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THE BRIDGE
MATERIALS ANALYSIS eNEWSLETTER
MAY 2016, ISSUE 35

Powder diffraction, thin film diffraction, SAXS, in-plane scattering

SmartLab®

The SmartLab is the most novel high-resolution X-ray diffractometer available today. Perhaps its most novel feature is the SmartLab Guidance software, which provides you with an intelligent interface that guides you through the intricacies of each experiment. It is like having an expert standing by your side. **For more >**

Interested in publishing your work in The Bridge?

Publish Your Work Here

The Bridge now welcomes manuscripts, communications, 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 send copy to the editor at Rigaku.newsletter@Rigaku.com

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 >**

Video of the Month

Shakespeare and Science Fiction

Arguably the first great science fiction film of the modern era was MGM's lavishly produced *Forbidden Planet* (1956), which was set in the 23rd century. The movie's most famous character was Robbie the robot, who has appeared in dozens of roles up to the present day. What many do not realize is that the plot is actually a retelling of Shakespeare's fourth and final romance play, *The Tempest* (1610). In the play, the main characters, Prospero and his daughter Miranda, have been living on a primitive island for some time. The play is infused with illusion and magic. Prospero has become a King on the island and is in control of Ariel, an airy spirit. In the movie, Dr. Morbius is Prospero, his daughter Alexia is Miranda, and Robby is Ariel. This two part documentary provides great insight into this most important film. **Watch video >**

Conferences and Workshops

Join Rigaku at future meetings

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

Bureau of International Recycling
Berlin, Germany
May 30 – 31, 2016

39th Canadian Chemistry Conference (CSC)
Halifax, NS, Canada
June 4 – 9, 2016

PPXRD-14
Fort Myers, FL, USA
June 6 – 9, 2016

Advanced Materials Characterization Workshop
Urbana-Champaign, IL, USA
June 7 – 8, 2016

See the complete list >

Useful link of the Month

Full Profile Search Match by L. Lutterotti

The "FPSM method" uses a Rietveld-like fitting procedure to test all possible crystal structures from a database, rank them and find the more probable in your diffraction pattern. In the end, a Rietveld phase quantification is done with the phases identified. Be aware that if a phase is not present in the database (COD is used here), it cannot be found nor quantified; so this method is limited to only the phases for which a crystal structure has been determined and has been uploaded to the COD database. This page has been constructed to permit other people to use the method and test it on their data. To use it you need to upload a datafile in proper format. Use a pm or .txt, double column format with no title line, first column contains the 2theta coordinates (it space for TOF), the second column the intensity (corrected for incident intensity for TOF). You need also to specify some additional instrument characteristics (wavelength, geometry etc.). If the selected instrumental broadening function matches the one of your instrument, then a reasonable analysis of crystallite sizes and microstrain is reported. **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 >**

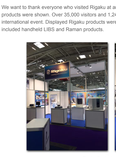
Rigaku's Materials Analysis eNewsletter, The Bridge

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 analytica® 2016 in Munich, where a variety of products were shown. Over 35,000 visitors and 1,244 exhibitors made for an important international event. Displayed Rigaku products were based on various X-ray technologies and also included handheld LIBS and Raman products.



Rigaku Booth at analytica 2016

Please come and see us at the following materials science events in June: Canadian Chemistry Conference (Halifax), PPXRD-14 (Fort Myers, FL) and European Conference on X-Ray Spectrometry (Gothenburg). We promise to have new and interesting things to discuss.

Our featured technical paper covers the "Determination of Crystalline Phase and Amorphous Phase in Refractory Material by X-ray Diffraction Analysis Using the Rietveld Refinement."

