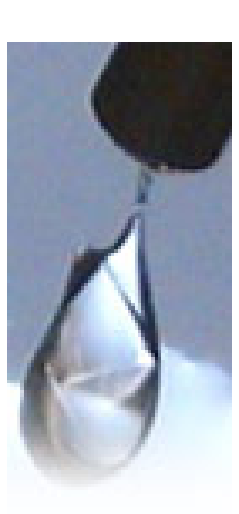
Welcome

Wednesday, September 2 marks the beginning of JASIS 2015, one of the largest Asian exhibitions of analytical and scientific instrumentation. All are invited to come and see the latest Rigaku products at the Makuhari Messe, Japan at booth #5A-101. The event runs through Friday, September 4, 2015. Rigaku will present six seminars at JASIS, with two presentations each day pertaining to new technologies.

For your continuing education, we offer the first installment of our new series "Introduction to single crystal X-ray analysis," entitled "What is X-ray crystallography?" Our featured technical X-ray diffraction (XRD) paper describes complete phase analysis of cement using a MiniFlex600 diffractometer. 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



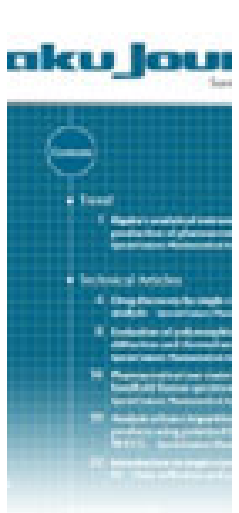
Introduction to single crystal X-ray analysis

What is X-ray crystallography?

Rigaku Corporation

This month we begin a serialized book entitled "Introduction to single crystal X-ray analysis." The first chapter covers "What is X-ray crystallography?"

Subsequent chapters, from September through February 2016, will cover the following topics (in order): mounting crystals, obtaining quality data from a microcrystal, data collection and processing, some key points of structure analysis by Rigaku's CrystalStructure, CIFs – alerts and how to handle them, and the refinement of disordered structure. **For more >**



Featured XRD Rigaku Journal Article

General features of GaN-related materials

Rigaku Corporation

In modern society where our daily environment is supported by various electronic devices, it is critical to pursue opto-electronic or power-electronic devices with less environment impact and with higher efficiency of energy conversion to ensure a sustainable society. GaN (gallium nitride) and related materials have been a focus of attention for the issue of sustainability. **For more >**

