisburg, Germany. With more than forty operational locations the company has one of the largest networks worldwide.

Protecting the environment is of particular concern to ELG who strives to treat our resources with care and prevent any danger to the environment.

and much more precise calibration, mainly containing international certified materials. By the beginning of 2014 this calibration had been fully optimized and completed.

PANalytical's Expertise will continue to be used in working to improve the calibration of Re, Hf, Ce and Ta. Batches containing these elements will be identified, quantified and sold separately. Last but not least measurements using the Omnia software will be tailored in order to cover odd samples, including filter material.

During the last 5 years PANalytical has been able to assist Jewometaal with a number of actions:

- Replacement of the induction furnaces by faster and more economical furnaces
- New ceramic crucibles which now prevent the inclusion of carbon
- Standardization of the sample preparation steps
- Reduction of operating staff
- Improved accuracy of both Ni and Cr analyses, the elements that often determine the prices
- Reduction of the measurement time with more than a minute per sample

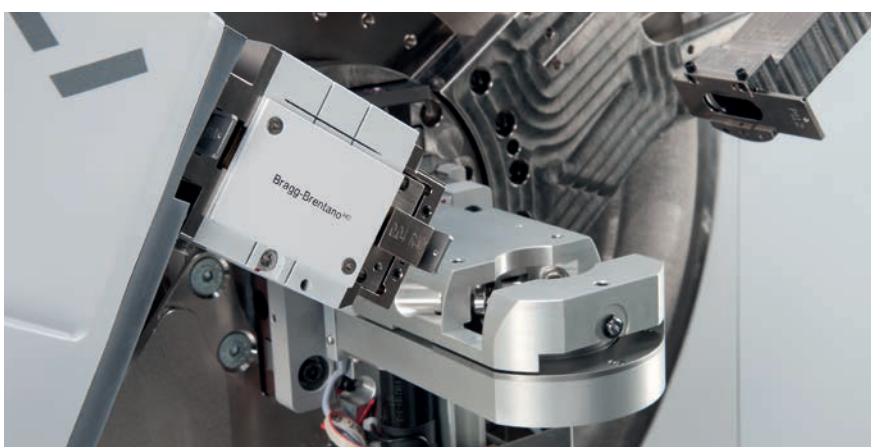
Setting a new standard for **high-quality** powder diffraction data

For users of PANalytical X-ray powder diffraction systems who need enhanced data quality we now offer our new Bragg-Brentano^{HD} module. This is the latest addition to PANalytical's extensive portfolio of PreFIX optical modules. For powder diffraction it combines high-speed data collection using 1D and 2D detectors with the traditional data quality of receiving slit diffractometers. In addition it can be successfully applied in thin film and nanoparticle analysis.

With Bragg-Brentano^{HD}, PANalytical again sets a new standard for recording high-speed, high-quality powder diffraction data, with the following key features: The new module delivers reduced wavelength spread with a higher signal-to-noise ratio than provided by the combination of divergence slits and beta filters. It also ensures a very smooth and featureless background for 1D scanning methods and improved detection limits. This enables a better quantification of trace phases and amorphous content. The low-angle performance is enhanced and last but not least there is minimal excitation of fluorescent radiation in the sample.

Additionally, the Bragg-Brentano^{HD} PreFIX module can be used for applications other than powder diffraction such as the analysis of thin films by grazing incidence diffraction and X-ray reflectometry or the analysis of nanoparticle size, shape and size distribution by small-angle scattering (SAXS). Users can profit from this extended range of measurement options without the need for other additional modules.

Following PANalytical's dedication to compatibility the Bragg-Brentano^{HD} module can of course be used with all of PANalytical's multipurpose powder diffractometers, both new and installed systems. Martijn Fransen, PANalytical's XRD product marketing manager, says: "Thanks to this new optical module users have now access to extremely high-quality X-ray diffraction data for their analyses. The higher signal-to-noise ratio, smoother background and reduction of fluorescent excitation in the sample achieve much improved detection limits for minor phases."

