



MiniFlex – qualitative and

quantitative analysis of

**Benchtop X-ray diffraction** (XRD) instrument

Ideally suited for today's fast-paced

XRD analyses, the fifth generation MiniFlex delivers speed and sensitivity through innovative technology enhancements such as the optional D/teX high speed detector coupled with a 600 W Xray 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 >

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that are of interest to fellow scientists in industry, academia, and government. Manuscripts, in 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 **NEX DE – High-resolution** 



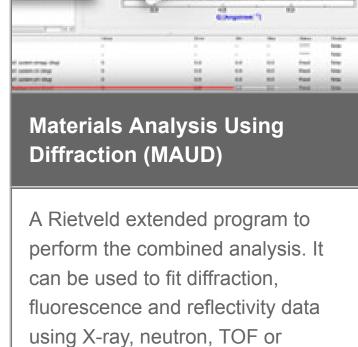
As a premium high-performance

analyzer, the new Rigaku NEX DE

benchtop EDXRF elemental

delivers wide elemental coverage with an easy-to-learn Windows®based QuantEZ software. Non-

destructively analyze from Na through U in almost any matrix,



**Conferences and Workshops** 

electrons. Watch video >

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XRD Crystallite Size Calculator using Scherrer Formula

**XRD Crystallite Size Calculator using Scherrer** Formula

The Scherrer equation, in X-ray

diffraction and crystallography, is a

formula that relates the size of sub-

micrometre particles, or crystallites,

in a solid to the broadening of a

peak in a diffraction pattern. It is

named after Paul Scherrer. It is

used in the determination of size of

particles of crystals in the form of powder. For more > **Planning to Submit a Grant?** 

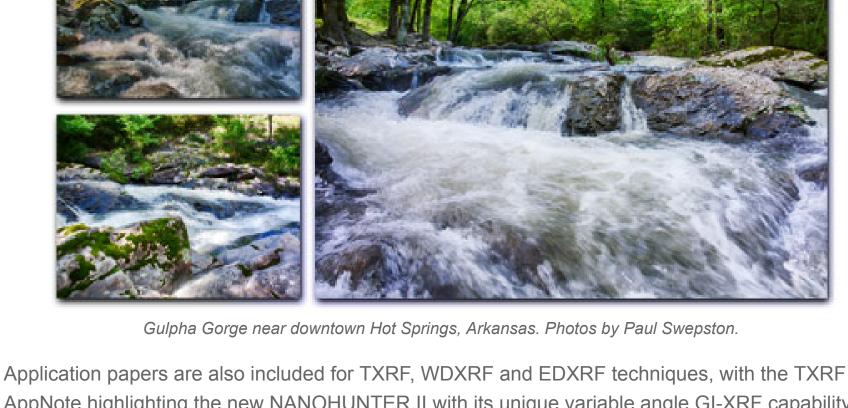
Rigaku is happy to assist If you are planning on submitting



crystallography. **Join us >** 

Thanks again to everyone who came by our booths at the fifteen conferences we attended this month. In June, we invite you to visit the various Rigaku divisions attending a variety of events scattered around the globe. There is a link to a complete list of upcoming conferences below.

computed tomography X-ray microscope (XRM), the Rigaku nano3DX. For XRD users, we offer an application note describing crystallite-size and size-distribution studies using a direct convolution technique.



Materials Analysis Using Diffraction (MAUD) software. 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

nku joui **Featured Rigaku Journal Article** In situ microscopic structural investigations with a three-dimensional X-ray

# It is well known that X-rays can penetrate opaque objects and show the internal

microscope: nano3DX

structure without destroying the object. Thus, X-rays are widely used for medical imaging, security and industrial inspection to name a few examples. In addition, X-

By Kazuhiko Omote, Yoshihiro Takeda, Raita Hirose and Joseph D. Ferrara

ray computed tomography (CT) is a powerful technique for visualizing internal structure of various specimens including the human body, in three dimensions (3D).

