



# 橋 THE BRIDGE

**MATERIALS ANALYSIS eNEWSLETTER**  
 AUGUST 2018, ISSUE 62

## A multi-functional single crystal X-ray diffractometer for a wide range of crystallographic applications



### XtaLAB Synergy-DW

One source with two high-flux wavelengths is the foundation of the revolutionary XtaLAB Synergy-DW single crystal X-ray diffractometer. It combines the increased flux of a rotating anode X-ray source with the flexibility of two different wavelengths, making it ideal for laboratories exploring a wide range of research interests. **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](mailto:Rigaku.newsletter@Rigaku.com)

## MiniFlex – qualitative and quantitative analysis of polycrystalline materials



### Benchmark 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 the 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



### Rigaku XtaLAB Synergy-S

The new video highlights the XtaLAB Synergy-S. With single or dual microfocus X-ray sources, this state-of-the-art single crystal X-ray diffractometer delivers exceptional performance for all your crystallographic needs. **Watch video >**

## Conferences and Workshops



### Join Rigaku at future meetings

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

**XTOP 2018 (the 14th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging)**  
 Bari, Italy  
 Sept 2 – 7, 2018

**JASIS 2018**  
 Tokyo, Japan  
 Sept 5 – 7, 2018

**Canadian Mineral Analysts (CMA2018)**  
 Rossland, BC, Canada  
 Sept 9 – 13, 2018

**See the complete list >**

## Useful Link of the Month



### Babylon – Japanese to English Translation

If it is an online Japanese to English translator you need, or you need to cross check Google Translate, this Japanese to English translator is free. Babylon, the world's leading provider of language solutions, puts at your disposal an automatic translator for instant Japanese to English translation of single words and phrases. **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 the Denver X-ray Conference, the two microscopy conferences, and the ECM that we attended in July. Rigaku will attend many events worldwide ([see full list](#)) in September. Of particular note is the annual Japan Analytical & Scientific Instruments Show (JASIS) from September 5 – 7 at the [Makuhari Messe](#) convention center outside Tokyo. Please come visit and see our latest technologies, including the new SmartLab 9 kW XRD system.



Sunflower field near Rigaku Yamanashi factory. Photos by Masa Watanabe, Rigaku Corporation.

This month's issue contains both a featured article and an event. The article continues the discussion from last month on data visualization in XRD, while the featured event is a report on the 2018 Denver X-ray Conference.

This month's featured XRD app note, *Operando measurement of Li ion battery positive electrode in charge/discharge process*, will be presented at JASIS 2018. Such *operando* measurements are very important for advanced battery engineering.

Application papers are also available for WDXRF and EDXRF. The book review covers *Energy: A Human History* by Richard Rhodes. The link of the month opens an alternative to Google Translate that many may find useful. Check out our new video on the XtaLAB Synergy-S single crystal X-ray diffraction system. 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

**SmartLab Studio II: Data Visualization plugin #2 – In-situ measurements**  
 By Dr. Akito Sasaki, Rigaku Corporation

It is very important for researchers and engineers involved in materials development to understand structural changes of a material associated with an external environment. Until recently, there were no good tools to display charts of changing temperature or humidity data coupled to X-ray diffraction (XRD) measurements of a sample other than for a few types of data. The Data Visualization plugin of SmartLab Studio II displays both a chart of temperature and/or humidity and that of XRD data sets in one window. **Full article >**

## Featured Event

**Denver X-ray Conference 2018**  
 Reported by Kosuke Kawakyu, WDXRF Application Laboratory, Rigaku Corporation

The 67<sup>th</sup> annual Denver X-ray Conference (DXC) was held from August 6 – 10 in Westminster, Colorado, USA. Located about 15 km northwest of the state capitol Denver, aka the Mile High City, Westminster's elevation is also about 1600 meters. The profile of the Rocky Mountains that can clearly be seen in the distance was incorporated into the conference logo. **Full article >**