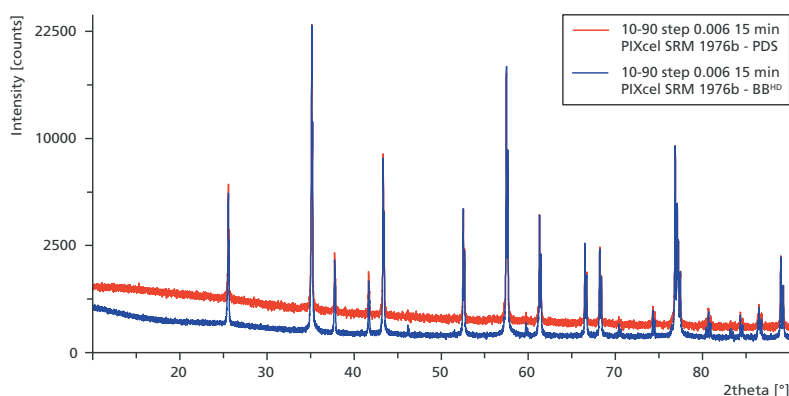


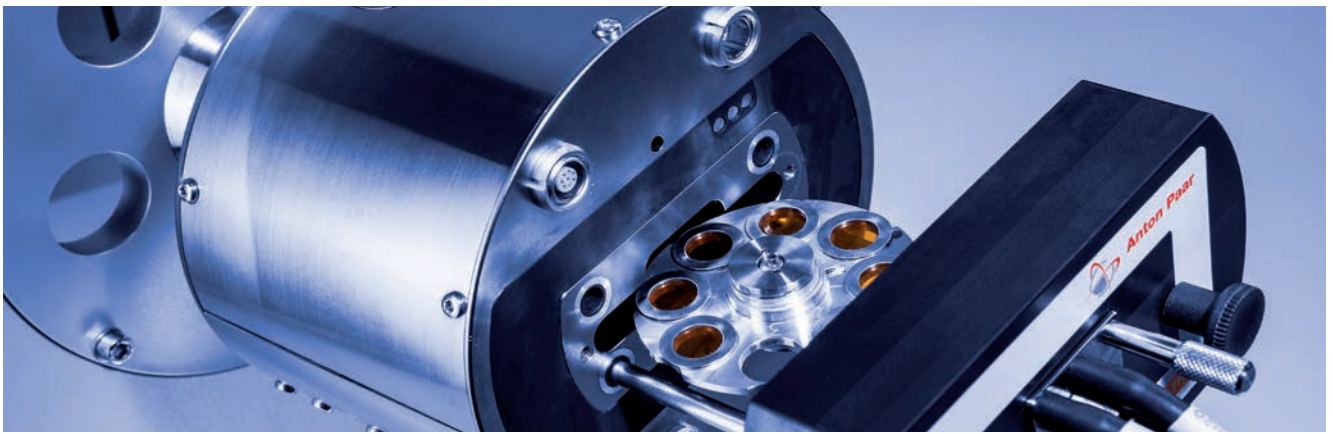
Bragg-Brentano^{HD}

Comparison of two data sets for NIST Al₂O₃ sample SRM1976b

For both measurements the optics settings were chosen to create matching peak shapes. The red data set was recorded with a conventional programmable divergence slit (PDS) set to 1/4°. The blue set was recorded with Bragg-Brentano^{HD} and shows a higher intensity and a lower background.

Both measurements employed the PIXcel^{3D} in 1D scanning mode. A scale factor of 1.96 was applied to the Bragg-Brentano (red) data in order to match the tops of the strongest peak. It can be clearly seen that the overall background from the Bragg-Brentano^{HD} data is considerably lower, improving the visibility of weaker reflections. (See, for example, the (202) reflection near 46°, 2θ).





MHC-trans

XRD experiments with **fully automated control** of temperature and humidity

X-ray diffraction (XRD) is usually the method of choice for *in situ* investigations of phase transitions. The sample is exposed to variable well-defined non-ambient conditions and diffraction patterns are recorded. For many years Anton Paar and PANalytical have been offering a variety of high- and low-temperature solutions with full software integration. We are now pleased to announce the addition of the fully automatic combined control of temperature and humidity in X-ray diffraction experiments using the existing CHC plus+ and the new MHC-trans chambers, both from Anton Paar.

