



**MiniFlex – qualitative and quantitative analysis of polycrystalline materials**



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

New sixth generation MiniFlex X-ray diffractometer (XRD) is a multipurpose analytical instrument that can determine: phase identification and quantification, percent (%) crystallinity, crystallite size and strain, lattice parameter refinement, Rietveld refinement, and molecular structure. It is widely used in research, especially in material science and chemistry, as well as in industry for research and quality control. It is the newest addition to MiniFlex series of benchtop X-ray diffraction analyzers from Rigaku, which began with the introduction of the original MiniFlex system decades ago. **For more >**

**Interested in publishing your work in The Bridge?**



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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 permitted to obtain permission to republish. Please send copy to the editor at [Rigaku.newsletter@Rigaku.com](mailto:Rigaku.newsletter@Rigaku.com)

**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 >**

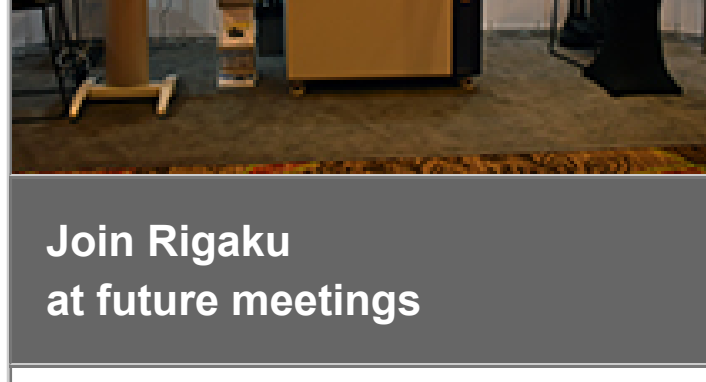
**Video of the Month**



**Top Science News**

Here is the top science news from the last three weeks by [SuspiciousObservers](#), an online community that investigates solar activity, earthquakes, astrophysics and weather. **Watch video >**

**Conferences and Workshops**



**Join Rigaku at future meetings**

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

- EPD/C16**  
Edinburgh, UK  
July 1 – 4, 2018
- SEMICON West**  
San Francisco, CA, USA  
July 10 – 12, 2018
- NANO Korea 2018**  
KINTEX, Gyeonggi-do, Korea  
July 11 – 13, 2018

**See the complete list >**

**Useful Link of the Month**

**General Differential Equation Solver**

Specify Differential Equation

**WolframAlpha Widgets**

Add live computational widgets to your website or blog. Search WolframAlpha Widget Gallery for hundreds of pre-built widgets. The embed code is easy to copy and paste—no programming skills are required. **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 >**

**Welcome**

As always, thanks to everyone who took the time to come and talk to us at the various events that we attended in May and early June. In July, Rigaku will attend many events worldwide ([see full list](#)). Of particular note are the [American Crystallographic Association \(ACA 2018\)](#) exhibit in Toronto (July 20 – 24), the [16th European Powder Diffraction Conference](#) in Edinburgh (July 1 – 4) and [SEMICON West](#) in San Francisco (July 10 – 12).

This month's issue contains a featured article on phase identification based on cluster analysis of Debye rings and a *Rigaku Journal* article introducing single crystal X-ray analysis.

Application papers are also available for XRD, EDXRF, and WDXRF. The book review covers *The Evolution of Scientific Knowledge: From Certainty to Uncertainty* by Edward R. Dougherty. Check out the news and papers sections at the bottom of the page for the latest developments in materials science.

R.C. Tisdale, Ph.D. – Editor

**Featured Article**  
**Phase Identification Based on the Result of Cluster Analysis of Debye Rings**  
By Dr. Akito Sasaki, Rigaku Corporation



One of the most utilized purposes of powder X-ray diffraction is "phase identification." If information on the compounds contained in the powder sample is available, it can be determined if each compound is included in the sample by comparing its powder X-ray diffraction pattern with the experimental diffraction data of the sample using a pattern-matching method. **Full article >**

**Featured Rigaku Journal Article**  
**Introduction to Single Crystal X-ray Analysis**  
**I. What is X-ray crystallography?**  
By Kimiko Hasegawa, Rigaku Corporation



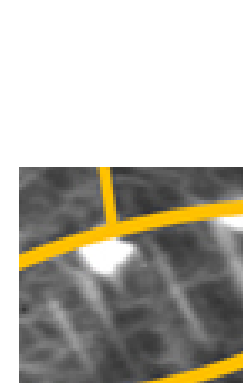
All substances around us consist of atoms. The types of atoms and their three-dimensional arrangement define the structure of materials, therefore the nature of materials. Since the properties and functions of materials relate directly to its structure, there exist extensive researches for various materials such as semiconductor, electronic, food, pharmaceutical, or life science related materials. **Full article >**