Featured XRD Rigaku Journal Article

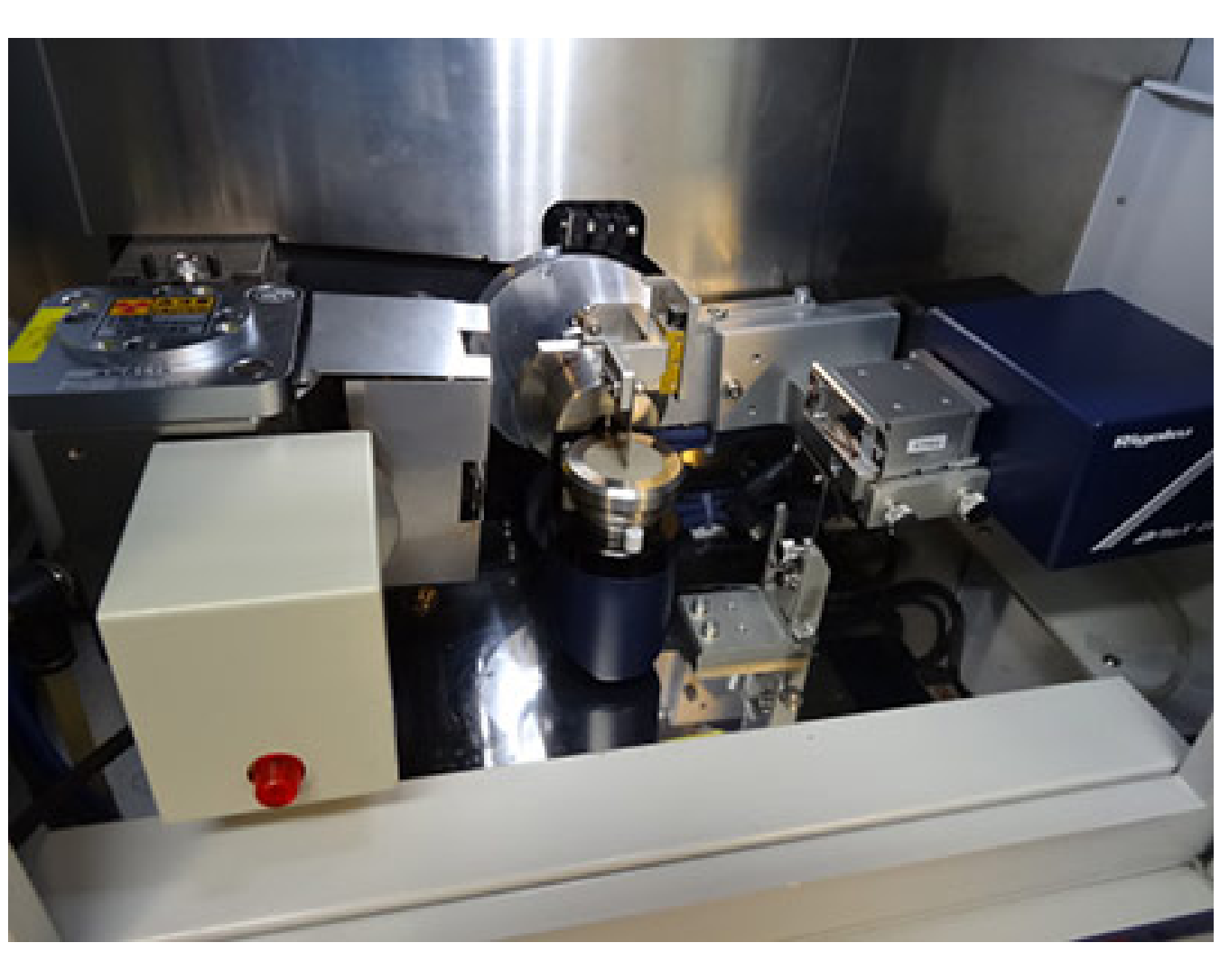
Integrated X-ray diffraction software

Rigaku Corporation

SmartLab Studio II is an integrated X-ray diffraction software package for SmartLab 3, an automated multi-purpose X-ray diffractometer. The package covers the full spectrum of operations required for X-ray diffraction analysis, including measurement, analysis, data display and reporting on a single platform. SmartLab Studio II is designed from the ground up with ease-of-use in mind, so that even novice users are able to quickly master their X-ray diffraction systems. This article introduces some of these features. **For more >**

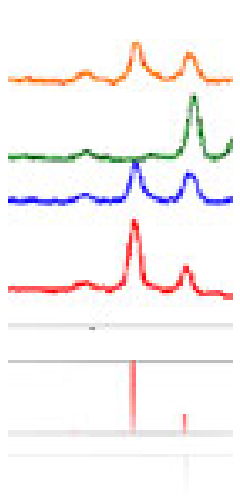
Featured Technical XRD Paper

Improved bench-top X-ray diffractometer for crystalline phase analysis of cement. Atsushi Ohbuchi, et al. Powder Diffraction. Dec2013, Vol. 28 Issue 04, pp 249-253. DOI:10.1017/S0885715613001206.



Interior of MiniFlex600 showing X-ray source (left) and detector (right)

This month's featured technical XRD paper, Improved bench-top X-ray diffractometer for crystalline phase analysis of cement by Dr. Atsushi Ohbuchi, et. al., covers the performance of the MiniFlex600 X-ray diffractometer – equipped with the D/teX Ultra silicon strip detector – for complete phase analysis of cement, including lime (CaO), in just 5 minutes. The system was comprised of a low-noise one-dimensional silicon strip detector, a variable slit, and a goniometer with a radius as small as 150 mm. A variable knife edge was used as a countermeasure for unwanted scattering, particularly in the low angle range. NIST 2686 standard reference material was analyzed and the quantitative analysis results for the major phases are in agreement with the certified values of the reference material. Dr. Ohbuchi uses XRD and XRF for analysis of municipal waste incineration ash as well as cement. Rigaku offers the benchtop MiniFlex XRD and benchtop Supermini200 WDXRF, including special sample holders, for cement analysis. Dr. Ohbuchi received his Doctor of Engineering from Meiji University. **For more >**

