Rigaku
Leading With Innovation

X-ray Diffraction & Elemental Analysis

Welcome

For all who came to see us exhibit the latest in X-ray analytical instrumentation at GSA, EAS, ACS and MRS, we thank you. Our staff was happy to see many new faces.

We warmly invite you to visit Rigaku (Sunday, December 2 to Wednesday, December 5, 2018, booth #2 – 4) at AsCA 2018/CRYSTAL 32, a combined conference of the Asian Crystallographic Association (AsCA) and the Society of Crystallographers in Australia and New Zealand (SCANZ).

Programs will showcase outstanding science from Asia, Australia and New Zealand, and from around the world, and will be presented in three streams covering diverse topics in structural biology, chemical crystallography, crystal engineering, materials science, physics and fundamental science, and methods including instrumentation, techniques and computation.

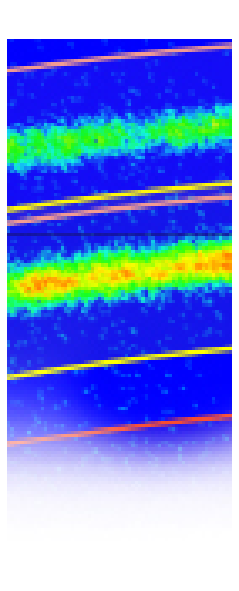
Landscape near Rigaku Yamanashi factory. Photos by Masayuki Watanabe, Rigaku Corporation.

The featured article this month discusses the Texture plugin of SmartLab Studio II.

This month's featured XRD technical note discusses crystallization behavior of ionic liquid at low temperatures. XRF application notes discuss the measurement of sulfur in crude and fuels by ASTM D2622-16 and the analysis of fiberglass by EDXRF spectroscopy.

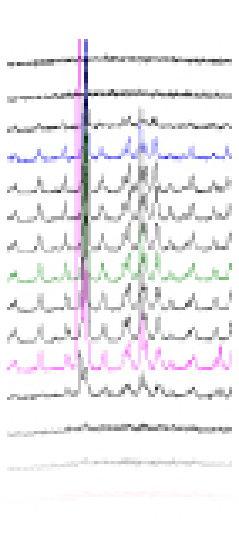
The book review covers *The Perfectionists: How Precision Engineers Created the Modern World* by Simon Winchester. Check out the two videos covering Japan's second space mission to an asteroid and NASA's 60th anniversary. And, as always, the news and papers sections are at the bottom of the page for a taste of the latest developments in materials science.

R.C. Tisdale, Ph.D. – Editor



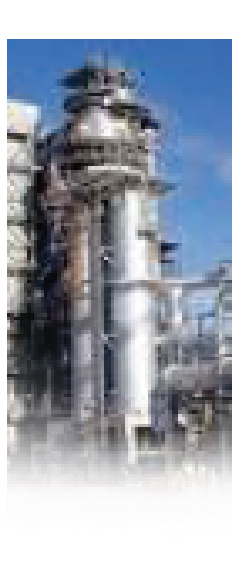
Featured Article
Texture plugin of SmartLab Studio II
Rigaku Corporation

The presence of crystallographic texture (preferred orientations) in polycrystalline materials has a significant effect on the anisotropy of the properties of such materials. That means that the quantitative description of the orientation distribution of crystallites, known as the orientation distribution function (ODF), is an important task for material characterization and prediction of their properties. Since direct measurement of the ODF is not possible, pole figures (PF) can be used to determine the ODF. Reconstruction of the ODF from measured PFs is a main goal of quantitative texture analysis. **Full article >**



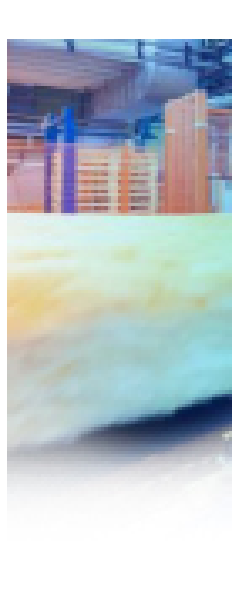
XRD Application Note
Crystallization behavior of ionic liquid at low temperatures (1)
Rigaku Corporation

Ionic liquids, consisting of molecular cations and anions, are regarded as the third most important liquid, following water and organic solvents. Due to their high electrical conductivity, they have especially gained attention in relation to electrochemical applications such as fuel cells or solar cells. However, research continues, as there are still many open questions regarding the relation between their structures and their physical properties. **For more >**