**XRD Application Note**  
**Qualitative Analysis of an Ancient Glass Bead with Rigaku's SmartLab**  
Research conducted by Tomomi Tamura, Nara National Research Institute for Cultural Properties, Center for Archaeological Operations, Conservation Science Section



The Oido tunnel tombs in Wakuyacho, Miyagi (Japan) were constructed between the late 7th century and the early 8th century. During scientific investigations between 1962 and 1964, a glass bead with a spotted pattern rare to Japan was excavated. By evaluating the colored portion of the glass bead using the SmartLab Automated Multipurpose X-ray Diffractometer, it was possible to determine its chemical composition and provide a scientific basis for assumptions on the fabrication technique and a reevaluation of its origin. **For more >**

**XRD Application Note**  
**Crystal Defect Analysis by X-ray Reflection Topography**  
**Observation of Magnesium Oxide Single Crystal Substrate**  
Rigaku Corporation



Crystal defects in epitaxial thin films may cause problems when producing high-performance semiconductor devices. Epitaxial thin films may inherit crystal defects from the single crystal substrate. It is important to evaluate the grains and crystal defects of the single crystal substrate before film growth on it. X-ray topography is an XRD imaging technique used to observe crystal defect distribution in a single crystal substrate. The SmartLab automated multipurpose X-ray diffractometer, equipped with an Xsight™ Micron FC high-sensitivity X-ray CCD camera, is capable of obtaining high-resolution topographs like those measured with dedicated equipment. **For more >**

**EDXRF Application Note**  
**Chemical Bath for Copper Foil Surface Treatment**  
Applied Rigaku Technologies



Measurement of aqueous chemical bath solutions containing nickel, cobalt, molybdenum, zinc and indium is demonstrated using Rigaku's NEX OL. **For more >**

**WDXRF Application Note**  
**Polymetallic Sulfide Ore Analysis with Supermini200**  
Rigaku Corporation



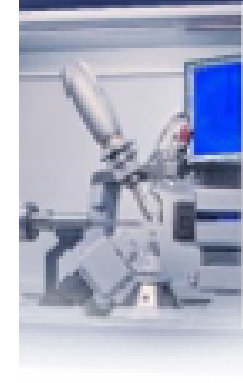
Polymetallic sulfide deposits are often major sources of copper, zinc, lead, gold and silver ore. Some of these deposits also contain many various metals such as co- or by-products and impurities. Laboratories in mining sites are often required to analyze large number of samples per day. Therefore, in order to determine multiple elements in ores, simple and fast analysis technique with high accuracy and precision is demanded. **For more >**

**Small Molecule Application Note**  
**Higher Flux from the XtaLAB Synergy-DW Leads to Improved Data for Small Crystals and Challenging Sample Types**  
Rigaku Oxford Diffraction



Single crystal X-ray diffraction is the preferred method for structure determination of small molecules as well as protein and larger biological macromolecules. The complexity of samples that can be studied using X-ray techniques has improved significantly over recent years. Samples that were previously too small to be considered for single crystal X-ray analysis are now fully amenable to study. Highly unstable and weakly diffracting samples may be studied immediately, samples do not need to be discarded or undergo further recrystallization attempts. **For more >**

**Book Review**  
**The Evolution of Scientific Knowledge: From Certainty to Uncertainty**  
by Edward O. Dougherty, SPIE Press, Bellingham, 2016  
Review by Joseph Ferrara, Deputy Director, X-ray Research Laboratory, Rigaku



I came across this title at the book shop at a conference for the International Society for Optics and photonics (SPIE). The author is on the faculty of Texas A&M in the department of Electrical Engineering and Computer Science, as well as an SPIE fellow. **Full review >**

**Material Analysis in the News**  
**News for June 2018**

**June 1, 2018.** A study by Yutaro Takaya of Waseda University, along with the University of Tokyo, and the Japan Agency for Marine-Earth Science and Technology, revealed that an estimated **16 million metric tons of Rare Earth Elements (REEs)** — enough to fulfill global demands potentially for hundreds of years on a semi-infinite basis — have been discovered in Japanese waters near Minami-Torishima, an island in the Ogasawara Island group located about 1,800 kilometers southeast of Tokyo.

**June 8, 2018.** Researchers at Japan's National Institute for Materials Science (NIMS) have reported that nanoporous, **amorphous silicon film anodes** can show excellent cycling stability with extremely high lithium storage capacity. These capacities are larger than those of conventional graphite anode materials.

