Rigaku
Leading With Innovation

X-ray Diffraction & Elemental Analysis

Welcome

Thanks again to everyone who came by our booth at AAPG and ACS Spring this month. It was great to see everyone and to have the chance to talk about our new and exciting products. In May, we invite members of the crystallography community to come see us at the Instruct Biennial Structural Biology Meeting 2017 (May 24 – 26, Brno, Czech Republic). Also, we will be at the American Crystallographic Association (ACA) 2017 conference at the Hyatt Regency Hotel in New Orleans (May 26 – 30, Booth 317 + 319). There is a link to a complete list of events below.

This month's issue contains three special feature articles. The first is "*Introduction of Rigaku Analytical Devices*," which describes the origins of the handheld products group in Wilmington, MA. The second paper reports on the recent SmartLab workshop organized in Oxford, UK. And we also feature an article on the "*Development History of the PDXL Structure Analysis Package*".

Sakura (cherry blossom) blooming season in Japan

Application papers are included for XRD, WDXRF and EDXRF techniques. The book review this month concerns *The Glass Universe: How the Ladies of the Harvard Observatory Took the Measure of the Stars* by Dava Sobel. This month"s video is an animation explaining the application and basic procedures of the Small Angle X-Ray Scattering (SAXS) experiment. Check out the news and papers sections at the bottom of the page for the latest developments in materials science.

Enjoy the newsletter.

R.C. Tisdale, Ph.D. – Editor

Featured Article

Introduction of Rigaku Analytical Devices

By Jen Lynch, Marketing Director, Rigaku Analytical Devices, Inc.

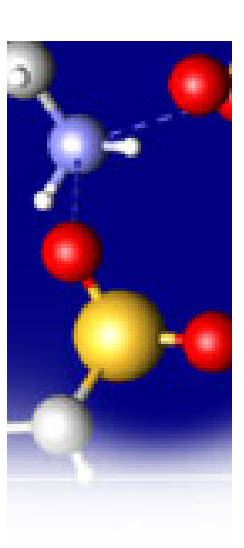
Rigaku Analytical Devices is a subsidiary of Rigaku Corporation, founded in 2011 (as Rigaku Raman Technologies) in response to a growing need for more rugged and technologically advanced mobile and handheld spectroscopic analyzers. Rigaku Analytical Devices is a leading innovator of solutions for use in the protection of public health and safety, to aid in the advancement of scientific and academic study, to enable the recycling and reuse of metal alloys, and to ensure quality of key metal alloy components in mission critical industries. **Full article >**

Featured Rigaku Event

User workshop for Rigaku "SmartLab"

Reported by Dr. Keisuke Saito, Regional Manager EMEA and North America, Rigaku Corporation

The objective of the workshop was to build the community of SmartLab users, especially in Europe. The objective was achieved through presentations given by invited speakers from different fields of application, contributed oral and poster presentations by users, technical presentations given by Rigaku application specialists, and hands-on training using the two SmartLab instruments at ISIS. **Full report >**

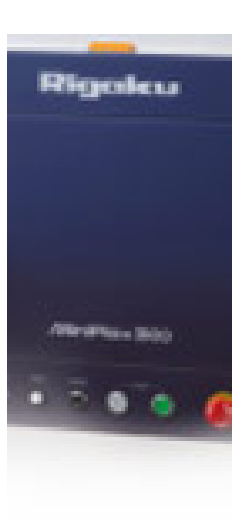


Integrated X-ray Powder Diffraction Software: PDXL

Development History of the PDXL Structure Analysis Package

By Dr. Akito Sasaki, Senior Manager XRD Application & Software Development Dept., X-ray Instrument Division, Rigaku Corporation

It was in 1999 that we tried crystal structure analysis from powder diffraction data ("SAPD") for the first time. At that time, we used strong X-rays generated from a rotating anode X-ray tube, a multilayer mirror and a parallel slit analyzer (PSA) with an extremely small aperture angle (0.057 deg) to create parallel beam optics, and collected diffraction data from a glass capillary filled with polycrystalline samples. The measurement took more than 60 hours. We believed that the data, which had a FWHM smaller than 0.1 deg, was some of the highest resolution data taken from laboratory-use diffractometers at the time. We used several third-party programs such as JADE, ITO, EXPO, to analyze the data. **For more >**