WDXRF Application Note
Sulfur Analysis in Crude Oil and High-Sulfur Fuels by Benchtop WDXRF According to ASTM D2622-16
Rigaku Corporation

This application note demonstrates quantitative analysis of high concentration sulfur in crude oil, high-sulfur diesel fuel and residual fuel oil according to ASTM D2622-16 on Rigaku Supermini200, a benchtop wavelength-dispersive X-ray fluorescence (WDXRF)spectrometer. **For more >**



EDXRF Application Note
Analysis of Fiberglass
Applied Rigaku Technologies

Fiberglass, also called glass wool, is used to make thermal insulation for houses, buildings, piping and ducts, and can also be used as a soundproofing material. Fiberglass-reinforced plastic is used to produce thermosetting polymers to make swimming pools, hot tubs, water tanks and surfboards, among many other types of products. Various fiberglass formulations are used which require elemental composition analysis to ensure proper physical and chemical properties during the manufacturing of fiberglass. Applied Rigaku Technologies offers NEX CG EDXRF analyzer to meet this industry need. **For more >**

Book Review
The Perfectionists: How Precision Engineers Created the Modern World
By Simon Winchester

Simon Winchester's *The Perfectionists: How Precision Engineers Created the Modern World* is a marvelous work of popular science, tracing the history of high-precision engineering from 1776 to present day. Precision engineering is a subdiscipline of effectively all other engineering disciplines. As the name suggests, precision is tantamount. High tolerances, repeatable results, and stability over time are the tenets of the practice. **Read review >**

Material Analysis in the News
News for November 2018

November 1, 2018. A transistor based on the 2-D material tungsten ditelluride (WTe_2) sandwiched between boron nitride can switch between two different electronic states – one that conducts current only along its edges, making it a topological insulator, and one that conducts current with no resistance, making it a superconductor.

November 2, 2018. Researchers at the National Institute for Materials Science, Japan, and Ehime University, Japan, discovered novel materials that exhibit superconductivity under high pressures using a materials informatics methodology. They took advantage of the AtomWork database, which contains more than 100,000 pieces of data on inorganic crystal structures.

November 5, 2018. A team of scientists at Ecole Polytechnique Fédérale de Lausanne (EPFL) led by Kyriakos Stylianou at the Laboratory of Molecular Simulation, have developed an MOF-based system that can perform two types of photocatalysis simultaneously: production of hydrogen, and cleaning pollutants out of water. The material contains cheap nickel phosphide (Ni_2P) and was found to carry out efficient photocatalysis under visible light.

November 15, 2018. Brazil President Michel Temer inaugurated the opening construction phase of a new particle accelerator called Sirius (Sirius Project in Campinas Brazil). It measures 518 meters (566 yards) in circumference and is expected to cost 1.8 billion reals ($477 million) to build. Only one other such accelerator exists in the world, the MAX IV in Sweden.

November 16, 2018. Scientists from around the world met at the General Conference on Weights and Measures in Versailles, France, and voted to change the definition of a kilogram, tying it to Planck's constant. The change will go into effect on May 20, 2019.

November 16, 2018. Chinese scientists unveiled the full conceptual design for the proposed Circular Electron Positron Collider (CEPC). The $5 billion, 100-kilometer-circumference machine will be designed to tackle the next big challenge in particle physics: studying the Higgs boson. Now, they're ready to develop detailed plans, start construction in 2022.

November 18, 2018. The Inamori Foundation announced that it has presented its 34th annual Kyoto Prize in Advanced Technology to Dr. Karl Deisseroth, M.D., Ph.D., a Stanford University neuroscientist and Howard Hughes Medical Institute Investigator. Deisseroth led the discovery of "optogenetics," a new methodological discipline in which cellular activity is controlled by light.

November 20, 2018. NASA has picked an ancient river delta as the landing site for its uncrewed Mars 2020 rover. Even though the Red Planet is now cold and dry, the landing site, Jezero Crater, was filled with a 1,600-foot (500-meter) deep lake that opened to a network of rivers some 3.5 to 3.9 billion years ago.

November 21, 2018. Researchers at the National Institute of Materials Science (NIMS), Japan, and the Toyota Technological Institute at Chicago, US, have jointly developed a computer-aided material design (CAMaD) system capable of extracting information vital to material design.

