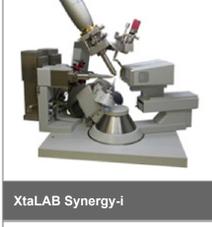




橋 THE BRIDGE
MATERIALS ANALYSIS eNEWSLETTER
MAY 2018, ISSUE 59

An upgradeable single crystal X-ray diffractometer for structural analysis of small molecule samples



XtaLAB Synergy-i

The XtaLAB Synergy-i single crystal X-ray diffractometer includes a high-flux, low-maintenance microfocus sealed tube source, a high-precision 4-circle kappa goniometer and one of Rigaku's own Hybrid Photon Counting (HPC) X-ray detectors, the HyPix Bantam. Containing the latest microfocus source technology the XtaLAB Synergy-i can be upgraded to dual source (Cu/Mo) to address a wider range of research interests. For ease of use and high performance, the system is controlled by the fully-integrated, user-inspired CrysAlis^{Pro} software package, which is capable of collecting and processing data efficiently and accurately, so you achieve the best data possible. **For more >**

Interested in publishing your work in The Bridge?



Publish Your Work Here

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

MiniFlex – qualitative and quantitative analysis of polycrystalline materials



Benchtop X-ray diffraction (XRD) instrument

New sixth generation MiniFlex X-ray diffractometer (XRD) is a multipurpose analytical instrument that can determine: phase identification and quantification, percent (%) crystallinity, crystallite size and strain, lattice parameter refinement, Rietveld refinement, and molecular structure. It is widely used in research, especially in material science and chemistry, as well as in industry for research and quality control. It is the newest addition to MiniFlex series of benchtop X-ray diffraction analyzers from Rigaku, which began with the introduction of the original MiniFlex system decades ago. **For more >**

Video of the Month



Mission to Minamata

The Minamata Convention on Mercury is a global treaty to protect human health and the environment from the adverse effects of mercury. It was agreed at the fifth session of the Intergovernmental Negotiating Committee on mercury in Geneva, Switzerland at 7 a.m. on the morning of Saturday, 19 January 2013 and adopted later that year on 10 October 2013 at a Diplomatic Conference (Conference of Plenipotentiaries), held in Kumamoto, Japan.

The Minamata Convention entered into force on 16 August 2017, on the 90th day after the date of deposit of the 50th instrument of ratification, acceptance, approval or accession.

The Convention draws attention to a global and ubiquitous metal that, while naturally occurring, has broad uses in everyday objects and is released to the atmosphere, soil and water from a variety of sources. Controlling the anthropogenic releases of mercury throughout its lifecycle has been a key factor in shaping the obligations under the Convention.

Major highlights of the Minamata Convention include a ban on new mercury mines, the phase-out of existing ones, the phase out and phase down of mercury use in a number of products and processes, control measures on emissions to air and on releases to land and water, and the regulation of the informal sector of artisanal and small-scale gold mining. The Convention also addresses interim storage of mercury and its disposal once it becomes waste, sites contaminated by mercury as well as health issues. **Watch video >**

Conferences and Workshops



Join Rigaku at future meetings

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

4th International Congress on 3D Materials Science (3DMS 2018)
Elsinore, Denmark
June 10 – 13, 2018

Synchrotron Radiation Instrumentation (SRI 2018)
Taipei, Taiwan
June 11 – 13, 2018

ACHEMA 2018
Frankfurt am Main, Germany
June 11 – 15, 2018

See the complete list >

Useful Link of the Month

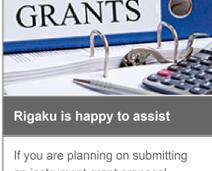


Pepsi-SAXS

Pepsi-SAXS

A new method called Pepsi-SAXS is presented that calculates small-angle X-ray scattering profiles from atomistic models. The method is based on the multiple expansion scheme and is significantly faster compared with other tested methods. In particular, using the Nyquist-Shannon-Kotelnikov sampling theorem, the multiple expansion order is adapted to the size of the model and the resolution of the experimental data. It is argued that by using the adaptive expansion order, this method has the same quadratic dependence on the number of atoms in the model as the Debye-based approach, but with a much smaller prefactor in the computational complexity. **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 X-ray crystallography. **Join us >**

