



A flexible system for small molecule 3D structure analysis



SuperNova

The SuperNova from the Rigaku Oxford Diffraction division combines our high-flux microfocus sources with one of our patented fast, self-optimizing S2 CCD detectors. This combination of high intensity and a fast, large active area CCD enables rapid data collection, with easy software switching between molybdenum and copper wavelengths. It is the ideal diffractometer for small molecule crystallography in research laboratories and leading analytical service facilities. **For more >**

Measurement of X-ray diffraction and scattering from materials



D/MAX RAPID II

D/MAX RAPID II is arguably the most versatile micro-diffraction XRD system in the history of materials analysis. In production for well over a decade and continuously improved during that time period, the success of the D/MAX RAPID II is a testament to the suitability of imaging plate technology for measuring diffraction patterns and diffuse scattering from a wide range of materials. **For more >**

Video of the Month



Wave-Particle Duality Animation

Feynman's double-slit experiment brought to life: an animation of the wave-particle duality through the double slit experiment with and without an observer. Like the Schrödinger's cat thought experiment, the double-slit experiment is often used to highlight the differences and similarities between the various interpretations of quantum mechanics. **Watch video >**

Conferences and Workshops



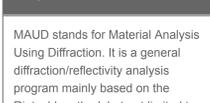
Join Rigaku at future meetings

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

- AWPA**
San Juan, Puerto Rico
May 1 – 3, 2016
- SIMC 2016**
Casablanca, Morocco
May 10 – 13, 2016
- Rigaku Symposium on X-ray Diffraction**
New Haven, CT, USA
May 18 – 20, 2016

See the complete list >

Useful link of the Month



MAUD

MAUD stands for Material Analysis Using Diffraction. It is a general diffraction/reflectivity analysis program mainly based on the Rietveld method, but not limited to. Main features are: Written in Java so it can run on Windows, MacOSX, Linux, Unix (needs Java VM 1.7 or later); Easy to use, every action is controlled by a GUI; Works with X-ray, synchrotron, neutron, TOF and electrons; Developed for Rietveld analysis, simultaneous multi spectra and different instruments/techniques supported. This software is the research result of Luca Lutterotti at University of Trento (Italy). **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 >**

Welcome

We want to thank everyone who visited Rigaku at exponim® in Santiago, Chile where a variety of X-ray based products for the mining industry were shown. Over 1,200 exhibitors and tens of thousands of attendees made for a great time.



Rigaku Booth at exponim 2016

Please come and see us at the following materials science events in May: 4th International Exhibition on Mining and Quarries (Casablanca), the Rigaku Symposium on X-ray Diffraction (Yale University) and analytica 2016 (Munich). We promise to have new and interesting things to discuss.

For your continuing education, we offer the ninth installment of our new series "Introduction to single crystal X-ray analysis," entitled "Protein structure analysis and small molecule structure analysis." Our featured technical paper is a primer on "Micro X-ray diffraction of cultural properties."

The Feynman's double-slit experiment is the video topic this month. Applications notes include XRD, WDXRF, EDXRF and RAMAN technologies. Check out the book reviews, 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 IX
Protein structure analysis and small molecule structure analysis
Rigaku Corporation

The previous series have discussed single crystal X-ray analysis of small molecules. This series will discuss structure analysis of proteins using X-ray diffraction. The explanation will focus in particular on differences between structure analysis of proteins and that of small molecules. **For more >**



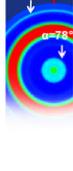
Featured XRD Rigaku Journal Article
Micro X-ray diffraction of cultural properties
Rigaku Corporation

There are two basic objectives in scientific analysis of tangible cultural properties: appraisal of authenticity, and investigation of materials for purposes of preservation or restoration. Targets of these analyses are buildings, sculptures, paintings, craft objects, old documents and so on. **For more >**



XRD Application Note
MiniFlex300/600: Suppression of the umbrella effect due to differences in Soller slits
Rigaku Corporation