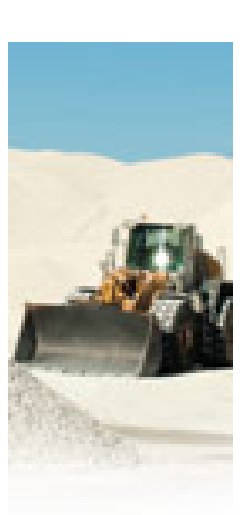


XRD Application Note

In-situ observation of structural changes accompanying charging-discharging of cathode materials of lithium ion batteries

Rigaku Corporation

Controlling the state of the charge-discharge process is believed to be crucial for extending the life of lithium ion batteries. Therefore, it is not enough to simply observe the electrode structure in the 100% charged and discharged states, and there is a need to carry out *in-situ* observation of the relationship between depth of charge, depth of discharge and electrode structure. However, if materials are removed once from sealed batteries, the materials will react with the atmosphere, and the charge-discharge state will change due to peeling of electrodes. Thus there is a risk of the material changing into another structure, irrespective of the charge-discharge situation. As a result, with previous methods, it was difficult to observe changes in materials accompanying charging-discharging via an X-ray diffraction measurement. However, with batteries made using lithium ion battery cells for evaluation and testing, X-ray diffraction can be performed simultaneously with charge-discharge testing. **For more >**



WDXRF Application Note

Quantitative Analysis of Dolomite and Limestone by Pressed Powder Method with Supermini200

Rigaku Corporation

Both dolomite and limestone are important mineral resources used in various industries such as cement, electronics, iron manufacturing, glass, paper and pulp, agriculture. X-ray fluorescence (XRF) analysis quickly and easily offers precise elemental analysis results allowing control of the components in the product during the manufacturing process. This application note demonstrates the excellent performance of Supermini200 for the analysis of dolomite and limestone. **For more >**

EDXRF Application Note

Sulfur and Chlorine in Activated Carbon

Applied Rigaku Technologies

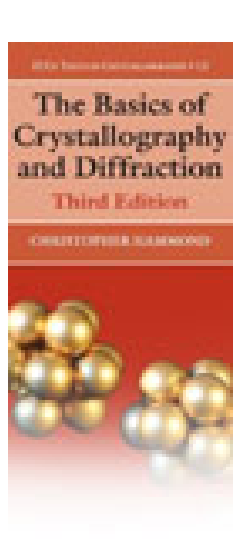
Sulfur and chlorine may occur naturally in charcoal and in the production and regeneration of activated carbon various solvents may be used, including sulfur-based and chlorine-based solvents. As the material is processed the sulfur and chlorine levels are monitored until they reach an acceptable content. EDXRF offers a fast and simple low cost method of measuring the sulfur and chlorine content with little or no sample preparation and relatively short analysis times.
For more >

Raman Application Note

Aseptic Identification of Polysorbates Using Handheld Raman

Rigaku Raman Technologies

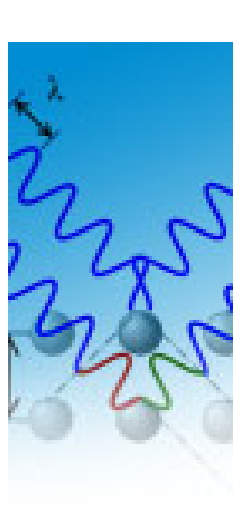
Polysorbates are used in a variety of industries including food, cosmetics, pharmaceuticals and biopharmaceuticals – specifically in the manufacturing of parenteral medication and cell culture growth. Due to industry regulations and quality standards, it is considered good practice to identify incoming materials prior to manufacturing. Handheld Raman is capable of identifying these materials without any sampling or preparation. **For more >**



Scientific Book Review

The Basics of Crystallography and Diffraction

I came across this book at a Royal Microscopy Society meeting and asked Oxford University Press to send me a copy for review. The title is very descriptive and you must remember there was crystallography long before diffraction by crystals was observed. This is a textbook for material scientists and geologists, although many crystallographers would find it a useful reference. One feature I really liked was the attention paid to history. There is a plethora of background information in the text, and the short biographic vignettes in Appendix 3 are very informative.
For more >



Material Analysis in the News

News for August 2015

August 2, 2015. Using X-ray diffraction, researchers at the Brazilian Synchrotron Light Source, led by Vesna Stanic and her colleagues, have discovered a never-before-seen component of human hair – an intermediate zone located between the cortex and cuticle. The findings were presented at the annual meeting of the American Crystallographic Association.