XRD Application Note

Lithium Analysis of Spodumene Ore by Quantitative X-Ray Diffraction

AXT, A Rigaku Distributor

Spodumene is a lithium-rich mineral. The importance of lithium is growing proportionally to the demand for lithium-ion rechargeable batteries, which are used in the ever-increasing number of portable electronic devices that are permeating our lives. **For more >**

WDXRF Application Note

NANOHUNTER II: Heavy Element Analysis with High Energy Excitation

Rigaku Corporation

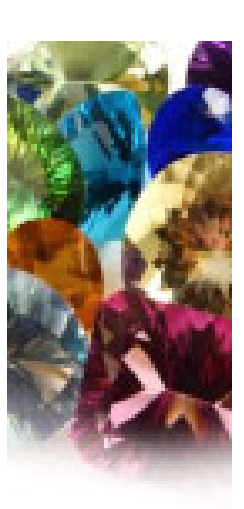
An incident X-ray beam impinges upon the sample at a shallow angle resulting in virtually complete reflection of the excitation beam away from the silicon drift detector. This affords dramatically reduced background contributions in the measured energy dispersive X-ray fluorescence spectra. In addition to the standard excitation, such as Mo-K line (about 17 keV), heavy element measurement can be carried out using high energy excitation such as 30 keV.
For more >

WDXRF Application Note

Analysis of Low Concentration Sulfur in Petroleum-based Fuels by WDXRF According to ASTM D2622-10

Rigaku Corporation

Sulfur in petroleum-based fuels contributes to atmospheric pollution. Sulfur content in fuels, especially in automobile fuels, is strictly controlled, and regulations of sulfur content in fuel oil such as diesel fuel and gasoline have been tightened. Therefore, control of sulfur content is very important in refinery plants. **For more >**

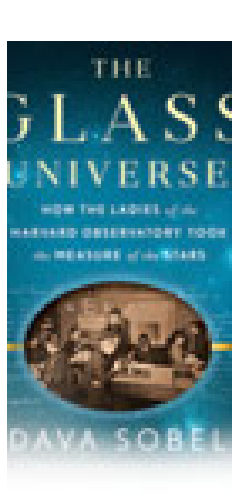


EDXRF Application Note

Analysis of Gemstones

Applied Rigaku Technologies

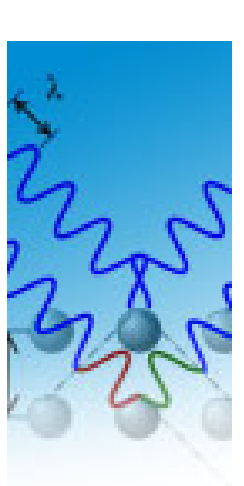
Elemental measurement is important in gemology for identification, classification and characterization of both natural and synthetic gemstones. Minor and trace levels of metals, especially the transition metals, as well as alkali elements and alkaline earth elements (such as Mg, K, Ca, Sr and Rb) help to establish the geographic region and environmental conditions during the formation of a gemstone. Other elements like Au and Pb can be used to indicate processing requirements of synthetics. **For more >**



Book Review

The Glass Universe: How the Ladies of the Harvard Observatory Took the Measure of the Stars by Dava Sobel

When we think of the scientists and astronomers who studied the far reaches of our universe, men like Galileo Galilei and Stephen Hawking often come to mind. But Dava Sobel's latest work tells the untold story of the women who worked at the Harvard Observatory during the late 19th and early 20th centuries, mapping the stars and paving the way for future generations of astronomers and astrophysicists to study the mysteries of our universe. **Full review >**



Material Analysis in the News

News for April 2017

April 3, 2017. X-ray fluorescence reveals van Eyck's original colours: elemental imaging shows alterations to famous Ghent Altarpiece by the van Eyck brothers. With the help of a homemade X-ray fluorescence scanner, researchers have shown that 70% of the original work has been covered with overpaintings for almost six hundred years.

