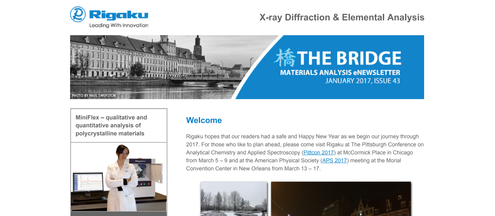

MiniFlex – qualitative and quantitative analysis of polycrystalline materials

Benchtop X-ray diffraction (XRD) instrument

Ideally suited for today's fast-paced XRD analyses, the fifth generation MiniFlex delivers speed and sensitivity through innovative technology enhancements such as the optional DTeX/Ultra high speed detector coupled with a 600 W X-ray source. Further used for teaching X-ray diffraction at the college and university level, or routine industrial quality assurance, the MiniFlex delivers both performance and value.
For more >

Interested in publishing your work in The Bridge?

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The Bridge now welcomes manuscripts, communications, and papers that describe techniques and applications of all forms of X-ray fluorescence (XRF) and X-ray diffraction (XRD, including SAXS) that are of interest to fellow scientists in industry, academia, and government. Manuscripts, in PDF format, are only accepted with the understanding that they are not commercial in nature. Authors are responsible for all statements made in their work. If illustrations or other material in a manuscript have been published previously, the author is responsible for obtaining permission to republish. Please send copy to the editor at Rigaku.newsletter@Rigaku.com

CT Lab GX series

Computed tomography (CT) for materials science

Rigaku recently introduced an ultra-high-speed, high-resolution 3D X-ray micro CT imager into the industrial CT market. The new "CT Lab GX" incorporates the "Sample-Stationary Method" and achieves CT scan in 8 seconds at top speed and maximum resolution of 4.5 μm.
For more >

Video of the Month

Is a new energy source a massive scientific fraud? Likely, but huge funding anyway!

Brillard Light Power, Inc. (BLP) of Cranbury, New Jersey is a company founded by Randell L. Mills, who claims to have discovered a new energy source. According to Wikipedia "The purported energy source is based on Mills' assertion that the electron in a hydrogen atom can drop below the lowest normal energy state as the ground state. Mills calls these hypothetical energy states that are in an energy state below ground level 'hydrinos'. Mills self-published a closely related book, *The Grand Unified Theory of Classical Physics* and has co-authored articles on claimed hydrino-related phenomena.

"Critics say it lacks corroborating scientific evidence, and is a relic of cold fusion. Critical analysis note that the proposed theory is inconsistent with quantum mechanics, and that the proposed hydrino states are unphysical and incompatible with key equations that have been experimentally verified many times. However, by 12/96, BLP raised more than $25 million from about 150 investors. By January 2009, BLP funding exceeded $60 million. In December 2013, BLP was one of 54 applicants to receive ~$1.1M grant from the New Jersey Economic Development Authority." **Watch video >**

Conferences and Workshops

Join Rigaku at future meetings

Rigaku will be sponsoring, attending or exhibiting at the following conferences and trade shows:

PITTCON 2017
Chicago, Illinois, USA
March 5 – 9, 2017

AWPA 2017
Las Vegas, Nevada, USA
April 9 – 11, 2017

MRO Americas 2017
Orlando, Florida, USA
April 25 – 27, 2017

See the complete list >

Useful link of the Month

The Materials Project

Harnessing the power of super-computing and state of the art electronic structure methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

A. Jain*, S.P. Ong*, G. Hautier, W. Chen, W.D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, K.A. Persson (*=equal contributions) The Materials Project: A materials genome approach to accelerating materials innovation. *APL Materials*, 2013, 1(1), 011002. DOI: 10.1063/1.4812323

For more >

Planning to Submit a Grant?

Rigaku is happy to assist

If you are planning on submitting an instrument grant proposal, Rigaku will be happy to assist you. We can help you determine the correct instrument and configuration best suited for your analytical needs. **Start the process >**

Rigaku's Materials Analysis eNewsletter, The Bridge

Join us

Each month, Rigaku distributes two eNewsletters: *The Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on life sciences. **Join us >**

Welcome

Rigaku hopes that our readers had a safe and Happy New Year as we begin our journey through 2017. For those who like to plan ahead, please come visit Rigaku at The Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon 2017) at McCormick Place in Chicago from March 5 – 9 and at the American Physical Society (APS 2017) meeting at the Moral Convention Center in New Orleans from March 13 – 17.