August 5, 2015. At Brookhaven National Laboratory, physicist Sanjit Ghose and his collaborators have been studying metal-organic frameworks (MOFs) designed for use in the separation of waste from nuclear reactors, which results from the reprocessing of nuclear fuel rods. He is targeting two waste products in particular: the noble gases xenon (Xe) and krypton (Kr). MOF studies were carried out by large multi-institution collaborations, using a combination of X-ray diffraction, theoretical modeling, and other methods.

August 6, 2015. A new scientific instrument at the Department of Energy's SLAC National Accelerator Laboratory promises to capture some of nature's speediest processes. It uses a method known as ultrafast electron diffraction (UED) and can reveal motions of electrons and atomic nuclei within molecules that take place in less than a tenth of a trillionth of a second – information that will benefit groundbreaking research in materials science, chemistry and biology.

August 13, 2015. The list of potential mechanisms that underlie an unusual metal-insulator transition has been narrowed by a team of researchers from Argonne and Lawrence Berkeley national laboratories and the University of Arkansas using a combination of X-ray techniques at the Advanced Photon Source (APS). This transition has ramifications for material design for electronics and sensors.

August 17, 2015. The world's newest and brightest synchrotron light source – the National Synchrotron Light Source II (NSLS-II) at the U.S. Department of Energy's Brookhaven National Laboratory – has discovered a new way to apply a widely used local-structure analysis tool – known as atomic pair distribution function (PDF) analysis – to X-ray scattering data from thin films, quickly yielding high-quality information on the films' atomic structure. The work creates new avenues for studies of nanocrystalline thin films.

August 17, 2015. Researchers at Oxford University's Department of Engineering Science have been investigating "smart gels" that can switch from a stable gel to a liquid suspension of very small particles (a "sol"). They have discovered a new family of gel-like materials whose behavior is extremely unusual; not only is their "shape-shifting" from gel to sol entirely reversible but it can be triggered by a range of stimuli.

August 19, 2015. All-plastic solar cells formulas unfortunately tend to form clumps with low surface areas. A new process called fluid enhanced crystal engineering (Fluence), by it inventors at Stanford University's Institute for Materials and Energy Sciences (SIMES), employs a micron-sized "rake" that can untangle these clumps to form nano-sized crystals that double the surface area and thus double output power.

August 19, 2015. Caltech's Thomas F. Rosenbaum and colleagues at the University of Chicago and the Argonne National Laboratory recently used a synchrotron X-ray source to investigate the existence of instabilities in the arrangement of the electrons in metals as a function of both temperature and pressure, and to pinpoint, for the first time, how those instabilities arise.

August 20, 2015. The Israeli Patent and Trademark Office (IL PTO) issued new working guidelines relating to the examination of patent applications claiming crystal and salt forms of known compounds. The guidelines reflect a significantly more restrictive approach than previously enunciated by the IL PTO regarding the patentability of polymorph and salt patents. Claims to new crystal forms must include the highest intensity X-ray powder diffraction (XRPD) peaks that conclusively characterize the crystal form

August 23, 2015. A Wilmington manufacturing company, Rigaku Analytical Devices, got a boost on Thursday with a visit from U.S. Rep. Seth Moulton, who toured the facility on Upton Drive. Moulton, a member of the Small Business Committee in the House of Representatives, praised the company's work as an innovator in the 6th Congressional District.

Recent Scientific Papers of Interest

Papers for August 2015

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

Anomalous X-ray diffraction study of Pr-substituted $BaCeO_{3-\delta}$. Basbus, Juan F.; Caneiro, Alberto; Suescun, Leopoldo; Lamas, Diego G.; Mogni, Liliana V. *Acta Crystallographica: Section B, Structural Science, Crystal Engineering & Materials*. Aug2015, Vol. 71 Issue 4, p455-462. 8p. DOI: 10.1107/S2052520615010203.