April 5, 2017. The future of energy technology as seen through X-ray eyes: the inner workings of batteries are being revealed by the assortment of X-ray microscopy tools used at SSRL. The latest innovations in photovoltaics are being examined and characterized with the aim of making sure that both energy storage and energy generation technologies can meet the demands of future generations.

April 10, 2017. Pushing X-ray imaging up against its physical limits: instead of sending X-rays through your imaging target and reading them on the other side, you can recreate an image using light that scatters back toward the source. The light that scatters from an object already carries all the information required to recreate an image of it: the scattering angle, amplitude, and phase of the light can be used to calculate the details of an object.

April 11, 2017. Carbonate analysis through X-ray diffraction (XRD) techniques has been well documented, and research into both carbonates and clays dates back many decades. An abudance of research has been published since the turn of the millennium, and even now new carbonate and clay-based research is coming to fruition through XRD analysis methods.

April 12, 2017. X-ray ptychography maps the 3D interior of integrated circuits: a team of researchers based in Switzerland is on the way to laying bare much of the secret technology inside commercial processors. They pointed a beam of X-rays at a piece of an Intel processor and were able to reconstruct the chip's warren of transistors and wiring in three dimensions.

April 12, 2017. For the first time ever a family of hydrogels has been created, with unique properties that allow them to be utilised in biological applications. The work, recently published in *Polymer*, could herald the introduction of a novel class of bio-inks or drug delivery vehicles. The properties of the novel polymer complexes were revealed by a host of techniques, including Small Angle X-ray Scattering (SAXS) at the Small Angle Scattering and Diffraction beamline (I22) at Diamond Light Source.

April 16, 2017. Researchers have come up with a new way to extract water from thin air. The new approach makes use of a substance called an MOF, a metal-organic framework. As the name suggests, these are materials made of metals mixed with organic compounds. Powders made from MOFs are very porous, so researchers have proposed using them to store hydrogen or methane fuels or to capture carbon dioxide.

April 21, 2017. Lowest density MOF to date: simple building blocks produce complex structure with a unit cell made up of 816 uranium nodes and 816 organic linkers. Omar K. Farha, a chemistry professor at Northwestern University who led the MOF-making effort, says his team didn't predict they would get such an elaborate structure based on first principles.

April 21, 2017. Focused Ion Beam Milling (FIB) applies a miniature beam of highly energetic particles to cut and analyze materials smaller than one thousandth of a strand of human hair. It was believed that the effects of FIB would not spread beyond this thin damaged layer. Revolutionary new results from the University of Oxford show that this is not true, and that FIB can in fact greatly change the structural identity of a material.

April 22, 2017. New knowledge has been gained about the behavior of metal nanoparticles when they undergo oxidation, by integrating X-ray imaging and computer modeling and simulation. This knowledge adds to our understanding of fundamental processes like oxidation and corrosion.

Recent Scientific Papers of Interest

Papers for April 2017

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

Direct Analysis of Metal Ions in Solutions with High Salt Concentrations by Total Reflection X-ray Fluorescence. Regadío, Mercedes; Riaño, Sofía; Binnemans, Koen; Vander Hoogerstraete, Tom. *Analytical Chemistry*. 4/18/2017, Vol. 89 Issue 8, p4595-4603. 9p. DOI: 10.1021/acs.analchem.7b00097.

4-Cyanopyridine, a versatile mono- and bidentate ligand. Crystal structures of related coordination polymers determined by X-ray powder diffraction. Zhao, Haishuang; Bodach, Alexander; Heine, Miriam; Krysiak, Yasar; Glinnemann, Jürgen; Alig, Edith; Fink, Lothar; Schmidt, Martin U. *CrystEngComm*. 4/28/2017, Vol. 19 Issue 16, p2216-2228. 13p. DOI: 10.1039/c7ce00425g.

