Rigaku
Leading With Innovation

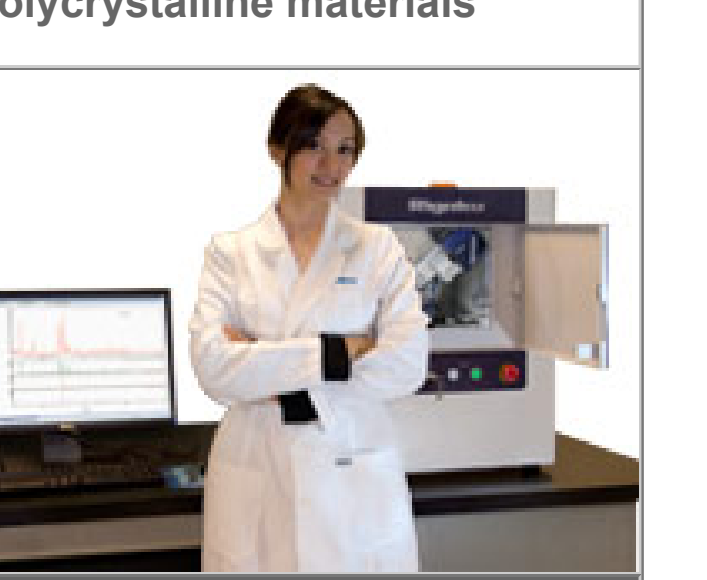
X-ray Diffraction & Elemental Analysis

High-power Benchtop Sequential WDXRF Spectrometer

Supermini200 – Elemental analysis of solids, liquids, powders, alloys and thin films

As the world's only high-power benchtop sequential wavelength dispersive X-ray fluorescence (WDXRF) spectrometer for elemental analysis of oxygen (O) through uranium (U) in almost any material, the Rigaku Supermini200 uniquely delivers low cost-of-ownership (COO) with high resolution and lower limits-of-detection (LLD). **For more >**

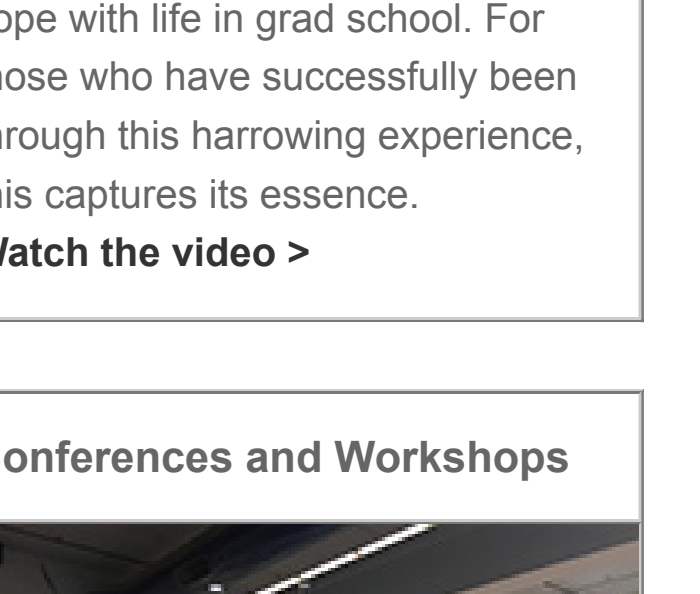
MiniFlex – qualitative and quantitative analysis of polycrystalline materials