***BINoculars*: data reduction and analysis software for two-dimensional detectors in surface X-ray diffraction.** Roobol, Sander; Onderwaater, Willem; Drnec, Jakub; Felici, Roberto; Frenken, Joost. *Journal of Applied Crystallography*. Aug2015, Vol. 48 Issue 4, p1324-1329. 6p. DOI: 10.1107/S1600576715009607

High-pressure phases of cordierite from single-crystal X-ray diffraction to 15 GPa. Finkelstein, Gregory J.; Dera, Przemyslaw K.; Duffy, Thomas S. *American Mineralogist*. Aug2015, Vol. 100 Issue 8/9, p1821-1833. 13p. DOI: 10.2138/am-2015-5073.

Grain size measurement from two-dimensional micro-X-ray diffraction: Laboratory application of a radial integration technique. Bramble, Michael S.; Flemming, Roberta L.; McCausland, Phil J.A. *American Mineralogist*. Aug2015, Vol. 100 Issue 8/9, p1899-1911. 13p. DOI: 10.2138/am-2015-5181.

Polycrystal orientation mapping using scanning three-dimensional X-ray diffraction microscopy. Hayashi, Yujiro; Hirose, Yoshiharu; Seno, Yoshiki. *Journal of Applied Crystallography*. Aug2015, Vol. 48 Issue 4, p1094-1101. 8p. DOI: 10.1107/S1600576715009899.

X-ray diffraction by phase diffraction gratings. Irzhak, D. V.; Knyasev, M. A.; Punegov, V. I.; Roshchupkin, D. V. Journal of Applied Crystallography (International Union of Crystallography – IUCr). Aug2015, Vol. 48 Issue 4, p1159-1164. 6p. DOI: 10.1107/S1600576715011607.

Thermal expansion behavior of $SrSiO_3$ and Sr_2SiO_4 determined by high-temperature X-ray diffraction and dilatometry. Thieme, Christian; Rüssel, Christian. *Journal of Materials Science*. Aug2015, Vol. 50 Issue 16, p5533-5539. 7p. 2 Diagrams, 2 Charts, 3 Graphs. DOI: 10.1007/s10853-015-9100-3.

A laboratory-based Laue X-ray diffraction system for enhanced imaging range and surface grain mapping. Whitley, William; Stock, Chris; Huxley, Andrew D. *Journal of Applied Crystallography*. Aug2015, Vol. 48 Issue 4, p1342-1345. 4p. DOI: 10.1107/S1600576715009097.

Analytical characterization of a new mobile X-ray fluorescence and X-ray diffraction instrument combined with a pigment identification case study. Van de Voorde, Lien; Vekemans, Bart; Verhaeven, Eddy; Tack, Pieter; De Wolf, Robin; Garrevoet, Jan; Vandenabeele, Peter; Vincze, Laszlo. *Spectrochimica Acta Part B*. Aug2015, Vol. 110, p14-19. 6p. DOI: 10.1016/j.sab.2015.05.002.

Statistical assessment of heavy metal pollution in sediments of east coast of Tamilnadu using Energy Dispersive X-ray Fluorescence Spectroscopy (EDXRF). Ravisankar, R.; Sivakumar, S.; Chandrasekaran, A.; Kanagasabapathy, K.V.; Prasad, M.V.R.; Satapathy, K.K. *Applied Radiation & Isotopes*. Aug2015, Vol. 102, p42-47. 6p. DOI: 10.1016/j.apradiso.2015.03.018.

Proton irradiation of Zr-1 wt.% Nb cladding material: A depth-wise assessment of inhomogeneous microstructural damage using X-ray diffraction line profile analyses. Neogy, S.; Mukherjee, P.; Srivastava, A.P.; Singh, M.N.; Gayathri, N.; Sinha, A.K.; Srivastava, D.; Dey, G.K. *Journal of Alloys & Compounds*. Aug2015, Vol. 640, p175-182. 8p. DOI: 10.1016/j.jallcom.2015.04.016.