Improving accuracy and capabilities of X-ray fluorescence method using intensity ratios. Garmay, Andrey V.; Oskolok, Kirill V. *Nuclear Instruments & Methods in Physics Research Section B*. Apr2017, Vol. 397, p67-74. 8p. DOI: 10.1016/j.nimb.2017.02.072.

X-ray diffraction and spectroscopy study of nano-Eu_2O_3 structural transformation under high pressure. Yu, Zhenhai; Wang, Qinglin; Ma, Yanzhang; Wang, Lin. *Journal of Alloys & Compounds*. Apr2017, Vol. 701, p542-548. 7p. DOI: 10.1016/j.jallcom.2017.01.143.

Influence of neutron irradiation on the microstructure of nuclear graphite: An X-ray diffraction study. Zhou, Z.; Bouwman, W.G.; Schut, H.; Pappas, C.; van Staveren, T.O.; Heijna, M.C.R. *Journal of Nuclear Materials*. Apr2017, Vol. 487, p323-330. 8p. DOI: 10.1016/j.jnucmat.2017.02.004.

Solution of an elusive pigment crystal structure from a thin film: a combined X-ray diffraction and computational study. Jones, Andrew O. F.; Röthel, Christian; Lassnig, Roman; Bedoya-Martínez, O. N.; Christian, Paul; Salzmann, Ingo; Kunert, Birgit; Winkler, Adolf; Resel, Roland. *CrystEngComm*. 4/14/2017, Vol. 19 Issue 14, p1902-1911. 10p. DOI: 10.1039/c7ce00227k.

Quantitative evaluation of statistical errors in small-angle X-ray scattering measurements. Sedlak, Steffen M.; Bruetzel, Linda K.; Lipfert, Jan. *Journal of Applied Crystallography*. Apr2017, Vol. 50 Issue 2, p621-630. 9p. DOI: 10.1107/S1600576717003077.

A New rGO-Overcoated Sb_2Se_3 Nanorods Anode for Na+ Battery: In Situ X-Ray Diffraction Study on a Live Sodiation/Desodiation Process. Ou, Xing; Yang, Chenghao; Xiong, Xunhui; Zheng, Fenghua; Pan, Qichang; Jin, Chao; Liu, Meilin; Huang, Kevin. *Advanced Functional Materials*. 4/5/2017, Vol. 27 Issue 13, pn/a-n/a. 10p. DOI: 10.1002/adfm.201606242.

NIST Standard Reference Material 3600: Absolute Intensity Calibration Standard for Small-Angle X-ray Scattering. Allen, Andrew J.; Zhang, Fan; Kline, R. Joseph; Guthrie, William F.; Ilavsky, Jan. *Journal of Applied Crystallography*. Apr2017, Vol. 50 Issue 2, p462-474. 12p. DOI: 10.1107/S1600576717001972.

Application of combined multivariate techniques for the description of time-resolved powder X-ray diffraction data. Taris, Alessandra; Grosso, Massimiliano; Brundu, Mariarosa; Guida, Vincenzo; Viani, Alberto. *Journal of Applied Crystallography*. Apr2017, Vol. 50 Issue 2, p451-461. 10p. DOI: 10.1107/S1600576717001753.

Real-time elemental imaging of large dimension paintings with a novel mobile macro X-ray fluorescence (MA-XRF) scanning technique. Romano, Francesco Paolo; Caliri, Claudia; Nicotra, Paolo; Di Martino, Sandra; Pappalardo, Lighea; Rizzo, Francesca; Santos, Hellen Cristine. *JAAS (Journal of Analytical Atomic Spectrometry)*. Apr2017, Vol. 32 Issue 4, p773-781. 9p. DOI: 10.1039/c6ja00439c.

Nondestructive X-ray diffraction measurement of warpage in silicon dies embedded in integrated circuit packages. Tanner, B. K.; Danilewsky, A. N.; Vijayaraghavan, R. K.; Cowley, A.; McNally, P. J. *Journal of Applied Crystallography*. Apr2017, Vol. 50 Issue 2, p547-554. 7p. DOI: 10.1107/S1600576717003132.