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 >

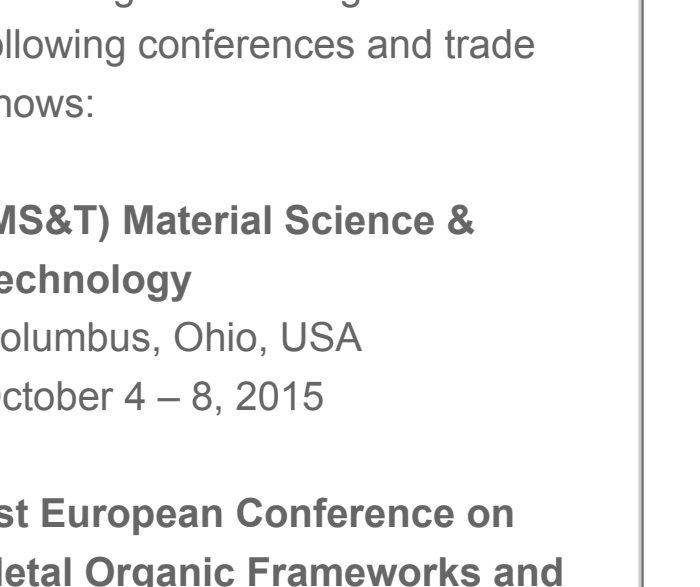
Video of the Month



Piled Higher and Deeper

Piled Higher and Deeper (Ph.D.) follows the lives of several science graduate students as they learn to cope with life in grad school. For those who have successfully been through this harrowing experience, this captures its essence.
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:

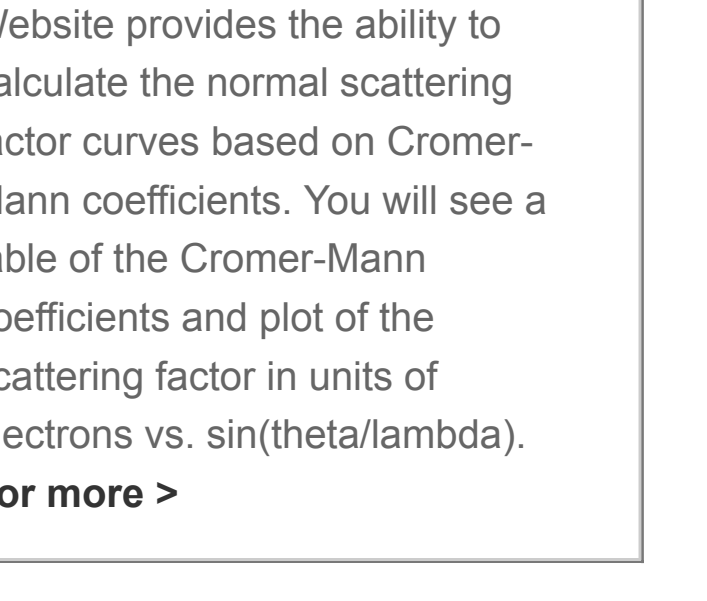
(MS&T) Material Science & Technology
Columbus, Ohio, USA
October 4 – 8, 2015

1st European Conference on Metal Organic Frameworks and Porous Polymers
Potsdam, Germany
October 11 – 14, 2015

(GCC) Gulf Coast Conference
Moody Gardens, Texas, USA
October 20 – 21, 2015

See the complete list >

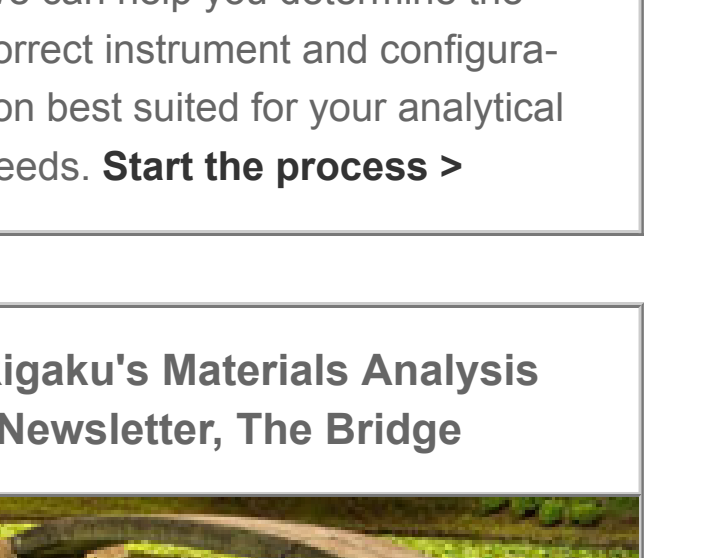
Useful link of the Month



Crystallographic Web Applets

Crystallographic Web Applets – Bernhard Rupp, BR's Macromolecular Crystallography Website provides the ability to calculate the normal scattering factor curves based on Cromer-Mann coefficients. You will see a table of the Cromer-Mann coefficients and plot of the scattering factor in units of electrons vs. sin(theta/lambda).
For more >