The CHC plus+ (Cryo & Humidity) chamber has proved its reliability and high performance for years. In addition to the temperature-humidity regime, this chamber can be also used for high- and low-temperature experiments.

The MHC-trans (Multi-Sample Humidity Chamber) is a new humidity chamber from Anton Paar for X-ray diffraction experiments in transmission geometry and includes an 8-position sample changer. The environmental heater offers a homogeneous temperature distribution around the sample. Having 8 samples loaded within the chamber saves time because humidity-induced phase transitions can be quite time-consuming. In addition, the same con-

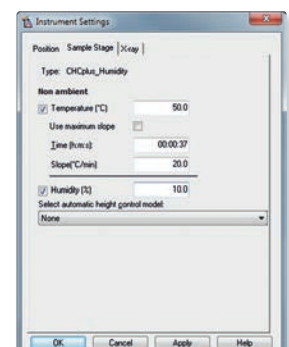
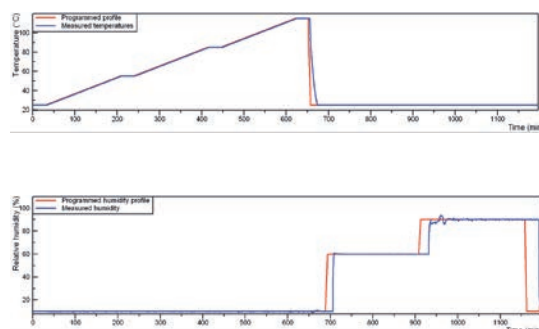
ditioning process for all samples is ensured. The transmission geometry is particularly suitable for pharmaceuticals where humidity studies are an industry requirement.

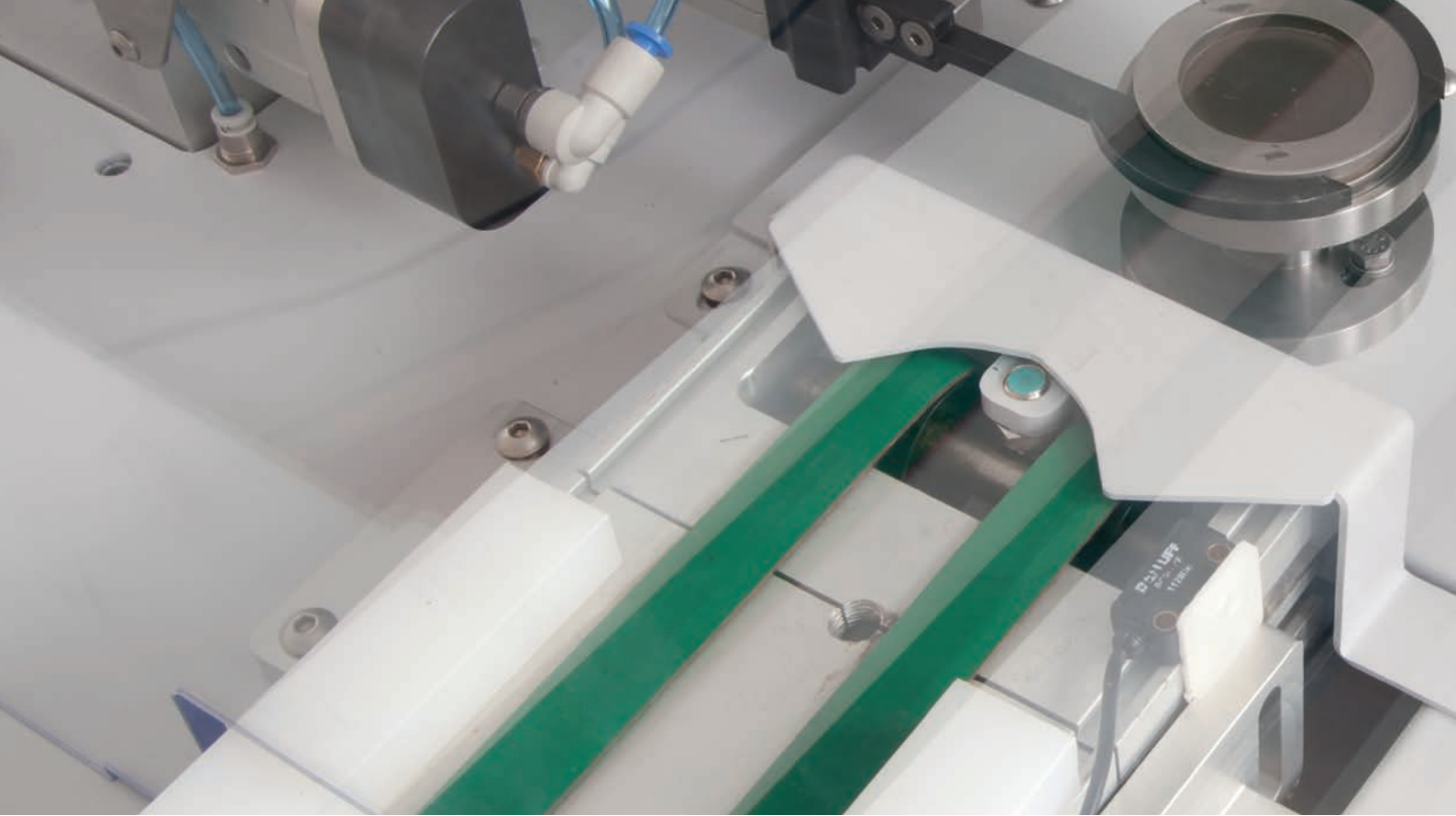
The new combined Relative Humidity-Temperature (RH-T) control tool is the result of our continued extensive collaboration with Anton Paar. The user can now define the exploration area of a RH-T regime and the software automatically controls both parameters to create a smooth path through the non-ambient parameter field. The thoroughly optimized control mechanism provides very smooth transition steps even at the highest temperature and humidity values, thus ensuring condensation-free experiments.