Hydration of mechanically activated blended cements studied by *in situ* X-ray diffraction. Kalinkin, A.; Krzhizhanovskaya, M.; Gurevich, B.; Kalinkina, E.; Tyukavkina, V. *Inorganic Materials*. Aug2015, Vol. 51 Issue 8, p828-833. 6p. DOI: 10.1134/S0020168515080099.

Adsorption isotherms of copper and zinc in clay minerals of calcareous soils and their effects on X-ray diffraction. Baghernejad, M.; Javaheri, F.; Moosavi, A.A. *Archives of Agronomy & Soil Science*. Aug2015, Vol. 61 Issue 8, p1061-1077. 17p. DOI: 10.1080/03650340.2014.982549.

On the determination of stress profiles in expanded austenite by grazing incidence X-ray diffraction and successive layer removal. Fernandes, Frederico A.P.; Christiansen, Thomas L.; Winther, Grethe; Somers, Marcel A.J. *Acta Materialia*. Aug2015, Vol. 94, p271-280. 10p. DOI: 10.1016/j.actamat.2015.04.040.

Use of a Field Portable X-Ray Fluorescence Analyzer for Environmental Exposure Assessment of a Neighborhood in Cairo, Egypt Adjacent to the Site of a Former Secondary Lead Smelter. Menrath, William; Zakaria, Yehia; El-Safty, Amal; Clark, C. Scott; Roda, Sandy M.; Elsayed, Essam; Lind, Caroline; Pesce, John; Peng, Hongying. *Journal of Occupational & Environmental Hygiene*. Aug2015, Vol. 12 Issue 8, p555-563. 9p. DOI: 10.1080/15459624.2015.1020382.

Determination of tungsten in tantalum–tungsten alloy by X-ray fluorescence spectrometry using fusion, thin layer, and pressed powder pellet techniques. Tian, Lunfu; Zou, Deshuang; Dai, Yichun; Tang, Guangping. *Spectrochimica Acta Part B*. Aug2015, Vol. 110, p136-138. 3p. DOI: 10.1016/j.sab.2015.06.007.

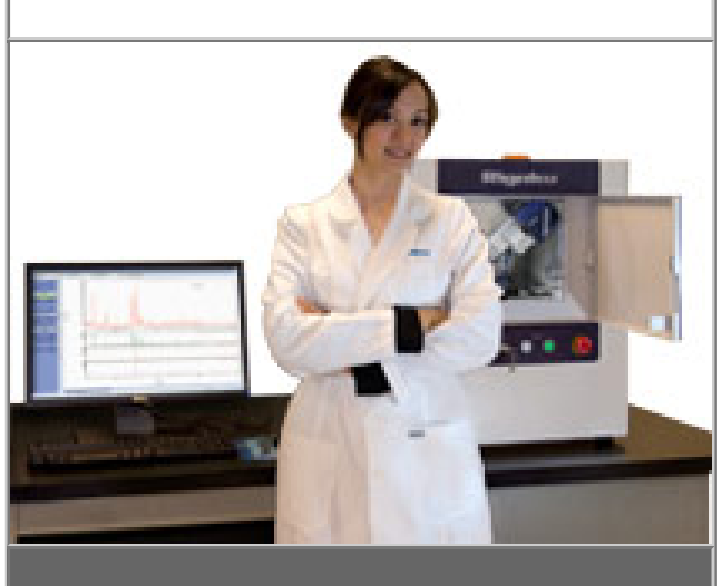
X-ray diffraction from bone employing annular and semi-annular beams. A J Dicken; J P O Evans; K D Rogers; N Stone; C Greenwood; S X Godber; D Prokopiou; J G Clement; I D Lyburn; R M Martin; P Zioupos. *Physics in Medicine & Biology*. 8/7/2015, Vol. 60 Issue 15, p1-1. 1p. DOI: 10.1088/0031-9155/60/15/5803.

Chemical and structural characterization of Zr-C-N-Ag coatings: XPS, XRD and Raman spectroscopy. Calderon V, S.; Cavaleiro, A.; Carvalho, S. *Applied Surface Science*. Aug2015, Vol. 346, p240-247. 8p. DOI: 10.1016/j.apsusc.2015.03.161.