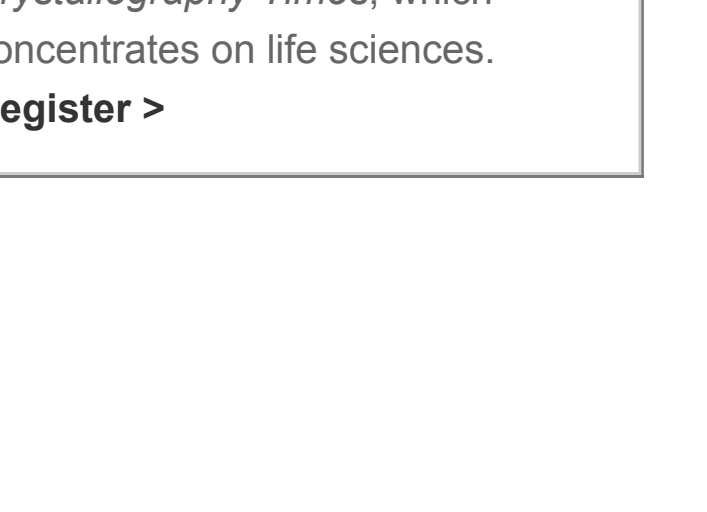
Planning to Submit a Grant?



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 >**

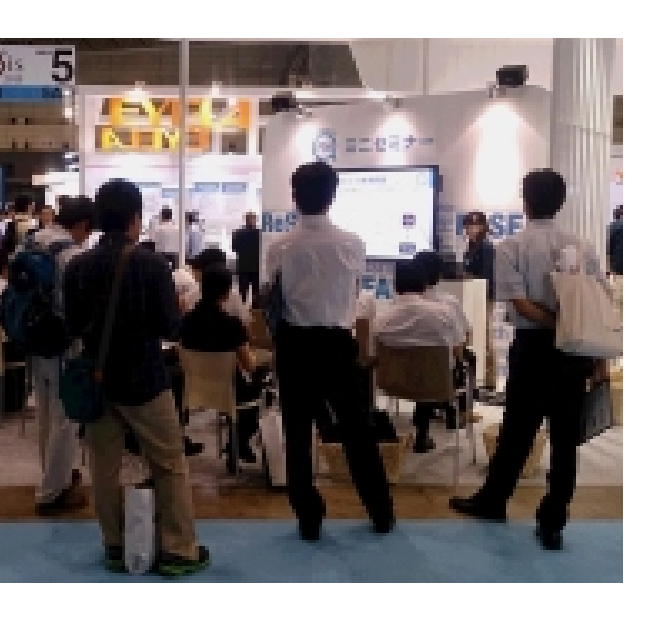
Rigaku's Materials Analysis eNewsletter, The Bridge



Join us

Each month, Rigaku distributes two eNewsletters: *The Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on life sciences.
Register >

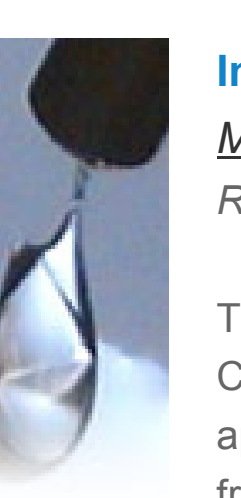
Welcome



The first week of the month heralded one of the largest Asian exhibitions of analytical and scientific instrumentation: JASIS 15. Over 23,000 visitors attended the events at Makuhari Messe, Japan. About 2300 people visited the Rigaku booth. We wish to thank all of those who took the time to come see the latest Rigaku products and to attend the various seminars highlighting new technologies.

For your continuing education, we offer the second installment of our new series "Introduction to single crystal X-ray analysis," entitled "Mounting Crystals." Our featured technical X-ray diffraction (XRD) paper describes characterization of GaN-related materials using high-resolution XRD. Check out the news and papers sections at the bottom of the page for the latest developments in materials science. Enjoy the newsletter.