Both CHC plus+ and MHC-trans chambers have the benefit of the complete user-friendly software integration with PANalytical's Data Collector. For each measurement, the RH-T values are saved in the file name and also in the XRDML file itself, together with the data and information about the measurement. The programmed and recorded RH-T profiles are saved in XRDML format in a separate file.

Control of RH-T can also be continued independently of Data Collector, enabling the sample to be kept at a required RH-T for days or weeks in between measurements, thus freeing up the diffractometer for other applications.

Example of programmed and measured temperature and humidity (graphs on the left) profiles and integration of the non-ambient parameters in the Data Collector (right)





New possibilities

PANalytical's new Epsilon 3^X benchtop X-ray fluorescence (XRF) spectrometers were presented to the public in early 2014 (as reported in X'Press 1/2014). These systems, upgraded from the proven Epsilon 3 range, satisfy users by their superb analytical results. In order to let more users profit from the systems' features we have now introduced two new application solutions: an automation option and the Oil-Trace analysis module.

Flexible and safe automation for process control

Historically, the automation of X-ray fluorescence (XRF) instruments has been limited to high-power wavelength dispersive (WD) XRF systems. However, more and more benchtop energy dispersive (ED) XRF spectrometers are sold into production control as cost-effective solutions because of improved performance. Recent advances in Epsilon 3^X (ED)XRF spectrometers make them an attractive alternative in automated environments.

The Epsilon 3^X Automation is a simple and flexible solution interfacing your existing Epsilon 3 or new Epsilon 3^X analyzer to any sample preparation equipment. The flexible sample introduction system is specifically designed to handle a variety of prepared samples coming from a belt, a robot or even from a manual input slide.

Epsilon 3^X Automation

Benchtop instrument enclosed in a sealed cabinet





“With these new additions PANalytical’s Epsilon 3^X and Epsilon 3^{XLE} benchtop spectrometers have evolved into mature XRF systems for dedicated analyses in industrial process control. Their superior performance and small footprint make them a very attractive solution close to the process.”

- Simon Milner, XRF product marketing manager at PANalytical

for Epsilon 3^X

Oil-Trace analysis module

The introduction of fuel emission regulations like Euro VI has led to more stringent norms for fuels and subsequently improved lubrication oil properties. Sulfur is the most prominent of the restricted elements in Euro VI. Its analysis with XRF is well established because sample preparation is simple and the results are accurate and reproducible. This is reflected in several international norms and standard test methods.