Powder X-ray diffractometers are used in many fields of industry and research, for substances ranging from inorganic materials such as ceramics and minerals, to pharmaceuticals and other organic materials. The MiniFlex Series is a line of benchtop instruments – with 1/20 the volume, and 1/10 the weight, of stand-alone powder X-ray diffractometers – that can operate with power from an AC 100 V outlet. The current models in the MiniFlex Series include a high-power model type with a maximum rated output of 600 W (MiniFlex600), and a reduced-utility model, which requires no water facilities and only generates 300 W of output power (MiniFlex300). **For more >**



XRD Application Note
Texture Analysis of a Cu Wiring Film using the Orientation Distribution Function (ODF)
Rigaku Corporation

Since there is a strong relation between the material characteristics and the crystal orientation of metals and many other industrial materials, quantitative analyses of crystallites orientation and their distributions are of great importance. Pole figure measurements are a common method to quantitatively analyze orientation. In this Application Note, we used the Orientation Distribution Function (ODF) to evaluate the crystallites orientation of a Cu wiring film from a pole figure measurement. **For more >**



WDXRF Application Note
Sulfur Analysis in Crude Oil and High-Sulfur Fuels by Benchtop WDXRF According to ASTM D2622-10
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 D2622-10 on Rigaku Supermini200, a benchtop wavelength-dispersive X-ray fluorescence (WDXRF) spectrometer. **For more >**



EDXRF Application Note
Analysis of Silver and Copper in Ore
Applied Rigaku Technologies

Silver naturally occurs in various ore and minerals, often as sulfides or chlorides or in combination with arsenic or antimony. A main source of silver is found in copper ore, as well as in copper-nickel, gold, lead and lead-zinc ores. Silver and other precious metals are also reclaimed from tailing piles or other recycled ore materials that would previously be discarded. Therefore the silver must often be measured at relatively low levels, as low silver levels can be considered profitable to extract. **For more >**



Raman Application Note
Cell Culture Media Identification in Biopharmaceuticals with Handheld Raman
Rigaku Analytical Devices

Cell culture media used for the growth of cells plays an important role in the quality and efficiency of biopharmaceutical production. Raman spectroscopy is a nondestructive, reliable, efficient, and cost-effective method to analyze cell culture media. Now recognized by the USP and EP as a viable technique for compendial identification, Raman analysis provides highly detailed chemical information on a variety of samples and requires little to no sample preparation. **For more >**



Scientific Book Review
Dark Money: The Hidden History of the Billionaires Behind the Rise of the Radical Right by Jane Mayer and *Dark Territory: The Secret History of Cyber War* by Fred Kaplan

This month we are turning to the dark side. No, I'm not talking about *Star Wars*, but rather Jane Mayer's *Dark Money* and Fred Kaplan's *Dark Territory*. **For more >**