November 22, 2018. Massachusetts Institute of Technology (MIT) engineers described successful flight tests at the duPont Athletic Center of an unmanned airplane powered by ion wind propulsion, also called electro-aerodynamic thrust. Called Version 2 EAD Airframe, or V2, it weighs only 2.45 kg and has a wingspan of 5 meters.

Recent Scientific Papers of Interest
Papers for November 2018

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

AMORPH: A statistical program for characterizing amorphous materials by X-ray diffraction. Rowe, Michael C.; Brewer, Brendon J. *Computers & Geosciences*. Nov2018, Vol. 120, p21-31. 11p. DOI: 10.1016/j.cageo.2018.07.004.

Combining XRD and Raman spectroscopy techniques to probe the solid solution and composite forms of $Pb_{1-x}Co_xTiO_3$ systems. Cunha, T.R.; Rodrigues, A.D.; Rodrigues, J.E.; da Costa, R.C.; Toledo, T.A.; Pizani, P.S. *Materials Research Bulletin*. Nov2018, Vol. 107, p462-467. 6p. DOI: 10.1016/j.materresbull.2018.08.007.

XRF scanning of discrete samples - A chemostratigraphic approach exemplified for loess-paleosol sequences from the Island of Susak, Croatia. Profe, Jörn Wacha, Lara; Frechen, Manfred; Ohlendorf, Christian; Zolitschka, Bernd. *Quaternary International*. Nov2018, Vol. 494, p34-51. 18p. DOI: 10.1016/j.quaint.2018.05.006.

Detachment of Cu (II) and Co (II) ions from synthetic wastewater via adsorption on Lates niloticus fish bones using LIBS and XRF. Rezk, R.A.; Galmed, A.H.; Abdelkreem, M.; Abdel Ghany, N.A.; Harith, M.A. *Journal of Advanced Research*. Nov2018, Vol. 14, p1-9. 9p. DOI: 10.1016/j.jare.2018.05.002.

A modified B_2O_3 containing Li_2O-Al_2O_3-SiO_2 glass with ZrO_2 as nucleating agent - Crystallization and microstructure studied by XRD and (S)TEM-EDX. Kleebusch, Enrico; Patzig, Christian; Höche, Thomas; Rüssel, Christian. *Ceramics International*. Nov2018, Vol. 44 Issue 16, p19818-19824. 7p. DOI: 10.1016/j.ceramint.2018.07.239.

***In-situ* xrd-investigation of electrolytic copper layer.** Schneider, M.; Weiser, M.; Matthey, B.; Herrmann, M. *Applied Surface Science.* Nov2018, Vol. 457, p815-820. 6p. DOI: 10.1016/j.apsusc.2018.06.175.

Analysis of phase composition of LiZn and LiTi ferrites by XRD and thermomagnetometric analysis. Lysenko, E.N.; Astafyev, A.L.; Vlasov, V.A.; Surzhikov, A.P. *Journal of Magnetism & Magnetic Materials*. Nov2018, Vol. 465, p457-461. 5p. DOI: 10.1016/j.jmmm.2018.06.010.

A Monte Carlo Model of a Benchtop X-Ray Fluorescence Computed Tomography System and Its Application to Validate a Deconvolution-Based X-Ray Fluorescence Signal Extraction Method. Ahmed, Md Foiez; Yasar, Selcuk; Cho, Sang Hyun. *IEEE Transactions on Medical Imaging*. Nov2018, Vol. 37 Issue 11, p2483-2492. 10p. DOI: 10.1109/TMI.2018.2836973.

Total Reflection X-Ray Fluorescence Analysis of Natural and Drinking Waters. Oskolok, K. V.; Monogarova, O. V.; Alov, N. V. *Journal of Analytical Chemistry*. Nov2018, Vol. 73 Issue 11, p1093-1097. 5p. DOI: 10.1134/S1061934818110084.

Total Reflection X-Ray Fluorescence Analysis of Solid Metallurgical Samples. Sharanov, P. Yu.; Alov, N. V. *Journal of Analytical Chemistry*. Nov2018, Vol. 73 Issue 11, p1085-1092. 8p. DOI: 10.1134/S1061934818110126.

Application of Energy Dispersive X-ray Fluorescence Spectrometry to the Determination of Copper, Manganese, Zinc, and Sulfur in Grass (*Lolium perenne*) in Grazed Agricultural Systems. Daly, Karen; Fenelon, Anna. *Applied Spectroscopy*. Nov2018, Vol. 72 Issue 11, p1661-1673. 13p. DOI: 10.1177/0003702818787165.