result of improvements in microfocus X-ray sources and high resolution X-ray detectors, making it possible to determine the precise internal 3D structure at micrometer resolution. Rigaku has developed a unique 3D X-ray microscope, the nano3DX, by the application of the quasi-parallel beam technique with a rotating anode high-power X-ray source and submicron-resolution X-ray detector. Full article > **Application of Integrated X-ray Powder Diffraction Software: PDXL** <u>Crystallite-size and size-distribution studies using a direct convolution</u> *technique* Crystallite size and its distribution are important information to investigate physical



Benchtop TXRF spectrometer NANOHUNTER II

measured energy dispersive X-ray fluorescence spectra. Furthermore, it is possible to obtain information depending on measuring depth with GI-XRF capability. For more >

**WDXRF** Application Note

Rigaku Corporation Major and trace component profiles in igneous rocks provide much information about rock history such as eruption or solidification, magma evolution, magma genesis and source materials as well as petrographical classification. In modern petrology, accurate determination of major and trace elements in silicate rocks is

throughput. X-ray fluorescence spectrometry is suitable for such requirements in

XRF analysis is currently a standard analytical method as well as the traditional wet

In the metallurgical production of metals and alloys it is important to ensure proper

balance of the major alloy metals, and it is critical to ensure certain harmful tramp

I first learned of Professor Krauss when he published *The Physics of Star Trek* in

1996. I have read most of the books he has published since then. When Krauss

was interviewed on Science Friday in March, I immediately pre-ordered my copy of

silicate rock analysis. For the determination of major elements in silicate rocks,



## elements are at sufficiently low concentration or not present. Applied Rigaku Technologies EDXRF systems offer a simple and *non-destructive* means of quickly testing ingots and sample slugs to ensure these properties are optimized. For

chemical technique. For more >

**EDXRF Application Note** 

Applied Rigaku Technologies

Ni:Fe Metallurgy

this title. Full review >

May 2, 2017. A team of Penn State researchers in the Department of Physics and the Center for Two-Dimensional and Layered Materials (2DLM) has developed a fast, nondestructive optical method for analyzing defects in 2D materials.



exchange heat with the environment. These materials show great promise for use in next-generation cooling devices.

alternatives to lithium-ion technology.

Society of Chemistry S F Boys – A Rahman Award. This biennial award from the London-based international organization for chemical scientists recognizes outstanding innovative research in the area of computational chemistry, including

May 9, 2017. Researchers at MIT have come up with a radically new way to make actuators that could be used in such extremely hot environments. The system relies on oxide materials similar to those used in many of today's rechargeable batteries, in that ions move in and out of the material during charging and discharging cycles.

designing optical and electronic properties of materials. Collective electrostatic effects are used to intentionally manipulate material properties. May 16, 2017. Silicon devices are prone to faltering and failing in difficult environments. Addressing these challenges, Jiangwei Liu, from Japan's National

Institute for Materials Sciences, and his colleagues describe new work developing

diamond-based transistors.

May 18, 2017. Chemists, materials scientists and nanoengineers at UC San Diego have created what may be the ultimate natural sunscreen. They report the development of nanoparticles that mimic the behavior of natural melanosomes, melanin-producing cell structures that protect our skin, eyes and other tissues from

**Recent Scientific Papers of Interest** Papers for May 2017 Recent Scientific Papers of Interest is a monthly compilation of material analysis papers appearing in recently released journals and publications. See below

Unified Theory for Decoding the Signals from X-Ray Fluorescence and X-Ray Diffraction of

Mixtures. Chung, Frank H. Applied Spectroscopy. May2017, Vol. 71 Issue 5, p1060-1068. 9p.

Persistence of Mixed and Non-intermediate Valence in the High-Pressure Structure of

Assessment of Ca and P content variation in enamel during an eight-week bleaching

Spectrometry. May/Jun2017, Vol. 46 Issue 3, p151-163. 13p. DOI: 10.1002/xrs.2732.

protocol using energy dispersive X-ray fluorescence. Sorozini, M.; Dos Santos, R.S.; Silva,

Silver(I,III) Oxide, AgO: A Combined Raman, X-ray Diffraction (XRD), and Density Functional



Identification of elemental composition of PM<sub>2.5</sub> collected in Makkah, Saudi Arabia, using **EDXRF.** Shaltout, Abdallah A.; Boman, Johan; Alsulimane, Mohammad E. XRS: X-ray

p1691-1700. 10p. DOI: 10.1002/cctc.201601665.