Material Analysis in the News
News for April 2016

- April 2, 2016.** The public now has **unlimited access to the complete 16-plus-year database** for Japan's Ministry of Economy, Trade and Industry (METI) Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) instrument, which images Earth to map and monitor the changing surface of our planet.
- April 4, 2016.** Researchers from the University of Vienna, led by Thomas Pichler, have presented a novel approach to grow and stabilize **carbon chains with a record length of 6,000 carbon atoms**, improving the previous record by more than one order of magnitude.
- April 4, 2016.** The SLAC National Accelerator Laboratory is **starting construction on a second X-ray laser** that will be even brighter and more intense than its first. The new hardware, based on a superconducting linear accelerator (or linac), will replace about a third of the length of the original accelerator and leave the facility's existing X-ray laser intact.
- April 8, 2016.** A research team led by the U.S. Department of Energy's (DOE's) Argonne National Laboratory has discovered that **only half the atoms in some iron-based superconductors are magnetic**, providing a conclusive demonstration of the wave-like properties of metallic magnetism in these materials. The discovery allows for a clearer understanding of the magnetism in some compounds of iron, the iron arsenides, and how it helps induce superconductivity.
- April 12, 2016.** A research team from the University of Barcelona, along with chocolatier Enric Rovira, undertook a study to **characterize the textures of the velvet effect in chocolate**. The work examined the effect by means of experiments conducted at the Alba Synchrotron Radiation Facility and UB Scientific and Technological Centres (CCiTUB).
- April 12, 2016.** Researchers from the University of Tokyo, in collaboration with a Spanish physicist, have used one of the world's most powerful computers to **analyze a special decay of calcium-48**, whose life, which lasts trillions of years, depends on the unknown mass of neutrons. This advance will facilitate the detection of this rare decay in underground laboratories.
- April 18, 2016.** Professor Takao Someya's research group at the University of Tokyo's Graduate School of Engineering has developed an **ultraflexible 'e-skin' film** and demonstrated its use by creating an organic light-emitting diode display.
- April 19, 2016.** Chemistry researchers, led by Ignacio Vargas Baca, an associate professor in McMaster University's Department of Chemistry and Chemical Biology, have managed to **coax molecules known as tellurazole oxides into assembling themselves into cyclic structures** – a major advance in their field that creates a new and promising set of materials.
- April 22, 2016.** Thin-film solar cells: **How defects appear and disappear in CIGSe cells**. Scientists have investigated the deposition of thin chalcopyrite layers. They were able to observe specific defects as these formed during deposition and under what conditions they self-healed using X-ray diffraction. The results of their research provide clues to optimizing fabrication processes.
- April 26, 2016.** A **unique rapid-fire electron source (HRES)**, originally built as a prototype for driving next-generation X-ray lasers, is helping scientists at the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) study ultrafast chemical processes and changes in materials at the atomic scale.



Recent Scientific Papers of Interest
Papers for April 2016

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

Feasibility of wavelength dispersive X-ray fluorescence spectrometry for the determination of metal impurities in pharmaceutical products and dietary supplements in view of regulatory guidelines. Figueiredo, Alexandra; Fernandes, Tânia; Costa, Isabel Margarida; Gonçalves, Luísa; Brito, José. *Journal of Pharmaceutical & Biomedical Analysis*. Apr2016, Vol. 122, p52-58. 7p. DOI: [10.1016/j.jpba.2016.01.028](https://doi.org/10.1016/j.jpba.2016.01.028).

Detection of short range order in SiO₂ thin-films by grazing-incidence wide and small-angle X-ray scattering. Kohki Nagata; Atsushi Ogura; Ichiro Hirose; Tomoyuki Suwa; Akinobu Teramoto; Tadaihiro Ohmi. *Journal of Applied Physics*. Apr2016, Vol. 119 Issue 15, p154103-1-154103-5. 5p. DOI: [10.1063/1.4947053](https://doi.org/10.1063/1.4947053).

Development of a ¹⁷⁰Tm based X-ray fluorescence monitoring studies in humans using XRF. Timmaraju, K. Phaniree; Fajurally, Bibi Najah; Armstrong, Andrea F.; Chettle, David R. *Applied Radiation & Isotopes*. Apr2016, Vol. 110, p70-73. 4p. DOI: [10.1016/j.apradiso.2015.12.066](https://doi.org/10.1016/j.apradiso.2015.12.066).

Progression of alignment in stretched CNT sheets determined by wide angle X-ray scattering. Severino, Joseph; Yang, Jenn-Ming; Carlson, Larry; Hicks, Robert. *Carbon*. Apr2016, Vol. 100, p309-317. 9p. DOI: [10.1016/j.carbon.2016.01.005](https://doi.org/10.1016/j.carbon.2016.01.005).

Analysis of heterogeneous gallstones using laser-induced breakdown spectroscopy (LIBS) and wavelength dispersive X-ray fluorescence (WD-XRF). Jaswal, Brj; Kumar, Vinay; Sharma, Jitendra; Rai, Pradeep; Gondal, Mohammed; Gondal, Bilal; Singh, Vivek. *Lasers in Medical Science*. Apr2016, Vol. 31 Issue 3, p573-579. 7p. DOI: [10.1007/s10103-016-1905-z](https://doi.org/10.1007/s10103-016-1905-z).