Preparation of standard materials of aerosol particles for X-ray fluorescence analysis using a small chamber sampling unit. Nakano, Kazuhiko; Oshiro, Yoshito; Azechi, Sotaro; Somada, Yuka; Handa, Daishi; Miyagi, Yoichi; Tanahara, Akira; Arakaki, Takemitsu; Itoh, Akihide. *XRS: X-ray Spectrometry*. Nov/Dec2018, Vol. 47 Issue 6, p450-458. 9p. DOI: 10.1002/xrs.2973.

A compositional analysis by energy dispersive X-ray fluorescence of Iberian copper-alloy votive figurines from southern Spain (fourth–third centuries BC). Roldán García, Clodoaldo; Vives-Ferrándiz Sánchez, Jaime. XRS: *X-ray Spectrometry*. Nov/Dec2018, Vol. 47 Issue 6, p441-449. 9p. DOI: 10.1002/xrs.2972.

Identification of weak peaks in X-ray fluorescence spectrum analysis based on the hybrid algorithm combining genetic and Levenberg Marquardt algorithm. Du, Hua; Chen, Wuhui; Zhu, Qingjun; Liu, Songlin; Zhou, Jianbin. *Applied Radiation & Isotopes*. Nov2018, Vol. 141, p149-155. 7p. DOI: 10.1016/j.apradiso.2018.07.009.

Multi-element determination of Cd, Pb, Cu, V, Cr, and Mn in ethanol fuel samples using energy dispersive X-ray fluorescence spectrometry after magnetic solid phase microextraction using $CoFe_2O_4$ nanoparticles. Meira, Lucilia A.; Almeida, Jorge S.; Dias, Fabio De S.; Pedra, Pablo P.; Costa Pereira, Amalia L.; Teixeira, Leonardo S.g. *Microchemical Journal*. Nov2018, Vol. 142, p144-151. 8p. DOI: 10.1016/j.microc.2018.06.025.

Temperature dependent Raman and X-ray diffraction studies of anhydrous milk fat. Lambert, A.; Bougrioua, F.; Abbas, O.; Courty, M.; El Marssi, M.; Faivre, V.; Bresson, S. *Food Chemistry*. Nov2018, Vol. 267, p187-195. 9p. DOI: 10.1016/j.foodchem.2017.09.006.

Thermal equation of state of $MgSiO_4H_2$ phase H determined by in situ X-ray diffraction and a multianvil apparatus. Nishi, Masayuki; Tsuchiya, Jun; Arimoto, Takeshi; Kakizawa, Sho; Kunimoto, Takehiro; Tange, Yoshinori; Higo, Yuji; Irifune, Tetsuo. *Physics & Chemistry of Minerals*. Nov2018, Vol. 45 Issue 10, p995-1001. 7p. DOI: 10.1007/s00269-018-0980-z.

Correlating deformation mechanisms with X-ray diffraction phenomena in nanocrystalline metals using atomistic simulations. Foley, Daniel J.; Coleman, Shawn P.; Tschopp, Mark A.; Tucker, Garritt J. *Computational Materials Science*. Nov2018, Vol. 154, p178-186. 9p. DOI: 10.1016/j.commatsci.2018.07.056.

Probing chemical heterogeneity of Li-ion batteries by in *operando* high energy X-ray diffraction radiography. Mühlbauer, M.J.; Schökel, A.; Etter, M.; Baran, V.; Senyshyn, A. *Journal of Power Sources*. Nov2018, Vol. 403, p49-55. 7p. DOI: 10.1016/j.jpowsour.2018.09.035.

Computer simulations of X-ray spherical wave dynamical diffraction in one and two crystals in the Laue case. Kohn, V. G.; Smirnova, I. A. *Acta Crystallographica. Section A, Foundations & Advances*. Nov2018, Vol. 74 Issue 6, p699-704. 6p. DOI: 10.1107/S2053273318012627.

Local structure and lattice covalency of complex perovskites $BaM_{0.2}Ta_{0.8}O_{3-x}N_x$ (M = Li, Na, Mg) studied by X-ray diffraction and X-ray absorption spectroscopy. Paek, Seung-Min; Kim, Young-Il. *Journal of Solid State Chemistry*. Nov2018, Vol. 267, p92-97. 6p. DOI: 10.1016/j.jssc.2018.08.011.