Welcome

As always, thanks to everyone who took the time to come and talk to us at Ceramics Expo 2018, as well as all of the other events that we attended in May. In June, Rigaku will attend many events worldwide ([see full list](#)). Of particular note are the Synchrotron Radiation Instrumentation (SRI 2018) exhibit in Taipei (June 11 – 13, booth #3SH2) and the European Conference on X-Ray Spectrometry 2018 in Ljubljana (June 24 – 29).

We are pleased to announce that Rigaku Corporation was recognized by [The Nature Index](#) as a Top Corporate Institution. The Nature Index is a database of information by author affiliation, collated from research articles published in an independently selected group of 68 renowned science journals. The database is compiled by the publishers of *Nature*, a leading weekly, international scientific journal. The Nature Index provides a close to real-time proxy for high-quality research output at the institutional, national and regional level.

Included in this month's edition is a special report from your humble editor regarding a recent International Distributors Meeting by [Nippon Instruments Corporation](#), Rigaku's mercury analysis division. The report chronicles the meeting and a special field trip to [Minamata, Japan](#), site of an environmental disaster that was first recognized in 1956.

This month's issue contains a featured new product: real-time search & match with Rigaku's SmartLab Studio II and a contributed article from Dr. Cameron Chai on hybrid pixel counting detectors.



Rigaku Yamanashi factory during May. Photos by Masa Watanabe, Rigaku Corporation.

Application papers are also available for XRD, USAXS, EDXRF, and WDXRF. The book review covers *Leonardo da Vinci* by Walter Isaacson. Check out the news and papers sections at the bottom of the page for the latest developments in materials science.

R.C. Tisdale, Ph.D. – Editor

Featured New Product

Real-time search & match with Rigaku's SmartLab Studio II
New integrated software package for SmartLab systems

SmartLab Studio II, a new integrated X-ray measurement and analysis software, incorporates a new search & match feature. It is a "real-time search & match" ([see online video](#)). During data collection, search & match algorithm provides the candidates of phases in the sample based on the peaks detected in the ongoing measurement. **Full article >**

Special Report

NIC International Distributors Meeting & Minamata Disease.
Article by Dr. Tisdale, Rigaku Corporation

Nippon Instruments Corporation (NIC) – a division of the Rigaku Corporation – held their biennial International Distributors Meeting from the 23rd to the 26th of April at the Hakata Excel Hotel Tokyu in Fukuoka, Japan. Founded in 1978, NIC designs and manufactures mercury (Hg) analyzers based on atomic absorption (AA) or atomic fluorescence (AF) spectrometric technologies. **Full article >**

Featured Article

Hybrid Pixel Counting Detectors
Article by Dr. Cameron Chai, AXT

AXT, a Rigaku distributor, recently published an article on Hybrid Pixel Counting (HPC) detectors in the *Australian X-ray Analytical Association Newsletter*. HPC detectors are next generation semiconductor detectors that directly measure all photons generated by your samples. They are the optimal hardware partner for researchers involved in diffraction experiments. **Full article >**

XRD Application Note

Measurement of Bulk Samples – Brake Pad of a Motorcycle
Rigaku Corporation

Bulk samples such as metal blocks, ceramic sintered bodies, or pharmaceutical tablets are aggregates of microcrystals that can be measured by powder X-ray diffraction. With Rigaku's bulk sample holder, thick bulk samples can be easily placed in the diffractometer without any need to cut or pulverize, making it possible to identify crystal phases of bulk surfaces in a non-destructive manner. **For more >**

USAXS Application Note

Average Particle Size and Size Distribution Analysis of Pigment Ink by Ultra-Small-Angle X-ray Scattering
Rigaku Corporation