## XRD Application Note

**Operando measurement of Li ion battery positive electrode in charge/discharge process**  
 Rigaku Corporation

Lithium ion secondary batteries are widely used in small portable devices such as mobile phones. Research and development of lithium ion batteries for use in automobiles and larger machines is an active field. To develop lithium ion secondary batteries with high capacity, high stability and long life, it is essential to evaluate the stability of the positive electrode material during the charge/discharge process. **For more >**

## WDXRF Application Note

**Elemental determination of whole coal by the pressed powder method**  
 Rigaku Corporation

Coal is the most abundant source of energy amongst the remaining fossil fuels in the world. Coal production is classified into two groups based on its usage. Thermal (steam) coal is used for generation of electricity, whereas metallurgical (coking) coal is mainly used for production of steel. **For more >**

## EDXRF Application Note

**Metals and alloys**  
 Applied Rigaku Technologies

Standard and specialty alloys vary in metal composition to give the alloy its specific physical, mechanical and chemical properties. Analyzing alloy composition by XRF is important to ensure the proper alloy grade meets the needs for its specific use. **For more >**

## Book Review

**Energy: A Human History** by Richard Rhodes.  
 Review by Jeanette S. Ferrara, MA

Richard Rhodes's *Energy* is a must-read. Although the title is tad misleading—it is by no means a comprehensive history of the relationship between energy and humanity—*Energy* is a delightful take on the modern history of that relationship. **Read review >**

## Material Analysis in the News

### News for August 2018

**August 2, 2018.** Despite being only slightly less stable than calcite, aragonite almost never crystallizes from solution in ambient conditions. Fiona Meldrum and her colleagues at the University of Leeds in the UK have shown that the secret may be much simpler: confinement. They found that [aragonite crystallizes inside submicron-diameter pores](#) of arbitrary depth without any special additives and in amounts that depend only on the diameter of the pore.

**August 6, 2018.** Scientists at Tokyo Institute of Technology have addressed one of the major disadvantages of all-solid-state batteries by developing [batteries with a low resistance at their electrode/solid electrolyte interface](#). The fabricated batteries showed excellent electrochemical properties that greatly surpass those of traditional and ubiquitous Li-ion batteries; thereby, demonstrating the promise of all-solid-state battery technology and its potential to revolutionize portable electronics.

**August 7, 2018.** Crystals containing ruthenium atoms often exhibit distinctive properties that arise from ruthenium's excited electronic states. In these states, the electrons are located far from the nucleus, which allows them to interact with their own spins and with neighboring electrons in unexpected ways. Prof. Je-Geun Park at Seoul National University, South Korea, and colleagues have studied the ruthenium-based crystal Na<sub>2</sub>7Ru<sub>4</sub>O<sub>9</sub> with X-ray diffraction and found that its [electrons arrange themselves in an unusual pattern](#), which affects the material's bulk properties, such as resistivity.

**August 13, 2018.** University of California, Berkeley, chemists have proved that three carbon structures recently created by scientists in South Korea and Japan are in fact the [long-sought schwarzites](#), which researchers predict will have unique electrical and storage properties like those now being discovered in buckminsterfullerenes (buckyballs or fullerenes for short), nanotubes and graphene.

**August 15, 2018.** Researchers have shown how to shuttle lithium ions back and forth into the crystal structure of a quantum material, representing a new avenue for research and potential applications in batteries, "smart windows" and brain-inspired computers containing artificial synapses. The [research centers on a material called samarium nickelate](#), which is a quantum material, meaning its performance taps into quantum mechanical interactions.

**August 16, 2018.** An international team of researchers from Columbia University, the National Institute for Materials Science in Tsukuba, Japan and the Centre National de Recherche Scientifique (CNRS) in France used boron-nitride-encapsulated graphene to demonstrate a [new class of electronic materials](#). They report a major advance that may revolutionize the field, a "twistronic" device whose characteristics can be varied by simply varying the angle between two different 2D layers placed on top of one another.

**August 16, 2018.** Controlling the excited electronic states in luminescent systems remains a challenge in the development of fluorescent and phosphorescent dyes. Now, scientists in Japan have developed a [unique organic fluorophore](#) that changes its emission color without loss of efficiency when externally stimulated.