Application of X- ray diffraction to study the grinding induced surface damage mechanism of WC/Co. Zhang, Quanli; Zhao, Qingliang; To, Suet; Guo, Bing. *International Journal of Refractory Metals & Hard Materials*. Apr2017, Vol. 64, p205-209. 5p. DOI: 10.1016/j.ijrmhm.2016.11.006.

Unveiling the Third Secret of Fátima: μ-XRF quantitative characterization and 2D elemental mapping. Manso, M.; Pessanha, S.; Guerra, M.; Figueirinhas, J.L.; Santos, J.P.; Carvalho, M.L. *Spectrochimica Acta Part B*. Apr2017, Vol. 130, p35-38. 4p. DOI: 10.1016/j.sab.2017.02.006.

Spectrophotometric analysis of hematite/magnetite nanocomposites in comparison with EDX and XRF techniques. Zayed, M.A.; Imam, N.G.; Ahmed, M.A.; El Sherbiny, Doaa H. *Journal of Molecular Liquids*. Apr2017, Vol. 231, p288-295. 8p. DOI: 10.1016/j.molliq.2017.02.007.

X-ray diffraction (XRD), thermogravimetric analysis (TGA) and impedance spectroscopy studies of PM-355 as a function of proton fluence. Al Garawi, M.S.; Al Salman, S.A.; Mansoor, Ali Syed; Kayani, A.; Al-Ghamdi, S.S.; Baig, M.R. *Radiation Measurements*. Apr2017, Vol. 99, p41-43. 3p. DOI: 10.1016/j.radmeas.2017.03.004.

XRF map identification problems based on a PDE electrodeposition model. Ivonne Sgura; Benedetto Bozzini. *Journal of Physics: D Applied Physics*. 4/20/2017, Vol. 50 Issue 15, p1-1. 1p. DOI: 10.1088/1361-6463/aa5a1f.

X-ray diffraction data-assisted structure searches. Gao, Pengyue; Tong, Qunchao; Lv, Jian; Wang, Yanchao; Ma, Yanming. *Computer Physics Communications*. Apr2017, Vol. 213, p40-45. 6p. DOI: 10.1016/j.cpc.2016.11.007.

Total reflection X-ray fluorescence as a fast multielemental technique for human placenta sample analysis. Marguí, E.; Ricketts, P.; Fletcher, H.; Karydas, A.G.; Migliori, A.; Leani, J.J.; Hidalgo, M.; Queralt, I.; Voutchkov, M. *Spectrochimica Acta Part B*. Apr2017, Vol. 130, p53-59. 7p. DOI: 10.1016/j.sab.2017.02.008.

$\lambda/2$ contamination in X-ray diffraction data – the impact of heavy atoms. Gianopoulos, Christopher G.; Chua, Zhijie; Zhurov, Vladimir V.; Pinkerton, A. Alan. *Journal of Applied Crystallography*. Apr2017, Vol. 50 Issue 2, p643-646. 3p. DOI: 10.1107/S160057671700317X.

Determining the structure of carbon black using Raman spectroscopy and X-ray diffraction. Dewa, Kazuki; Ono, Kiminori; Matsukawa, Yoshiya; Takahashi, Kaname; Saito, Yasuhiro; Matsushita, Yohsuke; Aoki, Hideyuki; Era, Koki; Aoki, Takayuki; Yamaguchi, Togo. *Carbon*. Apr2017, Vol. 114, p749-749. 1p. DOI: 10.1016/j.carbon.2016.09.074.

Race Differentiation Based on Raman Spectroscopy of Semen Traces for Forensic Purposes. Muro, Claire K.; Lednev, Igor K. *Analytical Chemistry*. 4/18/2017, Vol. 89 Issue 8, p4344-4348. 5p. DOI: 10.1021/acs.analchem.7b00106.