The application of thermal analysis, XRD and SEM to study the hydration behavior of tricalcium silicate in the presence of a polycarboxylate superplasticizer. Liu, Ming; Lei, Jiaheng; Guo, Liping; Du, Xiaodi; Li, Junsheng. *Thermochimica Acta*. Aug2015, Vol. 613, p54-60. 7p. DOI: 10.1016/j.tca.2015.05.020.

***Operando* NMR and XRD study of chemically synthesized LiC_x oxidation in a dry room environment.** Sacci, Robert L.; Gill, Lance W.; Hagaman, Edward W.; Dudney, Nancy J. *Journal of Power Sources*. Aug2015, Vol. 287, p253-260. 8p. DOI: 10.1016/j.jpowsour.2015.04.035.

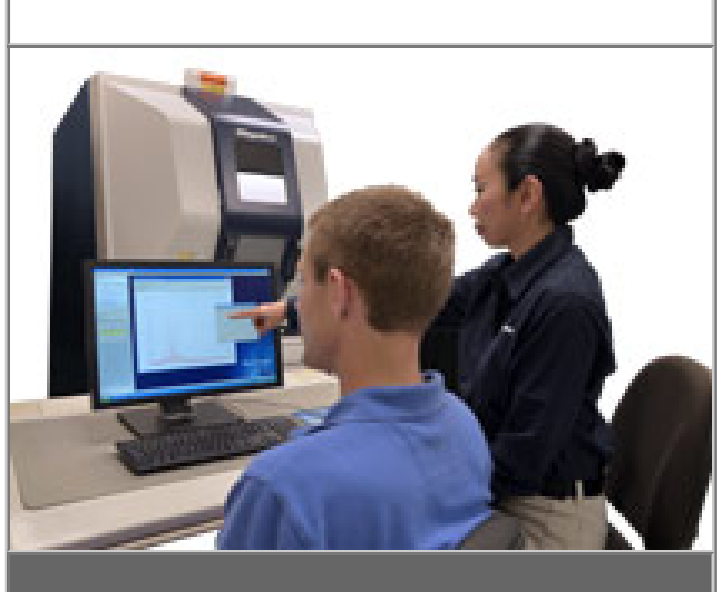
MiniFlex – qualitative and quantitative analysis of polycrystalline materials



Benchtop X-ray diffraction (XRD) instrument

Ideally-suited for today's fast-paced XRD analyses, the 5th generation MiniFlex delivers speed and sensitivity through innovative technology enhancements such as the optional D/teX high speed detector coupled with a 600 W X-ray source. Whether used for teaching X-ray diffraction at the college and university level, or routine industrial quality assurance, the MiniFlex delivers both performance and value.
For more >

SmartLab® Guidance™



Intelligent software that determines which optical units are best for an application, and performs automatic alignment, setup and measurement. Guidance delivers a completely automated measurement sequence.

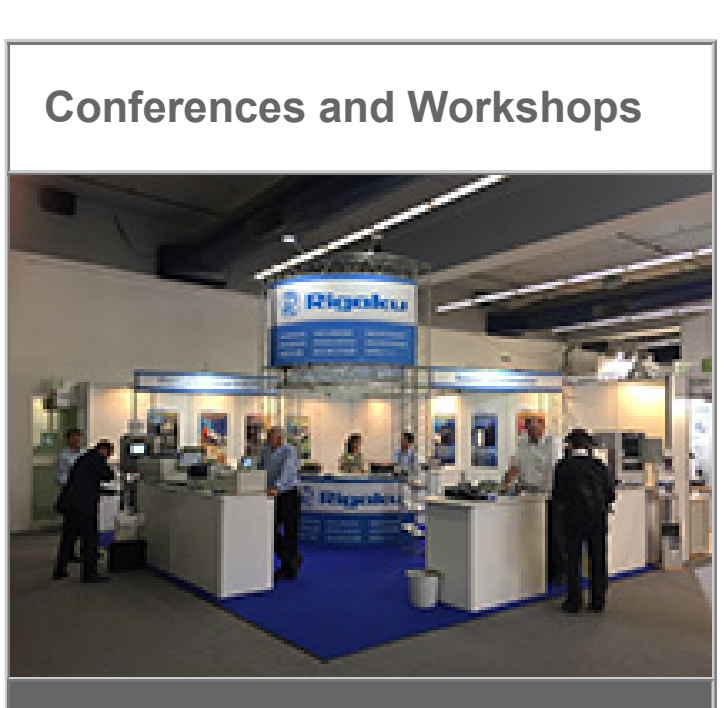
The **Guidance package**, based on built-in expertise, suggests the optimal hardware configuration and settings for specific application measurements. The program will determine which optics are most appropriate for a given application, determine the instrument settings and execute the measurement, offering a completely automated measurement sequence. Since the SmartLab has built-in component recognition, Guidance will not only tell you how you should configure the SmartLab for a given measurement, it will also warn you if you have not configured it properly. Expert advice coupled with hardware that will confirm the correct configuration is the foundation of the SmartLab system.
For more >