Using rule-based regression models to predict and interpret soil properties from X-ray powder diffraction data. Butler, Benjamin M.; O'Rourke, Sharon M.; Hillier, Stephen. *Geoderma*. Nov2018, Vol. 329, p43-53. 11p. DOI: 10.1016/j.geoderma.2018.04.005.

Atomic Imaging of Iron-Based Superconductor Parent FeTe Using X-Ray Fluorescence Holography. Paulus, Benedict; Hosokawa, Shinya; Stellhorn, Jens Rüdiger; Klee, Benjamin; Sowa, Katarzyna M.; Kudo, Kazutaka; Nishimoto, Naoki; Ota, Hiromi; Nohara, Minoru; de Boissieu, Marc; Blanc, Nils; Boudet, Nathalie; Pilgrim, Wolf-Christian. *Physica Status Solidi (B)*. Nov2018, Vol. 255 Issue 11, pN.PAG-N.PAG. 1p. DOI: 10.1002/pssb.201800200.

High-contrast, high-resolution computed micro-tomography

nano3DX

Rigaku has developed the nano3DX as a high-resolution 3D X-ray microscope that combines Rigaku's unique high-brightness rotating anode X-ray generator with a proprietary high-resolution CCD X-ray camera to provide high-contrast computed tomography at the submicron level. The nano3DX is able to observe an ultra-wide field-of-view while retaining high 2D/3D spatial resolution and providing improved density resolution compared to conventional X-ray microscopes. **For more >**

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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 email copy to the editor.

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 (1)

NASA 60th: Humans in Space

It is part of the human spirit to explore. During 60 years, NASA selected 350 people as astronauts to lead the way. For nearly two decades, humans have been living and working aboard the International Space Station in low-Earth orbit to enable future missions forward to the Moon and on to Mars while also leading discoveries that improve life on Earth. Congress passed the National Aeronautics and Space Act on July 16, and President Eisenhower signed it into law on July 29, 1958. NASA opened for business on Oct. 1, 1958. NASA's history tells a story of exploration, innovation and discoveries. **Watch video >**

Video of the Month (2)

Why Japan Is Landing Hopping Robots On An Asteroid

Japan has landed two hopping robots onto asteroid Ryugu as part of the Hayabusa2 mission. It's Japan's second mission to an asteroid, where it plans to return some samples of Ryugu to Earth by the early 2020s so that scientists can study the samples with more sophisticated instruments and hopefully uncover some of the biggest scientific mysteries of all. Following is a transcript of the video. **Watch video >**

Conferences and Workshops

Join Rigaku at future meetings

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

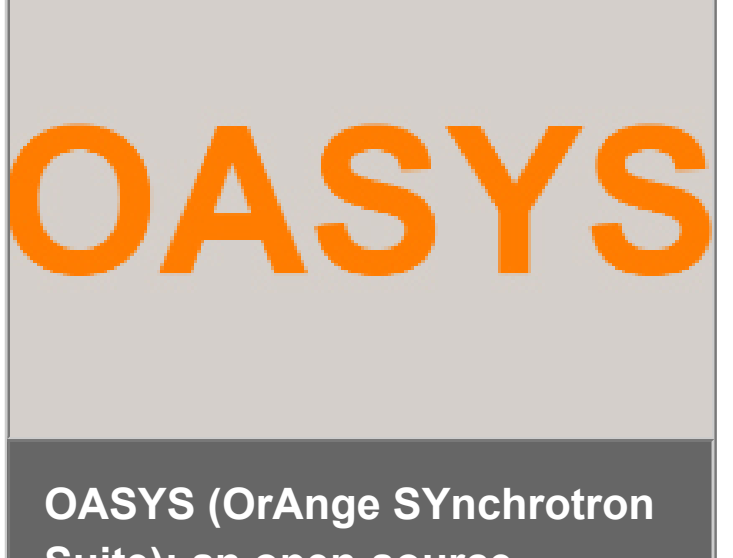
AsCA 2018
Auckland, New Zealand
December 2 – 5, 2018

AWA Global Release Liner Industry Conference & Exhibition 2019
Charlotte, NC, US
May 1 – 3, 2019

