Rigaku
Leading With Innovation

X-ray Diffraction & Elemental Analysis

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 >**

Interested in publishing your work in The Bridge?

Welcome

To begin 2019, please come visit us at the Florida Hazmat Conference (Jan. 15 – 17 in Daytona Beach), SEPEM Industries (Jan. 29 – 31 in Douai, France), and the National Narcotics Officers Association conference (Feb. 3 – 6 in D.C.).

Wishing you and your family health and prosperity for the New Year! We look forward to working with you in 2019.

A warm thanks to all who attended AsCA 2018/CRYSTAL 32, a combined conference of the Asian Crystallographic Association (AsCA) and the Society of Crystallographers in Australia and New Zealand (SCANZ) at the beginning of December. A few images below highlight the Rigaku booth and our friends down under.

The featured article this month was contributed by AXT and covers the *Examination of Bauxite Dehydroxylation Using In Situ XRD*. We also highlight a recent AXT press release.

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 email copy to the editor.

This month's featured XRD technical note discusses high-speed *in-situ* measurement of the Al metal melting process. The WDXRF application note discusses the measurement of trace elements in water using the "Ultra Carry" method while the EDXRF note covers the quantification of Co, Br and Mn in TPA and PTA.

The book review covers *The Tangled Tree: A Radical New History of Life* by David Quammen. Check out the new "advantage series video" covering the NEX DE VS energy dispersive X-ray fluorescence spectrometer. And, as always, the news and papers sections are at the bottom of the page for a taste of the latest developments in materials science.

R.C. Tisdale, Ph.D. – Editor

Featured Article

Examination of Bauxite Dehydroxylation Using In Situ XRD

By Hong Peng, James Vaughn and Cameron Chai

Bauxite is the primary raw materials used in the manufacture of aluminium. Australia produced 74.9 million tonnes of bauxite in 2011 accounting for 32% of global production in 2011, making us the largest producer in the world. To make aluminium, bauxite is first converted to alumina via the Bayer Process. Alumina can then be smelted into aluminium using the Hall-Heroult electrochemical process. The Bayer Process involves multiple steps to convert bauxite to alumina. One of these steps is digestion of the bauxite in hot caustic soda. It has been proposed that thermal activation of bauxite could enable this digestion process to take place at a lower temperature and that it would also reduce the organic content of resultant liquor. **Full article >**

Recent Press Release

University of Sydney First to Install a 6th Gen MiniFlex XRD in Australia

AXT Pty Ltd, a Rigaku Distributor

The University of Sydney has installed a new generation X-Ray Diffractometer (XRD) as a teaching tool within the School of Chemistry. The XRD is the sixth generation of Rigaku's MiniFlex benchtop instruments and will help prepare students for practical skills in industry and provide capacity to produce research-grade data for materials characterisation. The XRD was installed in partnership between the School of Chemistry and Sydney Analytical. **Full article >**

XRD Application Note

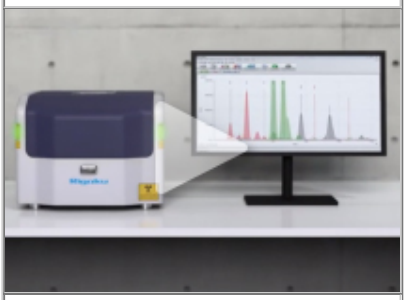
High-speed in-situ measurement of Al metal melting process

Rigaku Corporation

To capture the moment when materials change, such as during melting, solidification or crystal phase change, by *in-situ* X-ray diffraction measurement, the acquisition time of the X-ray diffraction images at each temperature needs to be as short as possible. 0D and 1D detectors take time to scan the detector and prepare for operation. Conventional 2D detectors also have a problem in that the X-ray shutter needs to be opened and closed between counting and reading the data. The HyPix-3000 hybrid pixel array multi-dimensional detector in 2D mode can acquire X-ray diffraction images without scanning the detector. The HyPix-3000 has two counters inside. Switching between them allows measurement without dead time. These features enable shutterless measurement of 2D X-ray diffraction images, which makes it possible to observe rapid changes in crystalline state. **For more >**

resolution and lower limits-of-detection (LLD). **For more >**

Video of the Month



NEX DE VS

A high performance small (variable) spot benchtop EDXRF elemental analyzer, the Rigaku NEX DE VS delivers wide elemental coverage with a easy-to-learn Windows®-based QuantEZ software. Small spot analysis, from sodium (Na) through uranium (U), of almost any matrix - from solids, thin films and alloys to powders, liquids and slurries. **Watch video >**