**June 8, 2018.** NASA's Curiosity rover has found new evidence preserved in **rocks on Mars that suggests the planet could have supported ancient life**, as well as new evidence in the Martian atmosphere that relates to the search for current life on the Red Planet.

**June 11, 2018.** A Japanese asteroid-sampling spacecraft has its target in sight. The **Hayabusa2 probe has photographed Ryugu**, the space rock it's scheduled to start orbiting late this month. The spacecraft will depart Ryugu in November or December 2018, and its collected samples will come back to Earth in a special return capsule in late 2020.

**June 12, 2018.** Yokohama National University researchers, led by Dr. Daisuke Yoshida, resolve the age-old **mystery of why silicon cannot replace carbon in organic compounds**. A new benchmark quantum chemical calculation of C<sub>2</sub>, Si<sub>2</sub>, and their hydrides for the first time reveals a qualitative difference in the topologies of core electron orbitals of organic molecules and their silicon analogues.

**June 13, 2018.** Research led by Kuhan Chandru and Jim Cleaves from the Earth-Life Science Institute at Tokyo Institute of Technology, Japan, has shown that reactions of alpha-hydroxy acids, similar to the **alpha-amino acids that make up modern proteins, form large polymers** easily under conditions presumed prevalent on early Earth.

**June 14, 2018.** A team of Japanese scientists led by Masahiro Kayama of Tohoku University's Frontier Research Institute for Interdisciplinary Science has discovered a **mineral known as moganite in a lunar meteorite found in a hot desert in northwest Africa**. This is significant because moganite is a mineral that requires water to form, reinforcing the belief that water exists on the Moon.

**June 14, 2018.** Everyone makes **mistakes, but when scientists do, the remedy goes** far beyond saying you're sorry. Two fresh examples show how some journals and universities react when the need arises to set the record straight.

**June 14, 2018.** The **melting of Antarctica is accelerating at an alarming rate**, with about 3 trillion tons of ice disappearing since 1992, an international team of ice experts said in a new study. From 1992 to 2011, Antarctica lost nearly 84 billion tons of ice a year; from 2012 to 2017, the melt rate increased to more than 241 billion tons a year.

**June 15, 2018.** In a fusion of mathematics and earth science, researchers from the International Institute for Carbon-Neutral Energy Research (I2CNER) and the Institute of Mathematics for Industry (IMI) of Kyushu University have now developed an **innovative method to characterize pore geometry**, based on a concept called persistent homology theory.

**Recent Scientific Papers of Interest**  
**Papers for June 2018**



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

**Quantitative X-ray diffraction and X-ray fluorescence analyses of mixtures – unified and simplified.** Chung, Frank H. *Journal of Applied Crystallography*. Jun2018, Vol. 51 Issue 3, p789-795. 6p. DOI: [10.1107/S1600576718005228](https://doi.org/10.1107/S1600576718005228).

**Accurate experimental determination of gallium K- and L3-shell XRF fundamental parameters.** Unterumtsberger, Rainer; Hönicke, Philipp; Colaux, Julien L.; Jaynes, Chris; Wansleben, Malte; Müller, Matthias; Beckhoff, Burkhard. *Journal of Analytical Atomic Spectrometry*. Jun2018, Vol. 33 Issue 6, p1003-1013. 11p. DOI: [10.1039/c8ja00046h](https://doi.org/10.1039/c8ja00046h).

**Recent advances in LIBS and XRF for the analysis of plants.** Arantes de Carvalho, Gabriel Gustinelli; Bueno Guerra, Marcelo Braga; Adame, Andressa; Nomura, Cassiana Seimi; Oliveira, Pedro Vitoriano; Pereira de Carvalho, Hudson Wallace; Santos, Dário; Nunes, Lidiiane Cristina; Krug, Francisco José. *JAAS (Journal of Analytical Atomic Spectrometry)*. Jun2018, Vol. 33 Issue 6, p919-944. 26p. DOI: [10.1039/c7ja00293a](https://doi.org/10.1039/c7ja00293a).

**Detection and quantitative determination of heavy metals in electronic cigarette refill liquids using Total Reflection X-ray Fluorescence Spectrometry.** Kariuki, Eleni; Farsalinos, Konstantinos; Poulas, Konstantinos; Kontoyannits, Christos G.; Orkoulas, Malvina G. *Food & Chemical Toxicology*. Jun2018 Part B, Vol. 116, p233-237. 5p. DOI: [10.1016/j.fct.2018.03.035](https://doi.org/10.1016/j.fct.2018.03.035).