The accurate analysis of sulfur in a variety of gasoline, ethanol, bunker fuels, diesel and biodiesels and their respective blends leads to the setup of many XRF calibrations, which also need to be maintained. Moreover, buying relatively expensive certified reference materials is costly. This is where PANalytical’s Oil-Trace module can help users to save time and money.

Not only can Oil-Trace deliver accurate results based on one single sulfur-in-mineral-oil calibration for many different fuel types. It also enables analysis of samples with different volume or weights than the initial weights used for calibration setup. This is especially handy for highly viscous samples like bunker fuels. The module can cater for differences in oxygen and hydrocarbon composition which influence accurate sulfur analysis and it can measure different additives in a variety of base oil classes without the need for specific calibrations.

Oil-Trace is very convenient for used oil as almost no standards exist to cater for all the variations that can occur in oxidized hydrocarbons composition. A single wear metal calibration is now sufficient to accurately quantify wear metal compositions allowing to perform machine monitoring and preventive maintenance with much more confidence.

The superior accuracy of Oil-Trace is achieved by the implementation of the 5th generation of PANalytical’s Fundamental Parameters program and a number of advanced corrections. The package has proven its advantages on PANalytical’s high-power Axios^{MAX}-Petro systems for many years and is now also available on the benchtop Epsilon 3^X instruments.



The Oil-Trace kit

PANalytical support for young scientists



Scientific research is one of the major contributors to furthering the development of mankind. In order to ensure the continuity of scientific research it is vital to support and encourage young scientists at the beginning of their career. Realizing this importance, PANalytical has created a number of possibilities for supporting promising young researchers.

The PANalytical Award

Founded in 2012 the PANalytical Award seeks to encourage and support one excellent young scientist per year. It praises groundbreaking research that required the use of a laboratory X-ray diffraction, X-ray fluorescence or X-ray scattering instrument as the primary analytical technique. The award is made to the first author of a publication and consists of € 5,000 cash prize, a trophy, and a certificate.



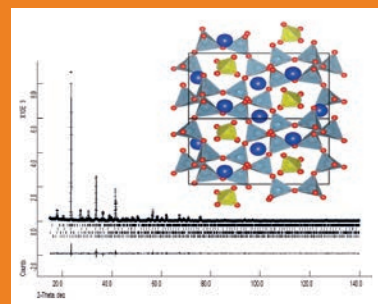
Ms. Ana María Cuesta García

In February 2014, Ms. Ana María Cuesta García from the department of Inorganic Chemistry at the University of Málaga (Spain) was elected as the next winner of the PANalytical Award. The decision was based on her publication 'Structure, Atomistic Simulations, and Phase Transition of Stoichiometric Yeelimite', which, according to the jurors, describes a splendid investigation that, although challenging, was thoroughly carried out. The committee was impressed by the level of understanding that Ms. Cuesta and her co-workers were able to extract from the combination of analytical techniques with a laboratory-scale X-ray technique being key to the structural characterization.

"The money will be very helpful in furthering my education as I would like to attend a number of additional specific courses before applying for a subsequent academic position in my current or a related research field."

- Ana Cuesta, winner of the 2nd PANalytical Award

Yeelimite (calcium sulfoaluminate) is the most important phase in calcium sulfoaluminate cements. The objective of Ms. Cuesta's paper was to establish the crystal structure of this phase with the aim of obtaining the best quantitative phase analysis of cements and hydrated pastes. The researchers have been able to understand the mechanisms of hydration of this yeelimite (and that of another polymorph of a doped-yeelimite). Currently the project is continued with work at a revised crystal structure of another polymorph of a doped-yeelimite (pseudo-cubic) by using the techniques described in the awarded article.



Top: Calculated crystal structure of the orthorhombic ye'elimite phase (Pcc2). Al denoted within light-blue tetrahedra, S within yellow tetrahedra, Ca are dark-blue and O are red.
Bottom: LXRPD Rietveld plot for synthetic ye'elimite using the orthorhombic structure.