Conferences and Workshops

Join Rigaku at future meetings

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

Florida Hazmat Conference
Daytona Beach, FL, US
January 15 – 17, 2019

Sepem Industries
Douai, France
January 29 – 31, 2019

WDXRF Application Note

Trace Element Analysis of Water Solution by Micro-Droplet Method Using "Ultra Carry" Filter Paper

Rigaku Corporation

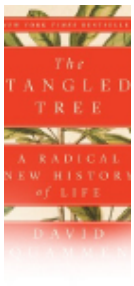
The influence on the environment of trace heavy elements such as Cd, Pb, As, Cr, Se, etc. in water is considered a serious social problem. In order to control this problem, it is essential to monitor water quality. Considering the large number of test samples required for assessment of water quality, the test method should be simple, rapid, and reproducible. X-ray fluorescence (XRF) analysis has many positive features, such as simple sample preparation, short analysis time, and high repeatability with low human error, compared to other elemental analysis methods, such as ICP-OES or AA. XRF is the best method for the above test. **For more >**

EDXRF Application Note

Co, Br, Mn in TPA and PTA

Applied Rigaku Technologies

The Rigaku NEX OL offers a simple and low maintenance on-line analytical technique for trending your process streams. Results are communicated to your plant DCS (distributed control system) via 4-20 mA current loops or MODBUS over Ethernet connection allowing for real time closed loop control. This application note demonstrates on-line measurement of cobalt (Co), bromine (Br) and manganese (Mn) in terephthalic acid (TPA). **For more >**

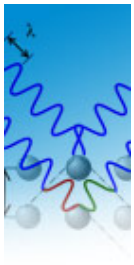


Book Review

The Tangled Tree: A Radical New History of Life

By David Quammen

David Quammen's *The Tangled Tree* is an absolute delight. In many ways, it feels like a biography of Carl Woese, the microbiologist who defined the domain of Archaea in 1977. Despite over 40 years having passed since then, Woese's definition challenged our fundamental understanding of evolutionary biology. **Read review >**



Material Analysis in the News

News for December 2018

December 1, 2018. Scientists explained how a particular phase-change memory (PCM) material can work much times faster and more durably than current flash computer memory. The basic idea and material were invented by Stanford Ovshinsky in 1975, but applications have lingered due to lack of clarity about how the material can execute the phase changes on such short time scales and technical problems related to controlling the changes with necessary precision.

December 3, 2018. A research team at Osaka University, Japan, has drawn inspiration from living cells to create a material that could improve the safety of rechargeable batteries while lowering their manufacturing costs.

December 3, 2018. Physicists from the Moscow Institute of Physics and Technology (MIPT) and Lomonosov Moscow State University have combined thermal analysis and X-ray scattering – two techniques for studying crystal structure – in one experimental setup to investigate semicrystalline polymers.

National Narcotics Officers Assocation Conference
Washington, D. C., US
February 3 – 6, 2019

See the complete list >

Useful Link of the Month

Whitehead BaRC public tools

Whitehead BaRC public tools consists of:

- Compare two lists
- Compare three lists
- Redundant list analysis
- Venn Diagram Generator (2-way)
- Venn Diagram Generator (3-way)
- UTR extractor
- Protein sequence visualization

Located in Cambridge, Massachusetts, Whitehead Institute was founded in 1982 by visionary industrialist and philanthropist Edwin C. “Jack” Whitehead, who was driven by a single vision: to assemble a cadre of the world's finest biomedical researchers under one roof and eliminate virtually any impediment to their pursuit of scientific discovery. He sought to create a wholly independent, self-governing institution with a close affiliation with a leading research university. His plans came to fruition with the help of Massachusetts Institute of Technology (MIT) biology professor and Nobel Laureate David Baltimore, who worked to structure an affiliation agreement with MIT and who would become Whitehead

December 4, 2018. Researchers with the Department of Energy's Oak Ridge National Laboratory have demonstrated a new level of control over photons encoded with quantum information. Research scientists with ORNL's Quantum Information Science Group, performed distinct, independent operations simultaneously on two qubits encoded on photons of different frequencies, a key capability in linear optical quantum computing.

December 5, 2018. What is X-ray spectroscopy? There are several different X-ray spectroscopy methods that are used in many disciplines of science and technology, including archaeology, astronomy and engineering.

December 6, 2018. Based on a rarely used X-ray visualization technique called COBRA, (coherent Bragg rod analysis) originally developed by a group in Israel, a team of materials scientists from Penn State, Cornell and Argonne National Laboratory have figured out how to expand and modify the technique to analyze one of the most complicated, least symmetrical material systems studied to date. This system is a strained three-dimensional perovskite crystal with octahedral tilts in all directions, grown on another equally complex crystal structure.