**Sheet beam x-ray fluorescence computed tomography (XFCT) imaging of gold nanoparticulates.** Dunning, Chelsea A. S.; Bazalova-Carter, Magdalena. *Medical Physics*. Jun2018, Vol. 45 Issue 6, p2572-2582. 11p. DOI: [10.1002/mp.12893](https://doi.org/10.1002/mp.12893).

**Differentiation of dental restorative materials combining energy-dispersive X-ray fluorescence spectroscopy and post-mortem CT.** Merriam, Tim; Kaufmann, Rolf; Ebert, Lars; Figi, Renato; Erni, Rolf; Pauer, Robin; Sieberth, Till. *Forensic Science, Medicine & Pathology*. Jun2018, Vol. 14 Issue 2, p163-173. 11p. DOI: [10.1007/s12024-018-9579-5](https://doi.org/10.1007/s12024-018-9579-5).

**Total reflection X-ray Fluorescence determination of interfering elements rubidium and uranium by profile fitting.** Dhara, Sangita; Khooha, Ajay; Singh, Ajit Kumar; Tiwari, M.K.; Misra, N.L. *Spectrochimica Acta Part B*. Jun2018, Vol. 144, p87-91. 5p. DOI: [10.1016/j.sab.2018.03.011](https://doi.org/10.1016/j.sab.2018.03.011).

**Determination of trace metals in spirits by total reflection X-ray fluorescence spectrometry.** Siverio, G.; Cinosi, A.; Monticelli, D.; Seralessandri, L. *Spectrochimica Acta Part B*. Jun2018, Vol. 144, p15-19. 5p. DOI: [10.1016/j.sab.2018.03.006](https://doi.org/10.1016/j.sab.2018.03.006).

**Bench-scale insight into the amenability of case barren copper ores towards XRF-based bulk sorting.** Li, Lixia; Li, Genzhuang; Li, Hui; Puzhen, Li; Guoqing; Zhang, Ding; Klein, Bern. *Minerals Engineering*. Jun2018, Vol. 121, p129-136. 8p. DOI: [10.1016/j.meng.2018.02.023](https://doi.org/10.1016/j.meng.2018.02.023).

**Sample preparation for total reflection X-ray fluorescence analysis using resist pattern technique.** Tsujii, K.; Yomogita, N.; Konyuba, Y. *Spectrochimica Acta Part B*. Jun2018, Vol. 144, p68-74. 7p. DOI: [10.1016/j.sab.2018.03.005](https://doi.org/10.1016/j.sab.2018.03.005).

**Effect of microwave treatment on structures of kaczmarek sodium carboxymethyl starch: FT-IR, FT-Raman and XRD investigations.** Kaczmarek, Karolina; Grabowska, Beata; Spychaj, Tadeusz; Zdanowicz, Magdalena; Bitar, Maciej; Bobrowski, Artur; Cukrowicz, Sylwia. *Spectrochimica Acta Part A: Molecular & Biomolecular Spectroscopy*. Jun2018, Vol. 199, p387-393. 7p. DOI: [10.1016/j.saa.2018.03.047](https://doi.org/10.1016/j.saa.2018.03.047).

**Near-surface clay authigenesis in exhumed fault rock of the Alpine Fault Zone (New Zealand): O-H Ar isotopic, XRD and chemical analysis of illite and chlorite.** Boles, Austin; Mulch, Andreas; van der Puijff, Ben. *Journal of Structural Geology*. Jun2018, Vol. 111, p27-41. 15p. DOI: [10.1016/j.jsg.2018.03.008](https://doi.org/10.1016/j.jsg.2018.03.008).

**Chemical Identification by Macroscopic X-ray Powder Diffraction (MA-XRPD) of Gogh's Sunflowers: Mapping of Areas with Higher Degradation Risk.** Vanmeert, Frederik; Hendriks, Ella; Van der Snickt, Geert; Monaco, Letizia; Dik, Joris; Janssens, Koen. *Angewandte Chemie International Edition*. 6/18/2018, Vol. 57 Issue 25, p7418-7422. 5p. DOI: [10.1002/anie.201713293](https://doi.org/10.1002/anie.201713293).

**Static strength of molybdenum to 92 GPa under radial X-ray diffraction.** Xiong, L.; Tu, P.; Li, B.; Wu, S. Y.; Hao, J. B.; Bai, L. G.; Li, X. D.; Liu, J. *International Journal of Modern Physics B: Condensed Matter Physics; Statistical Physics; Applied Physics*. Jun2018, Vol. 32 Issue 14, pN.PAG-N.PAG. 8p. DOI: [10.1142/S0217979218501771](https://doi.org/10.1142/S0217979218501771).