Identification of new psychoactive substances (NPS) using handheld Raman spectroscopy employing both 785 and 1064nm laser sources. Guirguis, Amira; Girotto, Sarah; Berti, Benedetta; Stair, Jacqueline L. *Forensic Science International*. Apr2017, Vol. 273, p113-123. 11p. DOI: 10.1016/j.forsciint.2017.01.027.

Development of nano-channel single crystals and verification of their structures by small angle X-ray scattering. Abbaspoor, Saleheh; Agbolaghi, Samira; Abbasi, Farhang. *Polymer Bulletin*. Apr2017, Vol. 74 Issue 4, p1103-1119. 17p. DOI: 10.1007/s00289-016-1766-4.

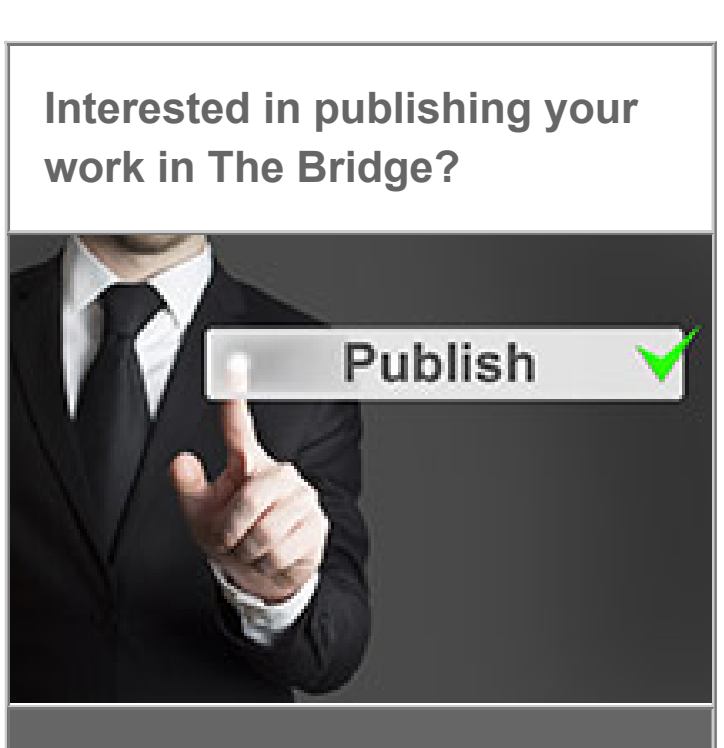
Basic X-ray scattering for soft matter. Rennie, Adrian R. *Crystallography Reviews*. Apr2017, Vol. 23 Issue 2, p152-153. 2p. DOI: 10.1080/0889311X.2016.1260560.

Elemental analysis of solids, liquids, powders, alloys and thin films

Supermini200

As the world's only high-power benchtop sequential wavelength dispersive X-ray fluorescence (WDXRF) spectrometer for elemental analysis of oxygen (O) through uranium (U) of almost any material, the Rigaku Supermini200 uniquely delivers low cost-of-ownership (COO) with high resolution and lower limits-of-detection (LLD). **For more >**

Interested in publishing your work in The Bridge?