The first serious science fiction movie, based on Shakespeare's *The Tempest*, 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

Lab in the Spotlight
An introduction to the latest article by Dr. Atsushi Obuchi

Quantitative analyses of components in refractories were carried out using the Rietveld refinement of X-ray diffraction patterns. Samples were sorted with a little powdering and rotated when they were analyzed by Co tube. **For more >**

Featured XRF Rigaku Journal Article
Sample preparation for X-ray fluorescence analysis
L. Quilitz of sample preparation
Rigaku Corporation

XRF (X-ray fluorescence) analysis as a technique is widely used in academia, research and development and industry as an analysis tool for the determination of elemental composition of materials. Unlike chemical and other instrumental techniques which require the use of hazardous chemicals and difficult preparation methods to dissolve samples for analysis purposes, the quick, accurate, sensitive non-destructive analysis technique of XRF makes it attractive as an analytical technique, this coupled with the fact that it can be used by non-technical users and does not require expert knowledge and high skill levels to produce good, reliable, reproducible analytical data. XRF is considered to be less labor intensive and more environmentally friendly that the aforementioned methods. **For more >**

XRD Application Note
MiniFlex300/600: Measurement of trace components using DtleX Ultra
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 120 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
Characterization of a Next-Generation Magnetic Recording Media (FePt) by In-Plane X-ray Diffraction
Rigaku Corporation

As next-generation ultra-density magnetic recording media, granular thin films in which metal nanoparticles are dispersed have been a focus of attention. Among these films, the regular phase (tetragonal crystal) of FePt has a particularly high magnetic anisotropy as well as good corrosion and oxidation resistances, so it is expected that it will be applied to actual devices. However, the irregular phase (cubic crystal) is created at the same time, depending on the film-forming conditions. For this reason, a technique to distinguish these crystalline phases at the nanoparticle and thin film level is required. **For more >**

WDXRF Application Note
Cement Analysis by the Fusion Method on Benchtop WDXRF Supermini200 According to ASTM C114-11
Rigaku Corporation

Cement is one of the most important materials for construction. Many kinds of hydraulic cements, including Portland cement, with various physical properties are produced by changing the composition of clinker minerals; therefore, it is important to control the chemical composition of cement products and interim products. **For more >**

EDXRF Application Note
Gold Recovery
Applied Rigaku Technologies

The measurement of gold is demonstrated in used ore material such as from ore dumps and tailing piles. The application note also shows the recovery of uranium from the used ore material. **For more >**

Featured Raman Rigaku Journal Article
Advantage of handheld Raman spectrometer with 1064 nm excitation in pharmaceutical raw material identification
Rigaku Corporation

Quality control is a top priority for the pharmaceutical industry. RMID (raw material identification) is an important part of quality control. Since health authorities of many countries including Japan joined PIC/S recently, quick and reliable RMID is becoming more important. **For more >**

Featured Software Rigaku Journal Article
Automated dislocation evaluation software for X-ray topography images
Rigaku Corporation

X-ray topography is a powerful technique for evaluating crystal defects such as dislocations, stacking faults, scratches, and so on. High-performance electronic devices such as microprocessors, solidstate memories, imaging processors are fabricated on dislocation-free Si single crystal wafers. However, device fabrication process often induce dislocations in the Si wafers that can affect the devices performance. Because X-ray topography can evaluate these crystal defects efficiently, it plays and important role in the Si industry. **For more >**

Scientific Book Review
Lab Girl by Hope Jahren

Jahren has an impressive resume. A geobiologist, she got her undergraduate degree at University of Minnesota and her PhD at the University of California at Berkeley. She has effectively built three laboratories from scratch, at three different universities: Georgia Tech, Johns Hopkins, and the University of Hawai'i at Manoa. Jahren really is, as the title of her book suggests, a "lab girl."
For more >

Material Analysis in the News
News for May 2016

May 2, 2016. Northwestern University's Mark Hersam discovered a way to stabilize exfoliated black phosphorene – or phosphorene – a layered semiconductor that chemically degrades in open air but shows great promise for electronics. Passivation was achieved by using organic chemistry to create nearly a single-molecule-thick layer onto phosphorene.

May 3, 2016. Researchers at KU Leuven have shed light on how adding limonene could improve the texture in low-fat versions of chocolate and the ability to melt. The researchers examined cocoa butter crystallization at 63°F and 88°F using differential scanning calorimetry and X-ray diffraction to examine cocoa butter profiles when limonene was added.