Wroclaw, Poland near Rigaku Oxford Diffraction facility (lower left)

Our featured article this month is "The Synergy Story," which chronicles Rigaku's acquisition of Agilent Corporation's single crystal business in April 2015 and the new synergies that were subsequently enabled throughout our global R&D operations. Flowing from this story is our *Rigaku Journal* article-of-the-month on the XtaLAB Synergy single crystal X-ray diffractometer.

Additional application papers include XRD, WDXRF and EDXRF technologies. This month we also include a special report on the PDXL software for powder XRD.

The book review this month addresses the very distressing problem of the (now) highly publicized "fake news" epidemic. Our book-selection may also fall into this category as it covers a CNN story about a supposed new energy source based on an unconventional hydrogen atom energy state. Check out the news and papers sections at the bottom of the page for the latest developments in materials science.

Happy New Year and enjoy the newsletter,

R.C. Tisdale, Ph.D. – Editor

XtaLAB Synergy
The Synergy Story
Reported by Paul Swepston, Global Manager, Rigaku Oxford Diffraction

At the end of April 2015, Rigaku acquired Agilent Corporation's single crystal business. From the beginning, the new combined single crystal division was named Rigaku Oxford Diffraction to pay homage to Oxford Diffraction, the original X-ray company that Agilent acquired. Our intent was to equally merge the two groups and create a synergistic effect in our single crystal product development. Aptly named, the first diffractometer to be developed by our combined group is called the XtaLAB Synergy. **Full article >**

Featured Rigaku Journal Article
XtaLAB Synergy: X-ray diffractometer system with single or dual PhotonJet microfocus sources
Rigaku Corporation

With your success utmost in our minds, the XtaLAB Synergy has been developed for single crystal X-ray diffraction. Using a combination of leading edge components and proven hardware best together through a highly parallelized architecture, the XtaLAB Synergy produces fast, precise data in an intelligent fashion. **Full article >**

14th Conference of the Asian Crystallographic Association
Report on AsCA 2016
Reported by Angela Criswell, VP, Life Science X-ray Products

The AsCA conference was held in Hanoi, Vietnam from December 4th to 7th. The conference was attended by 457 people from across Asia and beyond, with the largest attendance from Japan, Korea, Vietnam and India. **Full report >**

Application of Integrated X-ray Powder Diffraction Software: PDXL
Flufenamic Acid Nicotinamide Cocrystal
Rigaku Corporation

A cocrystal is a stoichiometric multicomponent crystal formed between two or more compounds. Cocrystals of an active pharmaceutical ingredient (API) have been attracting attention in the pharmaceutical industry because API cocrystals might have improved physicochemical properties, such as solubility, dissolution rate, and physical stability, compared with a single-component API crystal. **For more >**

XRD Application Note
Analysis of a stony-iron meteorite using a HyPix-3000 multi-dimensional detector
Rigaku Corporation

A stony-iron meteorite is like a single crystal. When using 0- or 1-dimensional detectors, only a few diffraction peaks are observed. In this situation, identification of crystalline phases cannot be conducted. Therefore, a stony-iron meteorite was analyzed using the multi-dimensional detector, HyPix-3000, which has an effective detection area for the identification of crystalline phases. **For more >**

WDXRF Application Note
Quantitative Analysis of Low Alloy Steel using the ZSX Primus III+
Rigaku Corporation

X-ray fluorescence spectrometers are the most common analysis tools to analyze steel owing to rapid analysis and the ability to measure both bulk metal and powders. This application note describes low alloy steel analysis using the ZSX Primus III+, which is optimized for process control. **For more >**

EDXRF Application Note
On-line Sulfur in Heavy Oils
Applied Rigaku Technologies

On-line, real time X-ray Transmission (XRT) measurement of sulfur (S) in heavy or light oils to satisfy the needs of refineries, pipelines, blending operations, bunkering terminals and ores industrial markets. Applications include bunker fuel testing to meet MARPOL Annex VI sulfur restrictions, interface detection of efficient grade fuels delivered via pipelines, refinery feedstock blending and monitoring, diesel/kerosene blending or production, and the quality monitoring of crude at remote collection and storage facilities. **For more >**