Video of the Month

Curiosity Rover Report (August 5, 2015): Three Years on Mars

It's a summer of milestones for Mars Exploration. Fifty years ago, Mariner 4 became the first spacecraft to take close-up pictures of Mars. Thirty-nine years ago, the Viking 1 Lander became the first spacecraft to successfully land on the Red Planet. And now, Curiosity celebrates 3 years on Mars – operating well over a thousand Martian days.
Watch the video >

Conferences and Workshops



Join Rigaku at future meetings

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

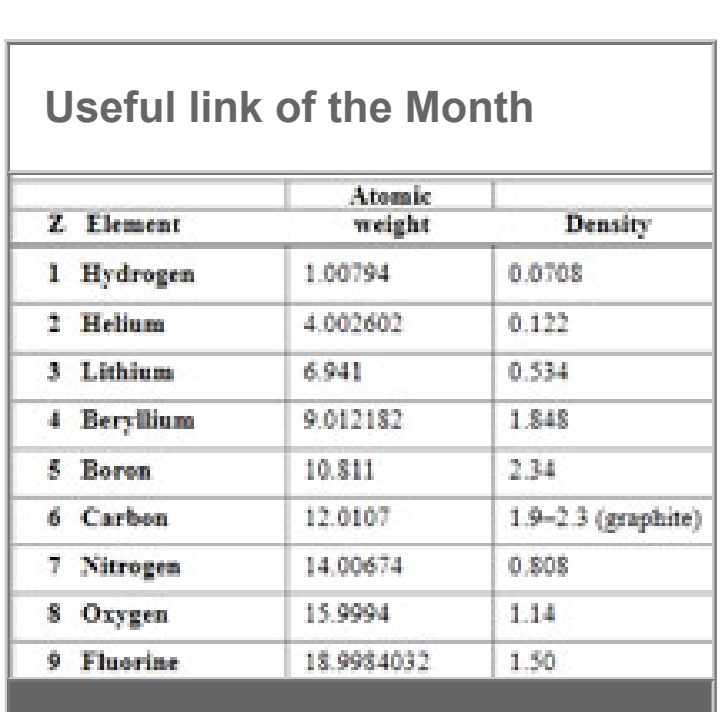
Canadian Mineral Analysts (CMA)
Ottawa, ON, Canada
September 14 – 15, 2015

DSEI – Defence & Security Equipment Internatioanl
London, UK
September 15 – 18, 2015

SPIE Security & Defense
Toulouse, France
September 21 – 24, 2015

See the complete list >

Useful link of the Month



Z	Element	Atomic weight	Density
1	Hydrogen	1.00794	0.0708
2	Helium	4.002602	0.122
3	Lithium	6.941	0.534
4	Beryllium	9.012182	1.848
5	Boron	10.811	2.34
6	Carbon	12.0107	1.9–2.3 (graphite)
7	Nitrogen	14.00674	0.808
8	Oxygen	15.9994	1.14
9	Fluorine	18.9984032	1.50

X-Ray Data Booklet

X-Ray Data Booklet: Section 5.2 Physical Properties of the Elements. This link lists several important properties of the elements. Atomic weights apply to elements as they exist naturally on earth; values in parentheses are the mass numbers for the longest-lived isotopes. Specific heats are given for the elements at 25°C and a pressure of 100 kPa. Densities for solids and liquids are given as specific gravities at 20°C unless other wise indicated by a superscript temperature (in °C); densities for the gaseous elements are given in g/cm^3 for the liquids at their boiling points.
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.
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