Publish Your Work Here

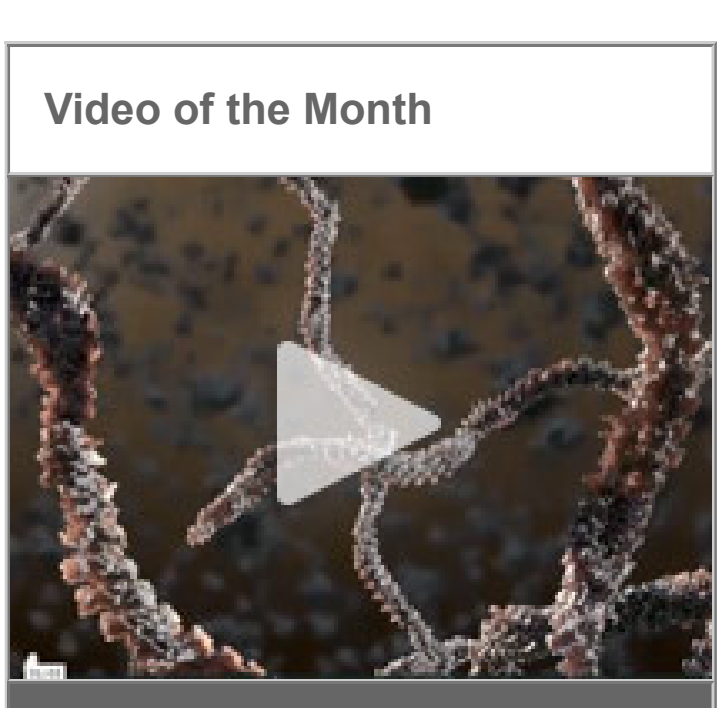
The Bridge now welcomes manuscripts, communications, and papers that describe techniques and applications of all forms of X-ray fluorescence (XRF) and X-ray diffraction (XRD, including SAXS) that are of interest to fellow scientists in industry, academia, and government. Manuscripts, in PDF format, are 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

Benchtop chemical crystallography system for 3D small molecule structure determination

XtaLAB mini II

The Rigaku XtaLAB mini II benchtop X-ray crystallography system is a compact single crystal X-ray diffractometer designed to produce publication-quality 3D structures. The perfect addition to any synthetic chemistry laboratory, the XtaLAB mini II will enhance research productivity by offering affordable structure analysis capability without the necessity of relying on a departmental facility. With the XtaLAB mini II, you no longer have to wait in line to determine your structures. Instead your research group can rapidly analyze new compounds as they are synthesized in the lab. **For more >**

Video of the Month



Small Angle X-ray Scattering animation – Project WeNMR

This is an animation for the WeNMR project (wenmr.eu), a science project funded by the European Commission. It explains the field of application and basic procedure of a Small Angle X-Ray Scattering Experiment, which can be used to study biological molecules. **Watch video >**

Conferences and Workshops

Join Rigaku at future meetings

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

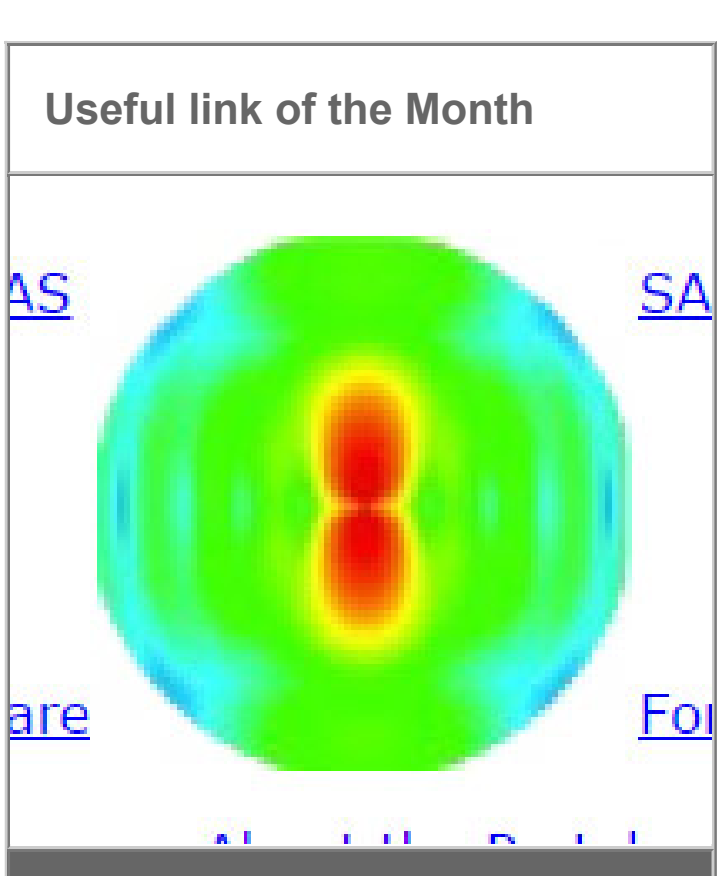
NYSCC Suppliers' Day 2017
New York, NY, USA
May 2 – 3, 2017