10.1007/s10751-017-1425-7.

10.1177/0003702816641421.

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DOI: 10.1177/0003702816664105.

A New Look at the Structural and Magnetic Properties of Potassium Neptunate K<sub>2</sub>NpO<sub>4</sub> Combining XRD, XANES Spectroscopy, and Low-Temperature Heat Capacity. Smith, Anna L.; Colineau, Eric; Jean-Christophe Griveau; Karin Popa; Kauric, Guilhem; Martin, Philippe;

Permeation and in situ XRD studies on PdCuAu membranes under H<sub>2</sub>. Jia, Haiyuan; Goldbach, Andreas; Zhao, Chenyang; Castro, German R.; Sun, Chenglin; Xu, Hengyong. Journal of Membrane Science. May2017, Vol. 529, p142-149. 8p. DOI: 10.1016/j.memsci.2017.01.062. X-Ray Fluorescence Analysis and Self-Organizing Maps Classification of the Etruscan Gold Coin Collection at the Monetiere of Florence. Arias, Claudio; Bani, Stefano; Catalli, Fiorenzo;

Lorenzetti, Giulia; Grifoni, Emanuela; Legnaioli, Stefano; Pagnotta, Stefano; Palleschi, Vincenzo.

Simplex Volume Maximization (SiVM): A matrix factorization algorithm with non-negative

constrains and low computing demands for the interpretation of full spectral X-ray

fluorescence imaging data. Alfeld, Matthias; Wahabzada, Mirwaes; Bauckhage, Christian;

Kersting, Kristian; van der Snickt, Geert; Noble, Petria; Janssens, Koen; Wellenreuther, Gerd;

Applied Spectroscopy. May2017, Vol. 71 Issue 5, p817-822. 6p. DOI:

May/Jun2017, Vol. 46 Issue 3, p164-170. 7p. DOI: 10.1002/xrs.2733.

Falkenberg, Gerald. Microchemical Journal. May2017, Vol. 132, p179-184. 6p. DOI: 10.1016/j.microc.2017.02.001. X-ray fluorescence determination of Cs, Ba, La, Ce, Nd, and Ta concentrations in rocks of various composition. Suvorova, Darya; Khudonogova, Elena; Revenko, Anatoly. XRS: X-ray Spectrometry. May/Jun2017, Vol. 46 Issue 3, p200-208. 9p. DOI: 10.1002/xrs.2747.

Seasonal determination of trace and ultra-trace content in Macrocystis pyrifera from San Jorge Gulf (Patagonia) by Total Reflection X-ray Fluorescence. Salomone, Vanesa N.; Riera, Marina; Cerchietti, Luciana; Custo, Graciela; Muniain, Claudia. Spectrochimica Acta Part B. May2017, Vol. 131, p74-78. 5p. DOI: 10.1016/j.sab.2017.03.009.

In situ analysis of the crystallization process of Sb<sub>2</sub>S<sub>3</sub> thin films by Raman scattering and X-ray diffraction. Parize, Romain; Cossuet, Thomas; Chaix-Pluchery, Odette; Roussel, Hervé; Appert, Estelle; Consonni, Vincent. *Materials & Design*. May2017, Vol. 121, p1-10. 10p. DOI: 10.1016/j.matdes.2017.02.034. Thermal expansion coefficient of carbon-supported Pt nanoparticles: *In-situ* X-ray

diffraction study. Leontyev, I. N.; Kulbakov, A. A.; Allix, M.; Rakhmatullin, A.; Kuriganova, A. B.; Maslova, O. A.; Smirnova, N. V. *Physica Status Solidi (B)*. May2017, Vol. 254 Issue 5, pn/a-n/a. 4p. DOI: 10.1002/pssb.201600695. Monitoring instability of linear amine impregnated UiO-66 by in-situ temperature resolved

Myoung Soo; Yavuz, Cafer T. Microporous & Mesoporous Materials. May2017, Vol. 243, p85-90. 6p. DOI: 10.1016/j.micromeso.2017.02.021. Measurement of residual stress in arc welded lap joints by cosa X-ray diffraction method. Lin, Jian; Ma, Ninshu; Lei, Yongping; Murakawa, Hidekazu. Journal of Materials Processing

powder X-ray diffraction. Song, Youngdong; Thirion, Damien; Subramanian, Saravanan; Lah,

Effect of draw ratio on fiber structure development of polyethylene terephthalate. Tomisawa, R.; Ikaga, T.; Kim, K.H.; Ohkoshi, Y.; Okada, K.; Masunaga, H.; Kanaya, T.; Masuda, M.; Maeda, Y. Polymer. May2017, Vol. 116, p357-366. 10p. DOI: 10.1016/j.polymer.2016.12.071.