May 5, 2016. Using a layer of molybdenum disulfide less than 1 nanometer thick, researchers at Rice University have designed a system that can absorb more than 35 percent of incident light in the 400- to 700-nanometer wavelength range.

May 5, 2016. Researchers at the University of Valencia have shown that the superconducting state can be maintained even when the material in question is reduced from three to two dimensions, making the efficiency gains needed for technologies like those underlying the frictionless train possible.

May 10, 2016. A team of scientists from Los Alamos National Laboratory has released a study that shows a new strategy could be extremely useful in developing new materials. Scientists have employed machine learning to cut down the trial-and-error period of testing out new materials that can be used for a wide range of applications.

May 10, 2016. An international team of scientists has used synchronized infrared and X-ray laser pulses to simultaneously manipulate and reveal the ultra-fast magnetic properties of this promising quantum landscape. The rapid, light-driven switching between magnetic states, explored here with unprecedented precision, could one day revolutionize the reading and writing of data in computers and other digital devices.

May 11, 2016. What does climate change look like? A spiraling animation from British climate scientist Ed Hawkins, which illustrates the data since 1850, captures a century and a half of change in just seconds.

May 11, 2016. Scientists have combined two different analytical methods at the BESSY II synchrotron source in order to extract more information about the chemistry of hydrogen metal catalysts in action. These hybrid catalyst compounds can act as catalysts to promote desirable reactions in energy materials, but their behavior has not been completely understood thus far.

May 16, 2016. Physicists have discovered a new form of light. Until now, it was thought that for all forms of light, the angular momentum would be a integer multiple of Planck's constant – a physical constant that sets the scale of quantum effects. But researchers led by Trinity College Dublin have now demonstrated that a new form of light exists, where the angular momentum is only half of this value.

May 17, 2016. Decommissioning the Fukushima Daiichi Nuclear Plant just got one step closer. Japanese researchers have mapped the distribution of boron compounds in a modeled control rod, paving the way for determining re-criticality risk within the reactor.

Recent Scientific Papers of Interest
Papers for May 2016

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

Combined X-ray diffraction and fluorescence analysis in the cultural heritage field. Lutterotti, Luca; Dell'Amico, Federica; Angelucci, Diego; Fontana, Raffaella; Pezzati, Giulianini; Stefano; *Microchemical Journal*. May2016, Vol. 126, p423-430. 8p. DOI: 10.1016/j.microc.2015.12.031.

Formation and dynamical theory of X-ray diffraction for perfect crystals in the Laue case using the Riemann surface. Saka, Tomoe; *Acta Crystallographica: Section A, Foundations & Advances*. May2016, Vol. 72 Issue 3, p338-348. 10p. DOI: 10.1107/S2053273316001005.

Combination of projection-based XRF, XAFS and XRD imagings for rapid spatial distribution analysis of a heterogeneous metal-bearing material. Shimura, Mitsuko; Hitomi, Sakae; Nakata, Kaoru; *Journal of Analytical Atomic Spectrometry*. May2016, Vol. 31 Issue 5, p1105-1111. 7p. DOI: 10.1039/c6ja00024j.

Elemental Analysis of Different Varieties of Rice Samples using XRF Technique. Kaur, Jaspreet; Kumar, Anil; *AIP Conference Proceedings*. 2016, Vol. 1728 Issue 1, p020350-1-020350-4. 4p. DOI: 10.1063/1.4946431.

Direct investigations on strain-induced cold crystallization behavior and structure evolutions in amorphous poly(lactic acid) with SAXS and WAXS measurements. Zhou, Chenghui; Li, Hongfei; Zhang, Wenyang; Li, Jingjing; Huang, Shaoqong; Meng, Yanfeng; Christiansen, Jesper deClaville; Yu, Donghong; Wu, Zhonghua; Jiang, Shichun. *Polymer*. May2016, Vol. 90, p111-121. 11p. DOI: 10.1016/j.polymer.2016.03.014.