Fire Australia
Sydney, Australia
May 3 – 5, 2017

Safeguarding Australia
Canberra, Australia
May 3 – 4, 2017

See the complete list >

Useful link of the Month



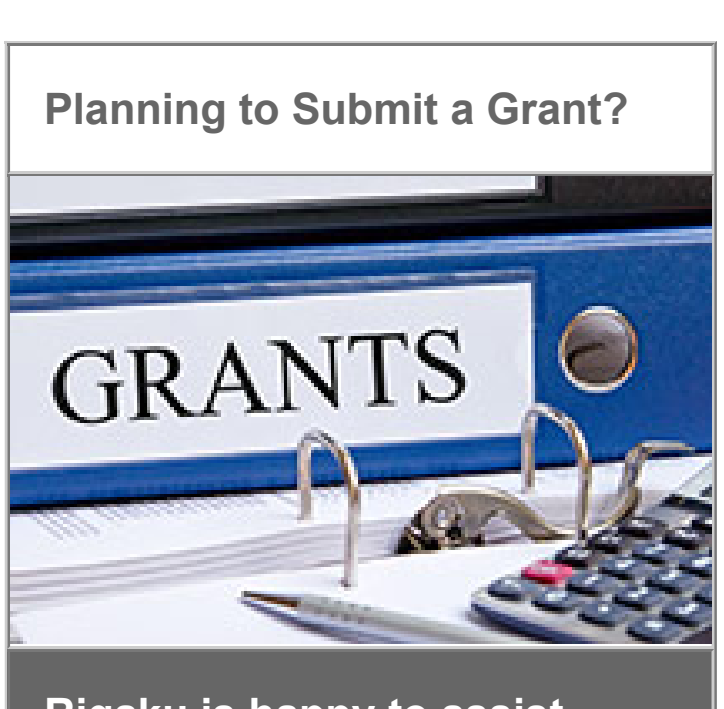
SAS Portal

The SAS Portal is a community attempt to gather some of the most relevant information about Small Angle Scattering, X-ray (SAXS) or neutron (SANS), in one place. A variety of resources are available to the small angle community:

- A nice neutron and X-ray SLD calculator based on code produced in the NSF DANSE project
- NIST also has a SLD calculator, as well as a table of neutron scattering lengths
- Other NIST tools on the web

For more >

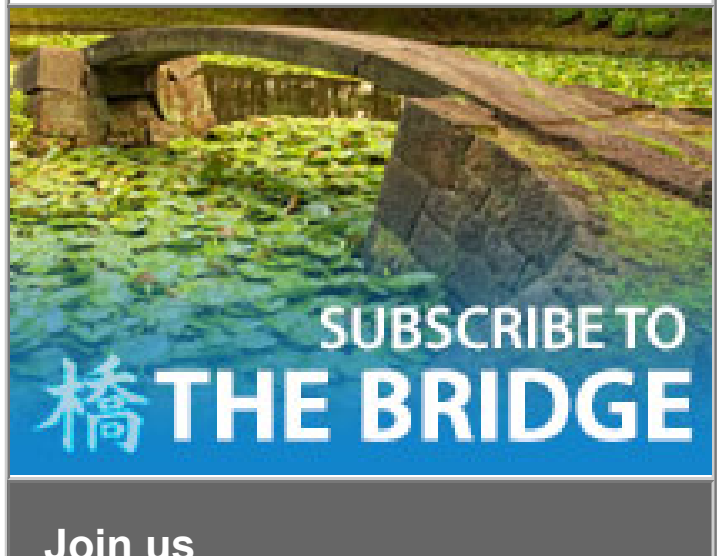
Planning to Submit a Grant?



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 >**