PEFTEC 2019
Rotterdam, The Netherlands
May 22 – 23, 2019

See the complete list >

Useful Link of the Month



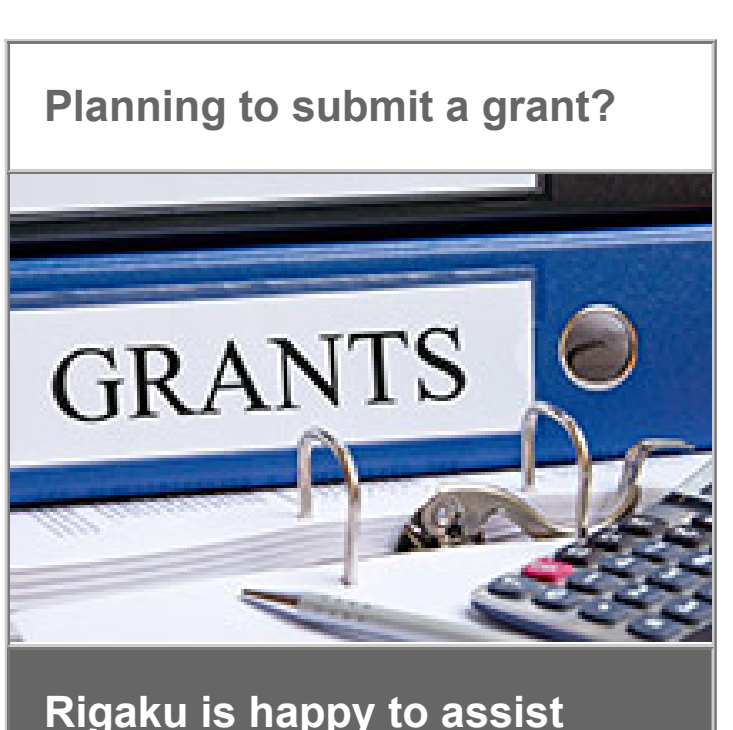
OASYS (OrAnge SYnchrotron Suite): an open-source graphical environment for X-ray virtual experiments

The implemented software architecture provides an intuitive and very-easy-to-use graphical interface, as well as high flexibility and rapidity for interactive simulations, making configuration changes to quickly compare multiple beamline configurations. Its purpose is to integrate in a synergetic way the most powerful calculation engines available. OASYS integrates different simulation strategies via the implementation of adequate simulation tools for X-ray Optics (e.g. ray tracing and wave optics packages). It provides a language so they can communicate by sending and receiving encapsulated data. Python has been chosen as the main programming language, because of its universality and popularity in scientific computing. The software Orange, developed at the University of Ljubljana (SLO), is the high level workflow engine that provides the interaction with the user and communication mechanisms.

OASYS (OrAnge SYnchrotron Suite): an open-source graphical environment for x-ray virtual experiments. Luca Rebuffi, Manuel Sanchez del Rio. *Proc. SPIE 10388, Advances in Computational Methods for X-Ray Optics IV*, 103880S (23 August 2017).
DOI: 10.1117/12.2274263

For more >

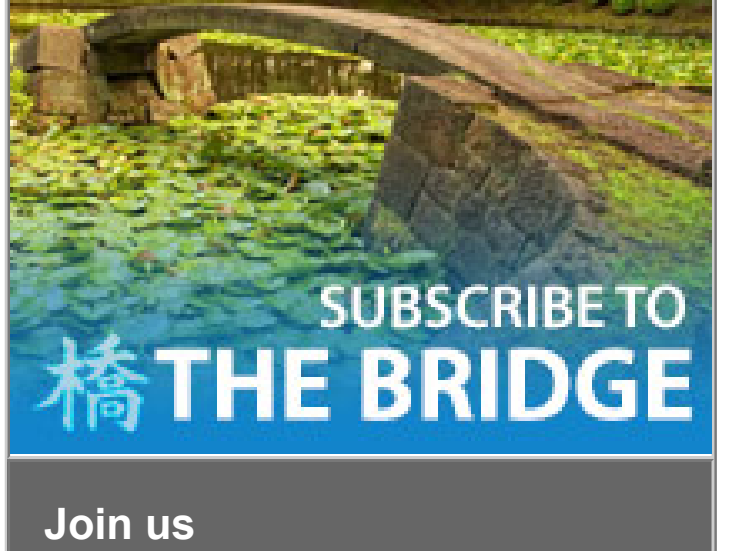
Planning to submit a grant?



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 >**