& Compounds. May 2017, Vol. 703, p344-353. 10p. DOI: 10.1016/j.jallcom.2017.01.293.

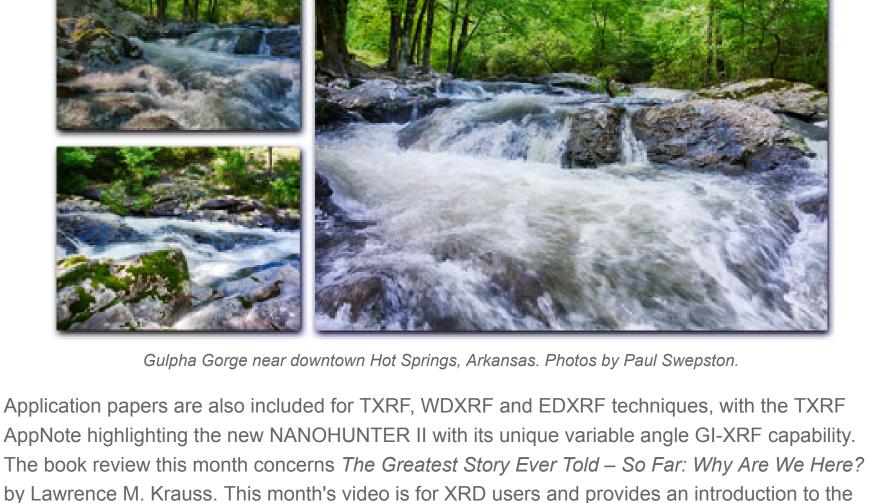
Miao, J.; Makineni, S.; Allison, J.E.; Shebanova, O.; Robson, J.D.; Lee, Peter D. *Journal of Alloys* 

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Recently, a high spatial resolution X-ray microscope has been developed as a

properties of materials. Precise determination of these values requires that the effect from instrument and strain should be separated. For this reason, it is suitable to use the whole powder pattern data which can evaluate the 2θ dependence of the peak shape. To eliminate the instrumental aberrations, we apply a convolution method between instrumental and physical profiles. For more >

**TXRF Application Note** Unique Variable Angle GI-XRF Capability 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

Silicate Rock Analysis by Fusion Method on ZSX Primus III+ essential. Elemental analysis of rocks requires high precision, sensitivity and high



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Y ARE WE HERE

## **Book Review** <u>The Greatest Story Ever Told – So Far: Why Are We Here?</u>

By Lawrence M. Krauss

more >

**Material Analysis in the News** News for May 2017

May 2, 2017. Scientists have produced novel electrolytes for rechargeable sodium and magnesium batteries. The research group's objective was to develop

May 3, 2017. Caloric materials are a class of materials that demonstrate interesting

May 5, 2017. Scientists have discovered a new nano-scale thin film material with

the highest-ever conductivity in its class. The new material could lead to smaller,

thermodynamic behavior: when they are exposed to an external field they

faster, and more powerful electronics, as well as more efficient solar cells.

May 9, 2017. Rice University chemist Gustavo Scuseria won the 2017 Royal



both quantum chemistry and molecular simulations.

May 9, 2017. Berkeley Lab researchers used structural characterization — both X-

ray crystallography and small angle X-ray scattering (SAXS) — to show that many

of the designs adopted the target oligomerization state and predicted structure.

May 10, 2017. Scientists have created the first-ever polarization gradient in thinfilm ferroelectrics, greatly expanding the range of functional temperatures for a key material used in a variety of everyday applications. May 12, 2017. Researchers have mapped out a radically new approach for

the harmful effects of ultraviolet radiation. May 19, 2017. Researchers at the Okinawa Institute of Science and Technology

Graduate University (OIST) have created self-assembling molecules that can be

broken down by ultraviolet light to recombine into novel macroscopic shapes.