Scientific Book Review
A Survival Guide to the Misinformation Age. Scientific Habits of Mind By David J. Helfand. Columbia University Press. ISBN: 9780231169724

Longtime Columbia University astronomy professor David Helfand's *Survival Guide* seems even more pertinent now, in the wake of the recent presidential election and the fake news epidemic, than it was almost a year ago at the time of its first publication. Helfand's book certainly isn't a "how to determine if the news you are reading is fake" guide, but many of the principles of scientific discovery he explores could certainly be applied to the aforementioned dilemma. **Full review >**

Material Analysis in the News
News for January 2017

January 2, 2017. An international team of scientists described the first synthetic ionic conductor – a transparent, self-healing, highly stretchable material that allows ions to flow through it. The material could someday be used to improve the lifespan of electronic devices or develop self-repairing robots.

January 4, 2017. Theoretical physicists at the Department of Energy's SLAC National Accelerator Laboratory used computer simulations to show how special light pulses could create robust channels where electricity flows without resistance in an atomically thin semiconductor.

January 5, 2017. Researchers from the Center for Organic Photonics and Electronics Research (OPERA), Japan Science and Technology Agency (JST), and Kyushu University (all in Fukuoka, Japan); Sumika Chemical Analysis Service (Niihama and Osaka, Japan); and the Institute of System Information Technology and Nanotechnology (ISIT; Sawara, Japan) discovered that organic light-emitting diodes (OLED) lifetime already increases when the time an OLED must spend in the vacuum chamber during fabrication is reduced.

January 9, 2017. Berkelium is one of the few elements that has yet to be characterized in detail, largely because the only available isotope, ^{249}Bk, has a half-life of only 320 days. Using single-crystal X-ray diffraction, researchers at Florida State University structurally characterized a complex containing berkelium. The findings, in which both the physical properties and electronic structure of berkelium were not anticipated, indicate that a lanthanide element is a poor choice for a berkelium surrogate.

January 12, 2017. Japanese scientists, led by Eiji Ohtani at Tohoku University, have revealed that silicon is likely the mystery element in the Earth's inner-core, claiming progress on solving one of the planet's deepest secrets.

January 17, 2017. Researchers at Argonne's Advanced Photon Source, a DOE Office of Science user facility, reveal they have captured – for the first time ever – images of the creation of structural defects in palladium when the metal is exposed to hydrogen.

January 19, 2017. The discovery of a new type of quantum phase transition has been announced by researchers at Oak Ridge National Laboratory. This unique transition happens at an elastic quantum critical point, or QCP, where the phase transition isn't driven by thermal energy but instead by the quantum fluctuations of the atoms themselves.

January 19, 2017. France's CEA and Japan's RIKEN institute announced a multi-faceted five-year collaboration to advance high performance computing generally and prepare for exascale computing.

January 23, 2017. Researchers at the Carnegie Institution for Science have discovered a new phenomenon of so-called metastability in a liquid phase. Reported are the first experimental evidence of creating a metastable liquid directly by melting a high-pressure solid crystal via a decompression process below its melting point.

January 23, 2017. With a comparable bandgap to aluminum-rich AlGaN, BAlN is a very promising alternative for making deep UV optical devices. One of its great attributes is a smaller lattice constant that can be used to tune the strain and thus enable optical polarization engineering.

January 27, 2017. Apollo 1 fire claimed lives of three astronauts on the ground 50 years ago. The three astronauts were scheduled to lift off in February 1967, the first manned mission of the program that had its sights set on placing American footprints on the moon. But three weeks before launch, a routine countdown rehearsal on the ground brought about the unthinkable.

Recent Scientific Papers of Interest
Papers for January 2017

Recent Scientific Papers of Interest is a monthly compilation of material analysis papers appearing in recently released journals and publications. *See below*

Anomalous dispersion X-ray diffraction study of Pb/Bi ordering/disordering states in PbTiO$_3$-based perovskite oxides. Lin, Kun; Wang, Nai; You, Li; Li, Qiang; Kato, Kenichi; Chen, Jun; Deng, Jinxia; Xing, Xianran; *Dalton Transactions: An International Journal of Inorganic Chemistry*, 1/21/2017, Vol. 46 Issue 3, p733-738. 6p. DOI: 10.1039/c6dt04364j.