December 7, 2018. Led by researchers at Monash University, an experiment conducted at the U.S. Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) has demonstrated, for the first time, electronic switching in an exotic, ultrathin material that can carry a charge with nearly zero loss at room temperature. Researchers demonstrated this switching when subjecting the material to a low-current electric field.

December 11, 2018. According to Pauling's rules, the fragments of the atomic lattice in inorganic materials are connected by vertices, because bonding by faces is the most energy-intensive way to form a chemical connection; therefore, it does not exist in nature. However, scientists have proved, both experimentally and theoretically, using NUST MISIS' supercomputer, that it is possible to form such a connections if the materials are at ultra-high pressure conditions. The obtained results open a completely new way in the development of modern materials science, showing that fundamentally new classes of materials exist at extreme conditions.

December 12, 2018. A team from Siberian Federal University modernized the Rietveld method to make it applicable for automated analysis. To do so, they developed a self-configuring evolutionary genetic algorithm – a program that uses the principle of biological natural selection to find optimal parameter values when modelling an X-ray image. First, a genetic algorithm uses random values, but then it optimizes the vast range of X-ray image and phase crystal structure parameters and manages the adjustment of only the best of them using the Rietveld method. Therefore, the algorithm is able to work without human involvement and self-learn.

December 13, 2018. Duke engineers have been tapped by the U.S. Department of Homeland Security to begin development of scanners that could soon become the standard in airports across the globe. The scanner will utilize a hybrid system combining the commonly-used X-ray technology with X-ray diffraction tomography.

December 13, 2018. Japan's space agency says more than 200 photos taken by two small rovers on an asteroid show no signs of a smooth area for the planned touchdown of a spacecraft early next year. Many of the photos show a rocky surface on the asteroid, presenting challenges for Hayabusa2's planned touchdown, which has already been postponed from late October after initial images showed the surface was rockier than expected.

Institute's Founding Director.

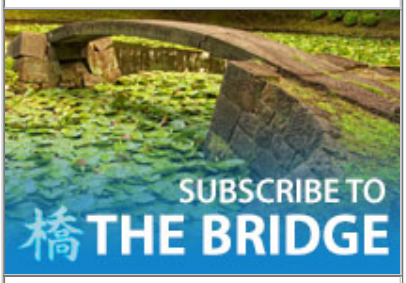
For more >

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 >**

December 13, 2018. Researchers led by Dr. Nobuhiko Hosono of Kyoto University's Institute for Integrated Cell-Material Sciences (iCeMS) in Japan were able to image the dynamic changes that occur on the surface of a porous coordination polymer in the presence of other molecules. In contrast to the common perception that crystals are hard and immobile, they were surprised to find that the porous coordination polymer surface is exceptionally flexible and constantly fluctuating in solution.

Recent Scientific Papers of Interest

Papers for December 2018

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

Applications of Powder X-Ray Diffraction in Small Molecule Pharmaceuticals: Achievements and Aspirations. Thakral, Naveen K.; Zanon, Roger L.; Kelly, Ron C.; Thakral, Seema. Journal of Pharmaceutical Sciences. Dec2018, Vol. 107 Issue 12, p2969-2982. 14p. DOI: 10.1016/j.xphs.2018.08.010.

Application of chemometric methods to XRF-data — A tutorial review. Panchuk, Vitaly; Yaroshenko, Irina; Legin, Andrey; Semenov, Valentin; Kirsanov, Dmitry. Analytica Chimica Acta. Dec2018, Vol. 1040, p19-32. 14p. DOI: 10.1016/j.aca.2018.05.023.

XRD and ATR/FTIR investigations of various montmorillonite clays modified by monocationic and dicationic imidazolium ionic liquids. Ahmed, A.; Chaker, Y.; Belarbi, El H.; Abbas, O.; Chotard, J.N.; Abassi, H.B.; Van Nhien, A. Nguyen; El Hadri, M.; Bresson, S. Journal of Molecular Structure. Dec2018, Vol. 1173, p653-664. 12p. DOI: 10.1016/j.molstruc.2018.07.039.

Emission and HR-XRD study of MBE structures with InAs quantum dots and AlGaInAs strain reducing layers. Torchynska, T.; Cisneros-Tamayo, R.; Vega-Macotela, L.; Polupan, G.; Escobosa-Echavarria, A. Superlattices & Microstructures. Dec2018, Vol. 124, p153-159. 7p. DOI: 10.1016/j.spmi.2018.10.005.

High-pressure angle-dispersive X-ray diffraction study of mechanically alloyed SnSe2. Borges, Z. V.; Poffo, C. M.; de Lima, J. C.; Souza, S. M.; Trichês, D. M.; de Biasi, R. S. Journal of Applied Physics. 12/7/2018, Vol. 124 Issue 21, pN.PAG-N.PAG. 11p. 2 Charts, 9 Graphs. DOI: 10.1063/1.5053220.