Pigments are used in various fields, such as paints, inks, cosmetics, foodstuffs, and so on. Among them, pigment ink has been used as the color component of inkjet printer ink for a long time because of its characteristics of high color stability, lightfastness, and gradation etc. Determining the primary particle size and size distribution of pigment ink is one of the most important processes in the pigment ink industry. In this application note, we illustrate the particle sizes and the size distributions of pigment inks analyzed from scattering profiles obtained by Ultra-Small-Angle X-ray Scattering (USAXS). **For more >**

EDXRF Application Note

Additive Elements in Lubricating Oils – ASTM D7751
Applied Rigaku Technologies

Controlling additive elements when blending new, fresh lubricating oils is vital to ensure correct lubrication properties and minimizing production waste and product rejection. Rigaku NEX CG offers compliance to D7751 Standard Test Method for Additive Elements in Lubricating Oils by EDXRF Analysis. **For more >**

WDXRF Application Note

Determination of Metals in Copper Concentrate by Advanced Correction Method for Fused Beads
Rigaku Corporation

Global copper supply and consumption has been growing in the past few decades. Copper is one of the important base metals for development of modern nations and it plays a significant role as an essential industrial material for construction, electronics, machinery, transportation and so on. This application note introduces an advanced correction technique for fusion method and application for copper concentrate analysis. **For more >**

Book Review

Leonardo da Vinci by Walter Isaacson
Review by Jeanette S. Ferrara, MA

Walter Isaacson's latest biography is an intimate venture into the life of Leonardo da Vinci: artist, sculptor, engineer, inventor, and even, one might argue, amateur coroner. **Full review >**

Material Analysis in the News

News for May 2018

May 2, 2018. Researchers led by Dr. Satoru Masubuchi at the University of Tokyo, Japan have created a [robot that can automatically assemble two-dimensional \(2D\) crystalline materials](#). Van der Waals heterostructures, which are assemblies of atomically thin 2D crystalline materials, are of interest in nanotechnology for their attractive conduction properties.

May 3, 2018. Researchers working on inorganic perovskites at the Energy Materials and Surface Sciences Unit at the Okinawa Institute of Science and Technology Graduate University (OIST) in Japan have found that [doping with manganese can significantly improve](#) the performance of wholly inorganic perovskite solar cells.

May 3, 2018. A mineral that requires the [presence of water to form has been discovered in a lunar meteorite](#). A team of Japanese scientists led by Masahiro Kayama at Tohoku University found the mineral, called moganite, in a lunar meteorite discovered in a desert in northwest Africa.

May 8, 2018. A research team led by Dr. Atsuko Kobayashi at Tokyo Institute of Technology (Tokyo Tech) has reported that magnetite (Fe₃O₄) particles (~50 nm in size, dispersed in pure water) which are [mechanically flocculated by external oscillating magnetic fields could disturb the water/crystal interface](#) and promote supercooling during the freezing process.

May 8, 2018. Researchers at The University of Tokyo's Institute of Industrial Science have successfully [created chiral nanostructures from particles of gold \(Au\)](#). The trick was to use circularly polarized (CP) light to generate electric fields, which localize differently depending on left CP or right CP. This in turn drove the chiral deposition of a dielectric material.

May 10, 2018. Scientists led by Professor Susumu Kitagawa at Kyoto University in Japan have created a [porous metal organic crystal that can change and retain its shape](#) depending on the prevailing conditions. Using single-crystal X-ray diffraction, the team studied the crystals' structure.

May 16, 2018. Japan's government proposed an energy plan Wednesday that sets [ambitious targets for nuclear energy use](#) in the coming decade despite challenges after the 2011 Fukushima disaster.

May 16, 2018. A trio of researchers centered at the Institute of Industrial Science at The University of Tokyo recently investigated [glass-forming behavior by simulating two model systems](#) whose glass-forming ability could be tuned by a single external parameter.