"The PANalytical Award provided me with international recognition of my work in X-ray diffraction. Such recognition, stemming from comparison of my work with others in the broad field by a panel of experts, is extremely difficult to access in the early stages of a career. Specifically, it provides research institutions with a highly accurate measure of the standard of one's research, which is invaluable when applying for academic positions."

- Dr. Thomas Bennett, first winner of the PANalytical Award

Shortly after the award, Thomas was elected to a highly competitive research fellowship at Trinity Hall, University of Cambridge. He was able to use the PANalytical award as evidence of his international standing, which can prove crucial in setting young academics apart from one another.



Dr. Thomas Bennett

Applications for the PANalytical Award 2014 can be submitted via www.panalytical.com/award.

Deadline is 1 December 2014. There are no restrictions on the manufacturer of the X-ray equipment that was used.

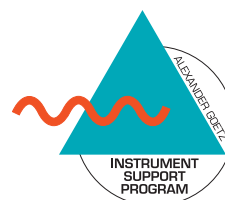
PANalytical Boulder student loan programs

The annual Alexander Goetz Instrument Support Program was established in 2007 by Analytical Spectral Devices (ASD) (now PANalytical Boulder) in recognition of their co-founder Alexander Goetz. This program seeks to inspire a creative research environment within the worldwide remote sensing and field spectroscopy community by offering graduate students the temporary use of a FieldSpec® spectroradiometer or a HandHeld 2 spectroradiometer.

Through the eight years of this program, instruments have been provided, free of charge to over 60 students across the globe who have used our near-infrared (NIR) spectrometers to further investigate their research applications.

A total of 12 students were selected for the 2014 calendar year program with topics of research including ancient cultures, climate change impacts, forensic science, forest analysis with satellite imagery, plant physiology, as well as the utility of NIR analysis for industrial polymerization.

Applications are now being accepted for the 2015 program and must be received by October 15, 2014 to be considered. More information about the Goetz Program is available on: www.asdi.com/service-and-support/goetz-instrument-support-program



Students in Mining TerraSpec Instrument Program

The success and popularity of the Goetz Program led to the development of the Students in Mining TerraSpec Instrument Program in 2013. Similar to the Goetz Program, the Students in Mining Program was developed to complement and strengthen student research.

However, the Students in Mining Program is dedicated specifically to studies that include mining education,

mining exploration or production, oil and gas and geothermal applications.

Participants of the Students in Mining Program receive temporary access to a TerraSpec® mineral analyzer and The Spectral Geologist (TSG®) Pro mineral analysis software.

For the 2014 program, four Ph.D. candidates in relevant fields of study have been granted the temporary use of a TerraSpec 4 mineral analyzer to complete their mining and energy research projects.

Proposals are now being accepted for the 2015 Students in Mining Program and must be submitted by November 15, 2014 to be considered. More information about the Students in Mining Program, is available on: www.terraspec.net



Successful IYCr 2014 OpenLab course in Ghana

PANalytical's first OpenLab event, celebrating the International Year of Crystallography (IYCr) 2014, took place at the 'Centre for African Wetlands', on the campus of the University of Ghana in Accra, Ghana, on 9-12 June. The OpenLab was organized by PANalytical B.V. together with F. Malawi Engineering Co. Ltd. and the Department of Physics at the University of Ghana.

The aim of the educational course was to make scientists familiar with crystallography and X-ray diffraction as described in the mission of IYCr 2014 (www.iycr2014.org, see also X'Press issue 1/2014). Thirty PhD students and young professionals attended the 4-day event consisting of presentations, hands-on sessions on software and practical sections on the Epyrean, which was recently installed at the university in the Department of Physics. Lectures and practical sessions were highly appreciated by the participants who enjoyed the interactive sessions.



The 14th EPDIC

The 14th European Powder Diffraction Conference (EPDIC-14) was held on 15-18 June at the Aarhus University (Denmark) and welcomed about 300 participants from all over the world.

PANalytical presented new hardware and software solutions during a lunch workshop. Visitors of the booth were introduced to some of the latest additions for PANalytical's diffractometers: the Bragg-Brentano^{HD} module, the Anton Paar MHC-trans chamber (see pages 8&9) and a Medipix3-based new detector. These, together with a number of poster contributions from our specialists inspired lively discussions with the conference delegates.