Characterization of x-ray imaging crystal spectrometer for high-resolution spatially-resolved x-ray Thomson scattering measurements in shock-compressed experiments. Lu, J.; Hill, K.W.; Bitter, M.; Pablant, N.A.; Delgado-Aparicio, L.F.; Efthimion, P.C.; Lee, H.J.; Zastrau, U. *Journal of Quantitative Spectroscopy & Radiative Transfer*, Jan2017, Vol. 187, p247-254. 8p. DOI: 10.1016/j.jqsrt.2016.10.001.

Direct Determination of Oxidation States of Uranium in Mixed-Valent Uranium Oxides Using Total Reflection X-ray Fluorescence X-ray Absorption Near-Edge Spectroscopy. Sanyal, Kaushiki; Khooha, Ajay; Das, Gangadhar; Tiwari, M. K.; Misra, N. L. *Analytical Chemistry*. 1/3/2017, Vol. 89 Issue 1, p871-876. 6p. DOI: 10.1021/acs.analchem.6b03945.

Small-angle X-ray and light scattering analysis of multi-layered Curdlan gels prepared by a diffusion method. Maki, Natsuyuki; Furusawa, Kazuya; Dobashi, Toshiaki; Sugimoto, Yasunobu; Wakabayashi, Katsuzo. *Carbohydrate Polymers*. Jan2017, Vol. 155, p136-145. 10p. DOI: 10.1016/j.carbpol.2016.08.061.

Three-dimensional Morphology and X-ray Scattering Structure of Aqueous Iso†-Butanol Mixtures: A Molecular Dynamics Study. Kaur, Supreet; Kashyap, Hemant. *Journal of Chemical Sciences*. Jan2017, Vol. 129 Issue 1, p103-116. 14p. DOI: 10.1007/s12039-016-1207-9.

Enhancing primary processing for small-angle X-ray scattering. Wei, Yanru; Li, Zhihong. *Instrumentation Science & Technology*. 2017, Vol. 45 Issue 1, p22-34. 13p. DOI: 10.1080/10739149.2016.1205084.

X-ray diffraction and Raman studies on Bi$_2$O$_3$-ZnO$_2$. K.A., Irshad; N.V., Chandra Shekar; T.R., Ravindran; V., Sithari; Pandey, K.K. *Journal of Molecular Structure*. Jan2017, Vol. 1128, p325-329. 5p. DOI: 10.1016/j.molstruc.2016.08.077.

Effect of reverted austenite on tensile and impact strength in a martensitic stainless steel-An in-situ X-ray diffraction study. Wessner, Manfred; Gamsjäger, Ernst; van der Zwaag, Sybrand; Angerer, Paul. *Materials Science & Engineering: A*. Jan2017, Vol. 682, p117-125. 9p. DOI: 10.1016/j.msea.2016.11.039.

Initial stages of Pt(111) electrodeposition: dynamic and structural studies by surface X-ray diffraction. Dinac, Jakub; Ruge, Martin; Rakowski, Finn; Rahn, Björn; Carla, Francesco; Felici, Roberto; Stettner, Jochim; Magnussen, Olaf M.; Harrington, David A. *Electrochimica Acta*. Jan2017, Vol. 224, p220-227. 8p. DOI: 10.1016/j.electacta.2016.12.028.

Using Similarity Metrics to Quantify Differences in High-Throughput Data Sets: Application to X-ray Diffraction Patterns. Hernández-Rivera, Efraín; Coleman, Shawn P.; Tschopp, Mark A. *ACS Combinatorial Science*. 1/9/2017, Vol. 19 Issue 1, p25-36. 12p. DOI: 10.1021/acscombsci.6b00142.

Texture evolution of orthorhombic α″ titanium alloy investigated by in situ X-ray diffraction. Elmay, W.; Berveiller, S.; Patoor, E.; Gloriant, T.; Prima, F.; Lahuerte, P. *Materials Science & Engineering: A*. Jan2017, Vol. 679, p504-515. 7p. DOI: 10.1016/j.msea.2016.10.072.