## Recent Scientific Papers of Interest

### Papers for August 2018

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

**Characterisation of structured and functionalised particles by small-angle X-ray scattering (SAXS).** Nirschl, Hermann; Guo, Xiaoli. *Chemical Engineering Research & Design: Transactions of the Institution of Chemical Engineers Part A*. Aug2018, Vol. 136, p431-446. 16p. DOI: [10.1016/j.cherd.2018.06.012](https://doi.org/10.1016/j.cherd.2018.06.012).

**Multivariate modeling of glaciomarine lithostratigraphy combining scanning XRF, multisensory core properties, and CT imagery: IODP Site U1419.** Penkrot, Michelle L.; Jaeger, John M.; Cowan, Ellen A.; St-Onge, Guillaume; Levay, Leah. *Geosphere*. Aug2018, Vol. 14 Issue 4, p1935-1960. 26p. DOI: [10.1130/GES01635.1](https://doi.org/10.1130/GES01635.1).

**Measurement of L XRF cross sections for elements with 33 ≤ Z ≤ 51 and their interpretation in terms of L<sub>i</sub> (i = 1–3) subshell vacancy decay parameters.** Duggal, Heena; Sharma, Veena; Kainth, H.S.; Kumar, Sanjeev; Shahi, J.S.; Mehta, D. *Nuclear Instruments & Methods in Physics Research Section B*. Aug2018, Vol. 429, p19-26. 8p. DOI: [10.1016/j.nimb.2018.05.013](https://doi.org/10.1016/j.nimb.2018.05.013).

**On the Calculation of SAXS Profiles of Folded and Intrinsically Disordered Proteins from Computer Simulations.** Skepö, Marie; Henriques, João; Lindorff-Larsen, Kresten; Arleth, Lise. *Journal of Molecular Biology*. Aug2018, Vol. 430 Issue 16, p2521-2539. 19p. DOI: [10.1016/j.jmb.2018.03.002](https://doi.org/10.1016/j.jmb.2018.03.002).

**Density fluctuations in amorphous pharmaceutical solids. Can SAXS help to predict stability?** Laggner, Peter; Paudel, Amrit. *Colloids & Surfaces B: Biointerfaces*. Aug2018, Vol. 168, p76-82. 7p. DOI: [10.1016/j.colsurfb.2018.05.003](https://doi.org/10.1016/j.colsurfb.2018.05.003).

**Characterisation of bare and tannase-loaded calcium alginate beads by microscopic, thermogravimetric, FTIR and XRD analyses.** Larosa, Claudio; Salerno, Marco; de Lima, Juliana Silva; Merijs Meri, Remo; da Silva, Milena Fernandes; de Carvalho, Luiz Bezerra; Converti, Attilio. *International Journal of Biological Macromolecules*. Aug2018, Vol. 115, p900-906. 7p. DOI: [10.1016/j.ijbiomac.2018.04.138](https://doi.org/10.1016/j.ijbiomac.2018.04.138).

**Nano-structural variations of ZnO:N thin films as a function of deposition angle and annealing conditions: XRD, AFM, FESEM and EDS analyses.** Savaloni, H.; Savari, Rojan. *Materials Chemistry & Physics*. Aug2018, Vol. 214, p402-420. 19p. DOI: [10.1016/j.matchemphys.2018.04.099](https://doi.org/10.1016/j.matchemphys.2018.04.099).

**Selective pore filling of mesoporous CMK-5 carbon studied by XRD: Comparison between theoretical simulations and experimental results.** Weinbrenner, Christian; Marschner, Marc; Ren, Sai; Sandberg, Thomas; Småt, Jan-Henrik; Tiemann, Michael. *Microporous & Mesoporous Materials*. Aug2018, Vol. 266, p24-31. 8p. DOI: [10.1016/j.micromeso.2018.02.035](https://doi.org/10.1016/j.micromeso.2018.02.035).

**Anisotropic broadening of XRD peaks of α-Fe: Williamson-Hall and Warren-Averbach analysis using full width at half maximum (FWHM) and integral breadth (IB).** Das Bakshi, S.; Sinha, D.; Ghosh Chowdhury, S. *Materials Characterization*. Aug2018, Vol. 142, p144-153. 10p. DOI: [10.1016/j.matchar.2018.05.018](https://doi.org/10.1016/j.matchar.2018.05.018).