The EPDIC Award for Young Scientists, sponsored by PANalytical, honors outstanding scientific achievements in the field of powder diffraction. It was presented to this year's winner, Dr. Jan Manuel Hinterstein from the University of New South Wales, Australia for his research at functional materials such as piezoceramics, battery materials and zeolites. Dr. Hinterstein presented his work during a talk at the closing ceremony.

- Dr. Hinterstein (left) receiving his award from PANalytical product manager Emphyrean Dr. Fabio Masiello

Finnish Mining Seminar

On 4 – 6 June the 9th Finnish Mining Seminar, organized by the Finnish Mining Entrepreneurs and the Oulu University Mining School took place in Oulu, Finland. PANalytical has been a sponsor of this event since its beginning nine years ago and held a special seminar focusing on the whole mining process, from exploration to end products. Here, laboratory automation solutions, the TerraSpec Halo near-infrared analyzer, XRD mining solutions and the CNA cross belt analyzer were presented.

Approximately 200 attendees from different mines and mining organizations enjoyed the highly informative talks, which were accompanied by live presentations of a number of PANalytical's systems on display at the booth and at the seminar.



Events calendar 2014

The list shows a selection of events where you will find us during the upcoming period. Please come and visit us if you attend any of these events. More information on www.panalytical.com/events

28 July–1 August	Denver Conference	Big Sky, MT, USA
4–9 August	IUCr	Montréal, Canada
11–13 August	VII National Congress of Crystallography	Johore Bahru, Malaysia
24–29 August	International Workshop on Nitride Semiconductors (IWN 2014)	Wrocław, Poland
3–5 September	JASIS 2014	Makuhari Messe, Japan
4–7 September	10 th International Conference on Minerals, Metals, Metallurgy & Materials	New Delhi, India
22–25 September	ICMA	Boston, MA, USA

Successful 3rd edition Dutch Technology Week

The 3rd Dutch Technology Week (DTW) titled 'Week of Wonders' was held on 18-24 May. The aim is to promote technology and technical education among students and the general public. PANalytical in Almelo and Eindhoven joined forces with other high-tech companies, participating in numerous events throughout the week.



The main event was the High-Tech Experience Day on 24 May, held at various locations in the Netherlands. PANalytical in Almelo participated in a general exhibition together with other high-tech companies located in the region. Highlight was Dutch astronaut André Kuipers' lively presentation for the young visitors.

PANalytical X-ray Tubes in Eindhoven, together with their plant neighbors, welcomed around 1,000 enthusiastic visitors. Guests could witness the development and manufacturing of X-ray tubes. Also on show were XRF spectrometers analyzing medicines and foodstuffs, making guests aware that everyday consumer goods like smart phones and head ache pills are reliable and safe because the materials inside are analyzed with X-ray diffraction and X-ray fluorescence.

With this year's experiences in mind, even more elaborate plans for the 2015 edition of DTW are already being made.

Colophon

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

PANalytical B.V.
Corporate Marketing
and Communications Department

Lelyweg 1, 7602 EA
PO Box 13, 7600 AA
Almelo, The Netherlands

T +31 (0) 546 534 444
F +31 (0) 546 534 598
info@panalytical.com
www.panalytical.com

Regional sales offices

Americas

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

Europe, Middle East, Africa

T +31 546 834 444
F +31 546 834 969

Asia Pacific

T +65 6741 2868
F +65 6741 2166

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Designed for the **mining** industry

How to control your process?

Monitoring your raw materials is key to efficient process control. The new CNA³ for mining provides the elemental composition of your entire conveyed matter in real time, giving you the full picture. No matter your belt width, load, variation or particle size, CNA³ will always deliver reliable results. A new feature is the possibility to check the system calibration without interrupting production.

- Rugged and compact - easy to install
- No moving parts - easy to maintain
- In factory calibration - accurate and reproducible
- Sodern electrical neutron source - stable and safe
- User-friendly interface - easy to use
- Available for iron, copper, nickel, coal

CNA³ cross belt analyzer