**Crystal Structure of Levofloxacin Anhydrides: A High-Temperature Powder X-ray Diffraction Study Versus Crystal Structure Prediction.** Freitas, Jennifer T. J.; de Melo, Cristiane C.; Viana, Olimpia M. M. S.; Ferreira, Fabio F.; Dorignetti, Antonio C. *Crystal Growth & Design*. 6/6/2018, Vol. 18 Issue 6, p3558-3568. 11p. DOI: [10.1021/acs.cgd.8b00363](https://doi.org/10.1021/acs.cgd.8b00363).

**Effect of the solid/liquid interface structure on X-ray diffraction in nano-biocomposites.** Zolotayabko, Emil. *Journal of Applied Crystallography*. Jun2018, Vol. 51 Issue 3, p849-853. 4p. DOI: [10.1107/S1600576718006167](https://doi.org/10.1107/S1600576718006167).

**In situ Bragg coherent X-ray diffraction during tensile testing of an individual Au nanowire.** Shin, J.; Cornelius, T. W.; Labat, S.; Lauraux, F.; Richard, M.-I.; Richter, G.; Blanchard, N. P.; Gianola, D. S.; Thomas, O. *Journal of Applied Crystallography*. Jun2018, Vol. 51 Issue 3, p781-788. 7p. DOI: [10.1107/S1600576718004910](https://doi.org/10.1107/S1600576718004910).

**Crystal structure analysis of a star-shaped triazine compound: a combination of single-crystal three-dimensional electron diffraction and powder X-ray diffraction.** Gorelik, Tatiana E.; van de Streek, Jacco; Meier, Herbert; Endermach, Lars; Opatz, Till. *Acta Crystallographica: Section B, Structural Science, Crystal Engineering & Materials*. Jun2018, Vol. 74 Issue 3, p287-294. 7p. DOI: [10.1107/S2052520618006686](https://doi.org/10.1107/S2052520618006686).

**X-Ray Diffraction of Iron Containing Samples: The Importance of a Suitable Configuration.** Mos, Yvonne M.; Vermeulen, Arnold C.; Buisman, Cees J. N.; Weijman, Jan. *Geomicrobiology Journal*. Jun2018, Vol. 35 Issue 6, p511-517. 7p. DOI: [10.1080/01490451.2017.1401183](https://doi.org/10.1080/01490451.2017.1401183).

**The composition, unit cell parameters and microstructure of quartz during phase transformation from alpha to beta as examined by in-situ high-temperature X-ray powder diffraction.** Karunadasa, Kohobhange S.P.; Manorathe, C.H.; Pitawala, H.M.T.G.A.; Rajapakse, R.M.G. *Journal of Physics & Chemistry of Solids*. Jun2018, Vol. 117, p131-138. 8p. DOI: [10.1016/j.jpcs.2018.02.028](https://doi.org/10.1016/j.jpcs.2018.02.028).

**A high-pressure X-ray diffraction study of the crystalline phases in calcium aluminato cement paste.** Geng, Guoqing; Li, Jiaqi; Zhou, Yang; Liu, Lin; Yan, Jinyuan; Kunz, Martin; Monteiro, Paulo J.M. *Cement & Concrete Research*. Jun2018, Vol. 108, p38-45. 8p. DOI: [10.1016/j.cemconres.2018.03.004](https://doi.org/10.1016/j.cemconres.2018.03.004).

**X-ray diffraction studies and dielectric properties of Ni doped Mg ferrites.** Chavan, Pradeep; Naik, L.R. *Vacuum*. Jun2018, Vol. 152, p47-49. 3p. DOI: [10.1016/j.vacuum.2018.03.007](https://doi.org/10.1016/j.vacuum.2018.03.007).

**Background radiation in inelastic X-ray scattering and X-ray emission spectroscopy. A study for Johann-type spectrometers.** Paredes Mellone, O.A.; Bianco, L.M.; Ceppi, S.A.; Goncalves Honnicke, M.; Stutz, G.E. *Nuclear Instruments & Methods in Physics Research Section A*. Jun2018, Vol. 894, p119-128. 10p. DOI: [10.1016/j.nima.2018.03.036](https://doi.org/10.1016/j.nima.2018.03.036).

**The dynamics of asphaltene aggregates in heavy crude oils on a nanometer scale studied via small-angle X-ray scattering in situ.** Larichev, Yu.V.; Martyanov, O.N. *Journal of Petroleum Science & Engineering*. Jun2018, Vol. 165, p575-580. 6p. DOI: [10.1016/j.petrol.2018.02.063](https://doi.org/10.1016/j.petrol.2018.02.063).