May 17, 2018. Researchers from Tokyo Metropolitan University and Shimane University have created a transparent hybrid film that combines natural clay minerals and dyes into a [material that changes color in response to environmental humidity](#). The color change does not involve breaking chemical bonds.

Recent Scientific Papers of Interest

Papers for May 2018

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

Authentication of two samples of ancient Chinese coins with component element depth analysis by confocal 3D XRF. Zhou, Peng; Liu, Zhiguo; Lin, Xiaoyan; Liu, Xin; Ye, Lei; Wang, Xingyi; Pan, Kai; Li, Yude. *Nuclear Instruments & Methods in Physics Research Section B*. May2018, Vol. 423, p37-41. 5p. DOI: [10.1016/j.nimb.2018.03.007](#).

Stretching-Induced Uniform Micropores Formation: An In Situ SAXS/WAXS Study. Caihong Lei; Ruijie Xu; Ziqin Tian; Henghui Huang; Jiayi Xie; Xiangqi Zhu. *Macromolecules*. 5/8/2018, Vol. 51 Issue 9, p3433-3442. 10p. DOI: [10.1021/acs.macromol.7b02335](#).

Simultaneous WAXS/SAXS study on semi-crystalline Poly(ethylene furanoate) under uniaxial stretching. Mao, Yimin; Bucknall, David G.; Krieger, Robert M. *Polymer*. May2018, Vol. 143, p228-236. 9p. DOI: [10.1016/j.polymer.2018.04.018](#).

A General Approach to Access Protocols of Polyoxometalates in Solution by Using SAXS: An Ab Initio Modeling Method. Li, Mu; Wang, Weiyou; Yin, Panchoa. *Chemistry – A European Journal*. 5/2/2018, Vol. 24 Issue 25, p6639-6644. 6p. DOI: [10.1002/chem.201800344](#).

Inter-technique comparison of PIXE and XRF for JAAS (Journal of Analytical Atomic Spectrometry). May2018, Vol. 33 Issue 5, p883-892. 10p. DOI: [10.1039/c8ja00019k](#).

Identifying the source of fluvial terrace deposits using XRF scanning and Canonical Discriminant Analysis: A case study of the Chihshang Chen reservoirs, eastern Taiwan. Chang, Queenie; Lin, Jian-Cheng; Hsiung, Jyh-Jaan; Wei, Kuo-Yen; Chen, Yue-Gau; Byrne, Timothy B. *Geomorphology*. May2018, Vol. 308, p204-214. 11p. DOI: [10.1016/j.geomorph.2018.02.011](#).

MA-XRF investigation of the Altenberg Retable from 1330. Hoffmann, P.; Flege, S.; Essinger, W.; Wolf, F.; Weber, C.; Seeborg, S.; Sander, J.; Schultz, J.; Kregel, R.; Wittkopf, A. *XRS: X-ray Spectrometry*. May/June2018, Vol. 47 Issue 3, p215-222. 8p. DOI: [10.1002/xrs.2829](#).

Prototype GaAs X-ray detector and preamplifier electronics for a deep seabed mineral XRF spectrometer. Loliou, G.; Barnett, A. M. *XRS: X-ray Spectrometry*. May/June2018, Vol. 47 Issue 3, p201-214. 14p. DOI: [10.1002/xrs.2818](#).

XRF characterization and source apportionment of PM10 samples collected in a coastal city. Manoyakas, M.; Diaphyllou, E.; Papaefthymiou, H.; Kantarelou, V.; Zarkadas, C.; Kalogridis, A.-C.; Karydas, A.-G.; Eleftheriadis, K. *XRS: X-ray Spectrometry*. May/June2018, Vol. 47 Issue 3, p190-200. 11p. DOI: [10.1002/xrs.2817](#).