A deblurring procedure for two-dimensional small angle X-ray scattering patterns. Chen, Ran; Yi, Zhi-yong; Liu, Jia-xue; Liu, Zhen-yu; Men, Yong-feng. *Chinese Journal of Polymer Science*. Apr2016, Vol. 34 Issue 4, p505-512. 8p. DOI: [10.1007/s10118-016-1767-7](https://doi.org/10.1007/s10118-016-1767-7).

A technique for determination of metallic impurities in Al₂O₃ matrix by EDXRF. Rajeswari, B.; Hon, N.; Kadam, R.; Mohapatra, M.; Natarajan, V. *Journal of Radioanalytical & Nuclear Chemistry*. Apr2016, Vol. 308 Issue 1, p357-362. 6p. 5 Charts, 3 Graphs. DOI: [10.1007/s10967-015-4589-0](https://doi.org/10.1007/s10967-015-4589-0).

The closed pores of tectonically deformed coal studied by small-angle X-ray scattering and liquid nitrogen adsorption. Pan, Jienan; Niu, Qinghe; Wang, Kai; Shi, Xinghua; Li, Meng. *Microporous & Mesoporous Materials*. Apr2016, Vol. 224, p245-252. 8p. DOI: [10.1016/j.micromeso.2015.11.057](https://doi.org/10.1016/j.micromeso.2015.11.057).

A new detector system for low energy X-ray fluorescence coupled with soft X-ray microscopy: First tests and characterization. Gianoncelli, Alessandra; Bufon, Jernej; Ahangarianbari, Mahdi; Altissimo, Matteo; Bellutti, Pierluigi; Bertuccio, Giuseppe; Borghes, Roberto; Carrato, Sergio; Cautero, Giuseppe; Fabiani, Sergio; Giacomini, Gabriele; Giuressi, Dario; Kourousias, George; Menker, Ralf Hendrik; Picciotto, Antonino; Piemonte, Claudio; Rachevski, Alexandre; Rashevskaya, Irina; Stofa, Andrea; Vacchi, Andrea. *Nuclear Instruments & Methods in Physics Research Section A*. Apr2016, Vol. 816, p113-118. 6p. DOI: [10.1016/j.nima.2016.01.076](https://doi.org/10.1016/j.nima.2016.01.076).

Green direct determination of mineral elements in artichokes by infrared spectroscopy and X-ray fluorescence. Mir-Marqués, Alba; Martínez-García, María; Garrigues, Salvador; Cervera, M. Luisa; de la Guardia, Miguel. *Food Chemistry*. Apr2016, Vol. 196, p1023-1030. 8p. DOI: [10.1016/j.foodchem.2015.10.048](https://doi.org/10.1016/j.foodchem.2015.10.048).

X-ray scattering from semiconductor p-n junctions. Noyan, I.C. *Crystallography Reviews*. Apr2016, Vol. 22 Issue 2, p142-144. 3p. DOI: [10.1080/089311X.2015.1094467](https://doi.org/10.1080/089311X.2015.1094467).

A bench-top K X-ray fluorescence system for quantitative measurement of gold nanoparticles for biological sample diagnostics. Ricketts, K.; Guazzoni, C.; Castoldi, A.; Royle, G. *Nuclear Instruments & Methods in Physics Research Section A*. Apr2016, Vol. 816, p25-32. 8p. DOI: [10.1016/j.nima.2016.01.084](https://doi.org/10.1016/j.nima.2016.01.084).

A XANES and XRD study of chalcocite bioleaching with pyrite. Yang, Yi; Liu, Weihua; Bhargava, Suresh K.; Zeng, Weimin; Chen, Miao. *Minerals Engineering*. Apr2016, Vol. 89, p157-162. 6p. DOI: [10.1016/j.mineng.2016.01.019](https://doi.org/10.1016/j.mineng.2016.01.019).