**Comparison of multiple X-ray fluorescence techniques for elemental analysis of particulate matter collected on air filters.** Bilo, Fabjola; Bichler, Diane M.; Tsuji, Kouchi; Rossi, Ahmad; Zacco, Annalisa; Federici, Stefania; Eichert, Biogene M.; Lauj, Wambui; Lucchini, Alberto G.; Placidi, Donatella; Bontempi, Elza; Depero, Laura E. *Journal of Aerosol Science*. Aug2018, Vol. 122, p1-10. 10p. DOI: [10.1016/j.jaerosci.2018.05.003](https://doi.org/10.1016/j.jaerosci.2018.05.003).

**Trace element determination in soy sauce: A novel plasma-reflection X-ray fluorescence procedure and comparison with inductively coupled total-mass spectrometry.** Monticelli, D.; Cinosi, A.; Siviero, G.; Seralessandri, L. *Spectrochimica Acta Part B*. Aug2018, Vol. 146, p16-20. 5p. DOI: [10.1016/j.sab.2018.04.022](https://doi.org/10.1016/j.sab.2018.04.022).

**High performance of yolk-shell structured MnO@nitrogen doped carbon microspheres as lithium ion battery anode materials and their in operando X-ray diffraction study.** Qin, Yanmin; Jiang, Zhongqing; Rong, Halbo; Guo, Liping; Jiang, Zhong-Jie. *Electrochimica Acta*. Aug2018, Vol. 282, p719-727. 9p. DOI: [10.1016/j.electacta.2018.05.118](https://doi.org/10.1016/j.electacta.2018.05.118).

**Quantitative study of the mineralogical composition of mineral dust emitted by X-ray diffraction.** Nowak, Sophie; Lafon, Sandra; Caquineau, Sandrine; Journet, Emilie; Laurent, Benoit. *Talanta*. Aug2018, Vol. 186, p133-139. 7p. DOI: [10.1016/j.talanta.2018.03.059](https://doi.org/10.1016/j.talanta.2018.03.059).

**Phase composition of copper nitride coatings examined by the use of X-ray diffraction and Raman spectroscopy.** Nowakowska-Langier, Katarzyna; Chodun, Rafał; Minikayev, Roman; Okrasa, Sebastian; Strzelecki, Grzegorz W.; Wicher, Bartosz; Zdunek, Krzysztof. *Journal of Molecular Structure*. Aug2018, Vol. 1165, p79-83. 5p. DOI: [10.1016/j.molstruc.2018.03.107](https://doi.org/10.1016/j.molstruc.2018.03.107).

**Glancing-incidence focussed ion beam milling: A coherent X-ray diffraction study of 3D nano-scale lattice strains and crystal defects.** Hofmann, Felix; Harder, Ross J.; Liu, Wenjun; Liu, Yuzi; Robinson, Ian K.; Zayachuk, Yevhen. *Acta Materialia*. Aug2018, Vol. 154, p113-123. 11p. DOI: [10.1016/j.actamat.2018.05.018](https://doi.org/10.1016/j.actamat.2018.05.018).

**Ni/GeSn solid-state reaction monitored by combined X-ray diffraction analyses: focus on the Ni-rich phase.** Quintero, Andrea; Gergaud, Patrice; Aubin, Joris; Hartmann, Jean-Michel; Reboud, Vincent; Rodriguez, Philippe. *Journal of Applied Crystallography*. Aug2018, Vol. 51 Issue 4, p1133-1140. 7p. DOI: [10.1107/S1600576718008786](https://doi.org/10.1107/S1600576718008786).

**X-ray powder diffraction and other analyses of cellulose nanocrystals obtained from corn straw by chemical treatments.** Hernandez, C.C.; Ferreira, F.F.; Rosa, D.S. *Carbohydrate Polymers*. Aug2018, Vol. 193, p39-44. 6p. DOI: [10.1016/j.carbpol.2018.03.085](https://doi.org/10.1016/j.carbpol.2018.03.085).