Dehydration of $AlPO_4$-34 studied by variable-temperature NMR, XRD and first-principles calculations. Varlec, Jure; Krajnc, Andraž; Mazaj, Matjaž; Ristić, Alenka; Venatalu, Katju; Oss, Andres; Samoson, Ago; Kaučič, Venčeslav; Mali, Gregor. *New Journal of Chemistry*. May2016, Vol. 40 Issue 5, p4178-4186. 9p. DOI: 10.1039/c5nj02838h.

Evolution of extended defects in polycrystalline UO_2 under heavy ion irradiation: combined TEM, XRD and Raman study. Cloet, C.; Sabathier, C.; Palancher, H.; Carlot, G.; Miro, S.; Servois, Y.; Desgardin, L.; Legros, M. *Nuclear Instruments & Methods in Physics Research Section B*. May2016, Vol. 374, p51-57. 7p. DOI: 10.1016/j.nimb.2015.08.091.

Measurement of L-XRF cross-sections and Coster–Kronig enhancement factors for ^{152}Sm at excitation energies 6.8, 7.4 and 8 keV. Kumar, R.; Rani, A.; Singh, R.M.; Tiwari, M.K.; Singh, A.K. *Journal of Electron Spectroscopy & Related Phenomena*. May2016, Vol. 209, p34-39. 6p. DOI: 10.1016/j.elspec.2016.03.008.

Combining XRF and GRT for the analysis of ancient silver coins. Ager, F.J.; Gómez-Tubío, B.; Paul, A.; Gómez-Morón, A.; Scrivano, S.; Ortiz-Repiso, I.; Respaldiza, M.A. *Microchemical Journal*. May2016, Vol. 126, p149-154. 6p. DOI: 10.1016/j.microc.2015.12.017.

Interaction of selenite with reduced Fe and/or S species: An XRD and XAS study. Finck, Nicolas; Dardenne, Kathy. *Journal of Contaminant Hydrology*. May2016, Vol. 186, p44-51. 8p. DOI: 10.1016/j.jconhyd.2016.03.001.

Extended and local structural description of a kaolinitic clay, its fired ceramics and intermediates: An XRD and XANES analysis. Andrini, L.; Gauna, M.R.; Conconi, M.S.; Suarez, G.; Requejo, F.G.; Agüero, E.F.; Rendtorff, N.M. *Applied Clay Science*. May2016, Vol. 124, p39-45. 7p. DOI: 10.1016/j.clay.2016.01.049.

Structural changes in SAPO-34 due to hydrothermal treatment. A NMR, XRD, and DRIFTS study. Arstad, Bjørnar; Lind, Anna; Cavka, Jasmina H.; Thorshaug, Karl; Akporiaye, Duncan; Wragg, David; Fjellvåg, Helmer; Grønvold, Arne; Fuglerud, Terje. *Microporous & Mesoporous Materials*. May2016, Vol. 225, p421-431. 11p. DOI: 10.1016/j.micromeso.2016.01.024.

Investigate of Atmospheric Arsenic, Cadmium, Chromium, Lead, and Mercury Levels in Moss Species Found around Zirkale by EDXRF Spectrometry. Akçay, Nükey; Batan, Necati; Çinar, Yunus. *AIP Conference Proceedings*. 2016, Vol. 1728 Issue 1, p1-5. 5p. 1 Chart, 1 Map. DOI: 10.1063/1.4945950.

Evaluation of EDXRF configurations for timing the effect of detection and exposure for *in vivo* quantification of gadolinium in tumor tissue. Santibáñez, M.; Vázquez, M.; Figueroa, R.G.; Valente, M. *Radiation Physics & Chemistry*. May2016, Vol. 122, p28-34. 7p. DOI: 10.1016/j.radphyschem.2016.01.015.

Determination of selenium in biological samples with an energy-dispersive X-ray fluorescence spectrometer. Li, Xiaoli; Ye, Zhaohui. *Applied Radiation & Isotopes*. May2016, Vol. 111, p45-49. 5p. DOI: 10.1016/j.apradiso.2016.02.010.