A combined X-ray and spectroscopic study on the multicolored pattern formation in gels containing FeCl₃ and K₂[Fe(CN)₆]. Hayashi, Hisashi; Abe, Hitoshi. *JAAS (Journal of Analytical Atomic Spectrometry)*. Apr2016, Vol. 31 Issue 4, p912-923. 12p. DOI: [10.1039/c5ja00481k](https://doi.org/10.1039/c5ja00481k).

Preparation of lead (Pb) X-ray fluorescence reference materials for the EPA Pb monitoring program and the IMPROVE network using an aerosol deposition method. Yatkın, Sinan; Amin, Hardik S.; Trzepla, Krystyna; Dillner, Ann M. *Aerosol Science & Technology*. Apr2016, Vol. 50 Issue 4, p309-320. 12p. DOI: [10.1080/02786826.2016.1150956](https://doi.org/10.1080/02786826.2016.1150956).

Speciation of inorganic chromium in water samples by energy dispersive X-ray fluorescence spectrometry. Pytlakowska, Katarzyna. *JAAS (Journal of Analytical Atomic Spectrometry)*. Apr2016, Vol. 31 Issue 4, p968-974. 7p. DOI: [10.1039/c5ja00495k](https://doi.org/10.1039/c5ja00495k).

Comparative study of inorganic elements determined in whole blood from Dmd^{mdx}/J mice strain by EDXRF and NAA analytical techniques. Redigolo, M.M.; Sato, I.M.; Metairon, S.; Zamboni, C.B. *Applied Radiation & Isotopes*. Apr2016, Vol. 110, p189-192. 4p. DOI: [10.1016/j.apradiso.2016.01.022](https://doi.org/10.1016/j.apradiso.2016.01.022).

JGIXA – A software package for the calculation and fitting of grazing incidence X-ray fluorescence and X-ray reflectivity data for the characterization of nanometer-layers and ultra-shallow-implants. Ingefelte, D.; Pepponi, G.; Meirer, F.; Wobruschek, P.; Strelli, C. *Spectrochimica Acta Part B*. Apr2016, Vol. 118, p20-28. 9p. DOI: [10.1016/j.sab.2016.02.010](https://doi.org/10.1016/j.sab.2016.02.010).

Electrochemical Mechanism for FeS₂/C Composite in Lithium Ion Batteries with Enhanced Reversible Capacity. Shengqing Wang; Jingxian Yu. *Energies*. Apr2016, Vol. 9 Issue 4, p391-9p. 1 Color Photograph, 1 Chart, 7 Graphs. DOI: [10.3390/en9040225](https://doi.org/10.3390/en9040225).

Combined Operando X-ray Diffraction/Raman Spectroscopy of Catalytic Solids in the Laboratory: The Co/TiO₂ Fischer-Tropsch Synthesis Catalyst Showcase. Cats, Korneel H.; Weckhuysen, Bert M. *ChemCatChem*. Apr2016, Vol. 8 Issue 8, p1531-1542. 12p. DOI: [10.1002/cctc.201600074](https://doi.org/10.1002/cctc.201600074).

Ultrafast and nonlinear surface-enhanced Raman spectroscopy. Gruenke, Natalie L.; Cardinal, M. Fernanda; McAnally, Michael O.; Frontiera, Renee R.; Schatz, George C.; Van Duyne, Richard P. *Chemical Society Reviews*. 4/21/2016, Vol. 45 Issue 8, p2263-2290. 28p. DOI: [10.1039/c5cs00763a](https://doi.org/10.1039/c5cs00763a).

Characterizing typical farmland soils in China using Raman spectroscopy. Xing, Zhe; Du, Changwen; Zeng, Yin; Ma, Fei; Zhou, Jianmin. *Geoderma*. Apr2016, Vol. 268, p147-155. 9p. DOI: [10.1016/j.geoderma.2016.01.029](https://doi.org/10.1016/j.geoderma.2016.01.029).