Artificial peaks in energy dispersive X-ray spectra: sum peaks, escape peaks, and diffraction peaks. Tanaka, Ryohei; Yuge, Koretaka; Kawai, Jun; Akawaldi, Hussain. *XRS: X-ray Spectrometry*. Jan/Feb2017, Vol. 46 Issue 1, p5-11. 7p. DOI: 10.1002/xrs.2697.

Crystal structure of dirubidium hydrogen citrate from laboratory X-ray powder diffraction data and DFT comparison. Rammohan, Alagappa; Kaduk, James A. *Acta Crystallographica: Section E*. 2017, Vol. 73 Issue 1, p69-73. 5p. DOI: 10.1107/S2056989016020166.

Characterization of Synthesized and Commercial Forms of Magnesium Stearate Using Differential Scanning Calorimetry, Thermogravimetric Analysis, Powder X-Ray Diffraction, and Solid-State NMR Spectroscopy. Delaney, Sean P.; Nethercott, Matthew J.; Hou, Christopher J.; Winquist, Nickolas T.; Arthur, Donia; Calahan, Julie L.; Sethi, Manish; Pardue, Daniel S.; Jungbunn Kim; Amidon, Gregory; Munson, Eric J. *Journal of Pharmaceutical Sciences*. Jan2017, Vol. 106 Issue 1, p338-347. 10p. 8 Graphs. DOI: 10.1016/j.xphs.2016.10.004.

Structure and thermal expansion of ($Cr_{1-x}V_x)_{n+1}AlC_n$ phases measured by X-ray diffraction. Halim, Joseph; Charter, Patrick; Basyuk, Tatyana; Prikhna, Tatyana; Caspi, El'ad N.; Barsoum, Michel W.; Caliovich, Thierry. *Journal of the European Ceramic Society*. Jan2017, Vol. 37 Issue 1, p15-21. 7p. DOI: 10.1016/j.jeurceramsoc.2016.07.022.

X-ray diffraction line profile analysis of nanostructured nickel oxide: Shape factor and convolution of crystallite size and microstrain contributions. Mansimar, K.; Madhu, G.; Biju, V. *Physica E*. Jan2017, Vol. 85, p224-232. 9p. DOI: 10.1016/j.physe.2016.08.024.

Development of a full micro-scale spatially offset Raman spectroscopy prototype as a portable analytical tool. Realini, Marco; Conti, Claudia; Botteon, Alessandra; Colombo, Chiara; Matousek, Pavel. *Analyst*. 1/21/2017, Vol. 142 Issue 2, p351-355. 5p. DOI: 10.1039/c6an02476j.

Temperature-controlled portable Raman spectroscopy of photothermally sensitive pigments. Ostrooki, I.; Mencaglia, A.A.; Siano, S. *Sensors & Actuators B: Chemical*. Jan2017, Vol. 238, p772-778. 7p. DOI: 10.1016/j.snb.2016.07.104.

X-ray micro computed tomography for characterization of cellular SiC foams for their applications in chemical engineering. Ou, Xiaoxia; Zhang, Xun; Lowe, Tristan; Blanc, Remi; Rad, Mansoureh Norouzi; Wang, Ying; Batal, Nelly; Pham, Charlotte; Shokri, Nima; Garforth, Arthur A.; Withers, Philip J.; Fan, Xiaolei. *Materials Characterization*. Jan2017, Vol. 123, p20-28. 9p. DOI: 10.1016/j.matchar.2016.11.013.

Generation of a realistic 3D seed assembly using X-ray micro-computed tomography and spherical harmonic-based principal component analysis. Zhou, B.; Wang, J. *International Journal for Numerical & Analytical Methods in Geomechanics*. Jan2017, Vol. 41 Issue 1, p93-109. 17p. DOI: 10.1002/nag.2548.

Measurement of Carbon Condensates Using Small-Angle X-ray Scattering During Detonation of High Explosives. Willey, T. M.; Bagge-Hansen, M.; Lauderbach, L.; Hodgin, R.; Hansen, D.; Ilavsky, J.; Benterou, T.; Dattelbaum, D. M.; Gustavsen, R. L.; Watkins, E. B.; Firestone, M. A.; Jensen, B. J.; Graber, T.; Bastea, S.; Fried, L. *AIP Conference Proceedings*. 1/10/2017, Vol. 1793, p1-5. 5p. 1 Diagram, 2 Graphs. DOI: 10.1063/1.4971470.