Optimized Compton fitting and modeling for light element determination in micro-X-ray fluorescence map datasets. O'Neil, L.P.; Catling, D.C.; Elam, W.T. Nuclear Instruments & Methods in Physics Research Section B. Dec2018, Vol. 436, p173-178. 6p. DOI: 10.1016/j.nimb.2018.09.023.

Time-resolved X-ray fluorescence analysis of element distribution and concentration in living plants: An example using manganese toxicity in cowpea leaves. Blamey, F. Pax C.; Paterson, David J.; Walsh, Adam; Afshar, Nader; McKenna, Brigid A.; Cheng, Miaomiao; Tang, Caixian; Horst, Walter J.; Menzies, Neal W.; Kopittke, Peter M. Environmental & Experimental Botany. Dec2018, Vol. 156, p151-160. 10p. DOI: 10.1016/j.envexpbot.2018.09.002.

Quantitative approaches to the determination of elements in lake sediments by total reflection X-ray fluorescence. Pashkova, Galina V.; Aisueva, Tatyana S.; Finkelshtein, Alexandr L.; Cherkashina, Tatyana Yu.; Shchetnikov, Alexandr A. Microchemical Journal. Dec2018, Vol. 143, p264-271. 8p. DOI: 10.1016/j.microc.2018.08.020.

Characterization of a 4-inch GaN wafer by X-ray diffraction topography. Kim, Jaemyung; Seo, Okkyun; Song, Chulho; Chen, Yanna; Hiroi, Satoshi; Irokawa, Yoshihiro; Nabatame, Toshihide; Koide, Yasuo; Sakata, Osami. CrystEngComm. 12/28/2018, Vol. 20 Issue 48, p7761-7765. 5p. DOI: 10.1039/c8ce01440j.

An analysis of orthopyroxene from Tsarev L5 meteorite using X-ray diffraction, magnetization measurement and Mössbauer spectroscopy. Maksimova, A.A.; Kamalov, R.V.; Chukin, A.V.; Felner, I.; Oshtrakh, M.I. Journal of Molecular Structure. Dec2018, Vol. 1174, p6-11. 6p. DOI: 10.1016/j.molstruc.2018.06.040.

Study of metallic Fe-Ni-Co alloy and stony part isolated from Seymchan meteorite using X-ray diffraction, magnetization measurement and Mössbauer spectroscopy. Oshtrakh, M.I.; Maksimova, A.A.; Goryunov, M.V.; Petrova, E.V.; Felner, I.; Chukin, A.V.; Grokhovsky, V.I. Journal of Molecular Structure. Dec2018, Vol. 1174, p112-121. 10p. DOI: 10.1016/j.molstruc.2018.06.039.

Non-conventional scans in high-resolution X-ray diffraction analysis of epitaxial systems. Dobrocka, E.; Hasenöhrl, S.; Chauhan, P.; Kuzmík, J. Applied Surface Science. Dec2018, Vol. 461, p23-32. 10p. DOI: 10.1016/j.apsusc.2018.07.009.

Fractal analysis of X-ray diffraction patterns of zirconia–alumina mixed oxides. Gordillo-Cruz, E.; Alvarez-Ramirez, J.; González, F.; de los Reyes, J.A. Physica A. Dec2018, Vol. 512, p635-643. 9p. DOI: 10.1016/j.physa.2018.08.057.

Poisson image denoising by piecewise principal component analysis and its application in single-particle X-ray diffraction imaging. Qiyu Jin; Osamu Miyashita; Florence Tama; Jie Yang; Jonic, Slavica. IET Image Processing. 2018, Vol. 12 Issue 12, p2264-2274. 11p. DOI: 10.1049/iet-ipr.2018.5145.

Misfit dislocations between boron-doped homoepitaxial films and diamond substrates studied by X-ray diffraction topography. González-Mañas, Marina; Vallejo, Beatriz. Journal of Applied Crystallography. Dec2018, Vol. 51 Issue 6, p1684-1690. 7p. DOI: 10.1107/S1600576718015388.

Quantitative X-ray diffraction of free, not chemically bound water with the PONKCS method. Scherb, Sebastian; Beuntner, Nancy; Thienel, Karl-Christian; Neubauer, Jürgen. Journal of Applied Crystallography. Dec2018, Vol. 51 Issue 6, p1535-1543. 9p. DOI: 10.1107/S1600576718012888.

Optimization of a table-top x-ray fluorescence computed tomography (XFCT) system. C A S Dunning; M Bazalova-Carter. Physics in Medicine & Biology. Dec2018, Vol. 63 Issue 23, p1-1. 1p. DOI: 10.1088/1361-6560/aaece9.