Biochemical characterization, low-resolution SAXS structure and an enzymatic cleavage pattern of BICel48 from *Bacillus licheniformis*. de Araujo, Evandro; Manzi, Livia Regina; Piadov, Vassili; Kadowlak, Marco Antonio; Seiki; Polikarpov, Igor. *International Journal of Biological Macromolecules*. May2018, Vol. 111, p302-310. 9p. DOI: [10.1016/j.ijbiomac.2017.12.138](#).

In situ macro X-ray fluorescence (MA-XRF) scanning as a non-invasive tool to probe for subsurface modifications in paintings by P.P. Rubens. Legrand, Stijn; Janssens, Koen; Van der Snickt, Geert; Slama, Ina; Gruber, Gerlinde; Oberhaier, Elke; Van Zuiwen, Eva; Van der Stighelen, Katlijne; Keens, Lize. *Microchemical Journal*. May2018, Vol. 138, p238-245. 8p. DOI: [10.1016/j.microc.2018.01.019](#).

The illuminated manuscript Corale 43 and its attribution to Beato Costanzo: Non-invasive analysis by FORS, XRF and hyperspectral imaging techniques. Cuccì, Costanza; Casini, Andrea; Innocenti, Silvia; Piccolo, Marcello; Stefani, Lorenzo; Bracci, Susanna; Rao, Ida Giovanna; Scudierri, Magnolia. *Microchemical Journal*. Vol. 138, p45-57. 13p. DOI: [10.1016/j.microc.2017.12.021](#).

Study of short range structure of amorphous Silica from PDF using Ag radiation in laboratory XRD system, RAMAN and NEXAFS. Biswas, Ripan K.; Khan, Prosenjit; Mukherjee, Smriti; Mukhopadhyay, Anoop K.; Ghosh, Jiten; Muraliedharan, K. *Journal of Non-Crystalline Solids*. May2018, Vol. 488, p1-9. 9p. DOI: [10.1016/j.jnoncrysol.2018.02.037](#).

Role of defectivity on the crystallography of martensitic transformations in Ti₅₀Ni₄₀Cu₁₀: an XRD investigation. Coduri, Mauro; Biffi, Carlo A.; Bassani, Paola; Tuisi, Ausonio. *Zeitschrift für Kristallographie*. Crystalline Materials. May2018, Vol. 233 Issue 5, p337-348. 12p. DOI: [10.1515/zkri-2017-2096](#).

Investigation of heavy metal distributions along 15 m soil profiles using EDXRF, XRD, SEM-EDX, and ICP-MS techniques. Özen, Songül Akbulut; Ozkalayci, Fatih; Çevik, Ugur; Van Grieken, Rene. *XRS: X-ray Spectrometry*. May/June2018, Vol. 47 Issue 3, p231-241. 11p. DOI: [10.1002/xrs.2832](#).

XRD, SEM/EDX and micro-Raman spectroscopy for mineralogical and chemical characterization of iron slags from the Roman archaeological site of Forca (Biscay, North Spain). Portillo, Haizea; Zuluaga, Maria Cruz; Ortega, Luis Angel; Alonso-Olazabal, Ainhoa; Murelaga, Xabier; Martínez-Salcedo, Ana. *Microchemical Journal*. May2018, Vol. 138, p246-254. 9p. DOI: [10.1016/j.microc.2018.01.020](#).

Inelastic X-ray scattering of RTA₃ (R = La, Ce, T = Cu, Au). Tsutsui, Satoshi; Kaneko, Koji; Pospisil, Jiri; Haga, Yoshinori. *Physica B*. May2018, Vol. 536, p24-27. 4p. DOI: [10.1016/j.physb.2017.09.087](#).

Assessment of collagen fiber orientation dispersion in articular cartilage by small-angle X-ray scattering and diffusion tensor imaging: Preliminary results. Tadimalla, Sirisha; Tourel, Monique C.; Knott, Robert; Momot, Konstantin I. *Magnetic Resonance Imaging*. May2018, Vol. 48, p115-121. 7p. DOI: [10.1016/j.mri.2017.12.032](#).