Functionalized metal-organic-framework CMFrO@MIL-101(Cr) as a stable and selective rare earth adsorbent. Decker, Jensen; Clancy, Jeriffa; Vermeer, Pieter; Voort, Pascal. Journal of Materials Science. May2016, Vol. 51 Issue 10, p5019-5026. 8p. 1 Color Photograph, 2 Diagrams, 2 Charts, 5 Graphs. DOI: 10.1007/s10853-016-9807-9

Suitability of Transportable EDXRF for the On-site Assessment of Ancient Silver Coins and Other Silver Artefacts. Corsi, Damiano; Cotten, Gabriel. *Archaeometry*. May2016, Vol. 70 Issue 5, p940-951. 12p. DOI: 10.1111/arcm.12238.

Innovative combination of spectroscopic techniques to reveal nanoparticle fate in a crop plant. Lanoux, Cécile; Castillo-Michel, Hiram; Rivasseau, C. Fayard; Lefebvre, Pierre; Emetline, Villanova; Julie; Magnin, Valérie; Pradas del Real, Ana-Elena; Trona, Nicolas; Legros, Samuel; Sorieul, Stéphanie; Sarret, Géraldine. *Spectrochimica Acta Part B*. May2016, Vol. 119, p17-24. 8p. DOI: 10.1016/j.sab.2016.03.005.

Direct reduction of synthetic rutile using the FFC process to produce low-cost novel titanium alloys. Benson, L.; Mellor, I.; Jackson, M.; Wang, Z.; Nixon, M.A. *Journal of Materials Science*. May2016, Vol. 51 Issue 9, p4250-4261. 12p. DOI: 10.1007/s10853-015-9718-1.

Experimental observation and numerical simulation of the spectra of solid-anode X-ray tubes. Vidow, P.; Kondratenko, S.; Nikolaev, V.; Sorokin, V. *Journal of Analytical Chemistry*. May2016, Vol. 71 Issue 5, p471-475. 5p. DOI: 10.1134/S1061934816030151.

X-ray diffraction of crystallization of copper (II) chloride for improved energy utilization in hydrogen production. Jiang, O.A.; Lescaux, M.; Wang, Z.; Rosen, M.A.; Naterer, G.F. *International Journal of Hydrogen Energy*. May2016, Vol. 41 Issue 19, p7848-7853. 6p. DOI: 10.1016/j.ijhydene.2015.12.213.

Effects of calcium and ferric ions on struvite precipitation: A new assessment based on quantitative X-ray diffraction analysis. Yan, Haichu; Shih, Kaimin. *Water Research*. May2016, Vol. 95, p310-318. 9p. DOI: 10.1016/j.watres.2016.03.032.

Conformational change in the C form of palmitic acid investigated by Raman spectroscopy and X-ray diffraction. de Souza, F.F.; Nogueira, C.E.S.; Freire, P.T.C.; Moreira, S.G.C.; Teixeira, A.M.R.; de Sousa, A.A.; Mendes Filho, J.; Sasaki, J.C.D. *Spectrochimica Acta Part A: Molecular & Biomolecular Spectroscopy*. May2016, Vol. 161, p162-169. 8p. DOI: 10.1016/j.saa.2016.02.035.

A direct correlation of x-ray diffraction orientation distributions to the in-plane stiffness of semi-crystalline organic semiconducting films. Brigoux, Zhao; Awartani, Omar; O'Connor, Brendan; Zikry, Mohammed A. *Applied Physics Letters*. 2016, Vol. 108 Issue 18, p181902-1-181902-3. 3p. 1 Diagram, 1 Chart, 2 Graphs. DOI: 10.1063/1.4948533.

Materials identification using a small-scale pixelated x-ray diffraction system. D'Flynn, C.; Crews, I.; Drakos, C.; Christodoulou, M.D.Wilson; M.C.Veale; P.Seller; R.D Speller. *Journal of Physics: D Applied Physics*. 5/5/2016, Vol. 49 Issue 17, p1-1. 1p. DOI: 10.1088/0022-3727/49/17/175304.