Theory (DFT) Study. Grzelak, Adam; Gawraczynski, Jakub; Jaron, Tomasz; Somayazulu, Maddury; Derzsi, Mariana; Struzhkin, Viktor; Grochala, Wojciech. *Inorganic Chemistry*. 5/15/2017, Vol. 56 Issue 10, p5804-5812. 9p. DOI: 10.1021/acs.inorgchem.7b00405.

Scheinost, Andreas C.; Cheetham, Anthony K.; Konings, Rudy J. M. *Inorganic Chemistry*. 5/15/2017, Vol. 56 Issue 10, p5839-5850. 12p. DOI: 10.1021/acs.inorgchem.7b00462. In Situ XRD Study on Promotional Effect of Potassium on Carburization of Spray-dried Precipitated Fe<sub>2</sub>O<sub>3</sub> Catalysts. Niu, Liwei; Liu, Xingwu; Liu, Xi; Lv, Zhengang; Zhang, Chenghua; Wen, Xiaodong; Yang, Yong; Li, Yongwang; Xu, Jian. ChemCatChem. 5/10/2017, Vol. 9 Issue 9,

Mössbauer and XRD characterization of the effect of heat treatment and the tribological test

Sanchez, H.; Pérez Alcazar, G. *Hyperfine Interactions*. 5/4/2017, Vol. 238 Issue 1, p1-8. 8p. DOI:

TG/DTA and XRD study on structure and chemical transformation of the Cs-P-W oxides.

Zhang, Guoliang; Wu, Hui; Peng, Zhijian; Li, Chunshan. Journal of Thermal Analysis &

on the physical and mechanical properties of a Fe-Mn-Al-C alloy. Ramos, J.; Piamba, J.;

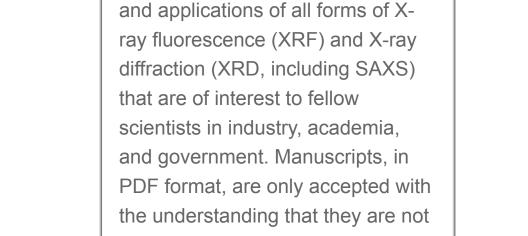
Calorimetry. May2017, Vol. 128 Issue 2, p947-956. 10p. DOI: 10.1007/s10973-016-5990-9.

A comparative study on the total reflection X-ray fluorescence determination of low Z elements using X-ray tube and synchrotron radiation as excitation sources. Sanyal, K.; Kanrar, B.; Misra, N. L.; Czyzycki, M.; Migliori, A.; Karydas, A. G. XRS: X-ray Spectrometry.

Operando X-ray diffraction during battery cycling at elevated temperatures: A quantitative analysis of lithium-graphite intercalation compounds. Cañas, Natalia Andrea; Einsiedel, Philipp; Freitag, Oliver Thomas; Heim, Christopher; Steinhauer, Miriam; Park, Dong-Won; Friedrich, Kaspar Andreas. *Carbon*. May2017, Vol. 116, p255-263. 9p. DOI: 10.1016/j.carbon.2017.02.002.

Technology. May2017, Vol. 243, p387-394. 8p. DOI: 10.1016/j.jmatprotec.2016.12.021.

Characterising precipitate evolution in multi-component cast aluminium alloys using smallangle X-ray scattering. Panagos, P.; Wang, Y.; McCartney, D.G.; Li, M.; Ghaffari, B.; Zindel, J.W.;



elemental analysis of sodium (Na) through uranium (U)

from solids and alloys to powders, liquids and slurries. For more > Video of the Month

Meeting Hershey, PA, USA June 4 – 6, 2017

Green Bay, WI, USA

June 15 – 16, 2017

**Training** 

See the complete list >

**Useful link of the Month** 

Source wavelength, A (Angstroms): Peak FWHM. Psq (decrees): Peak Position, 20 (degrees):

an instrument grant proposal,

Rigaku will be happy to assist you.

We can help you determine the

correct instrument and configura-

tion best suited for your analytical

needs. **Start the process >** 