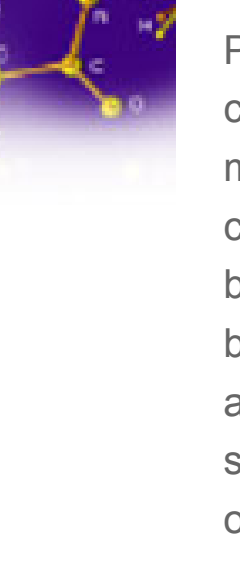
R.C. Tisdale, Ph.D. – Editor



Introduction to single crystal X-ray analysis

Mounting Crystals
Rigaku Corporation

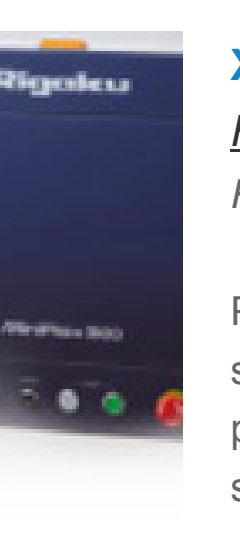
This month we cover mounting samples for single crystal X-ray diffraction. Conventionally, a crystal is glued to the tip of a glass fiber. This method is still applicable for a wide range of crystals. However, it is not appropriate for unstable, fragile or very small crystals. These days, sticking crystals to a polyimide film or a fiber loop, and measuring under low temperature, is becoming the common practice for diffraction experiments. With this method, the crystal can be readily attached and detached. **For more >**



Featured XRD Rigaku Journal Article

Characterization of GaN-related materials using high-resolution XRD
Rigaku Corporation

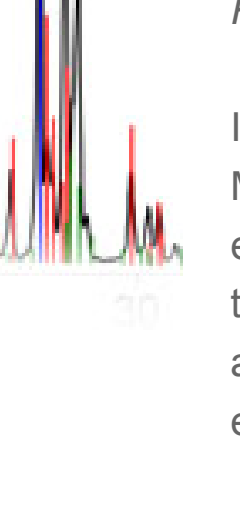
Although high-resolution X-ray diffraction (HR-XRD) has been commonly employed for the crystallinity characterization of GaN-related materials, special care is required due to the complexities resulting from peculiar features in GaN-related materials. **For more >**



XRD Application Note

Analysis of powder crystal structures of organic crystals using a high-resolution convergent beam optical system
Rigaku Corporation

Previously, it was typical to conduct crystal structure analysis using the single crystal method. However, analysis of crystal structure using the single crystal method is difficult in the case of samples for which it is hard to produce single crystals, and samples for which crystal growth is difficult even if single crystals can be produced. In recent years, the precision of powder X-ray diffractometers has been improving, and thus it is becoming possible to conduct crystal structure analysis using powder samples. Here we show an example where a powder sample was measured, and structural analysis was conducted based on the obtained diffraction pattern. **For more >**



XRD Application Note for Beginners – 1

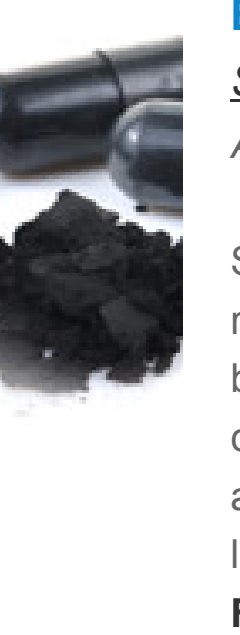
Features of the MiniFlex300
Rigaku Corporation

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 5th generation Rigaku MiniFlex series of benchtop XRD instruments – with 1/20 the volume and 1/10 the weight of stand-alone powder X-ray diffractometers – can operate with power from a standard single phase AC outlet. **For more >**

XRD Application Note for Beginners – 2

MiniFlex300/600
Rigaku Corporation

Ideally suited for today's fast-paced XRD analyses, the new 5th generation MiniFlex delivers speed and sensitivity through innovative technology enhancements such as the optional D/teX Ultra high speed detector coupled with the new 600 W X-ray source. By using this detector, it is possible to obtain intensity a few tens to roughly 100 times greater than with a scintillation counter and thus enabling a dramatic shortening of measurement times. **For more >**



WDXRF Application Note

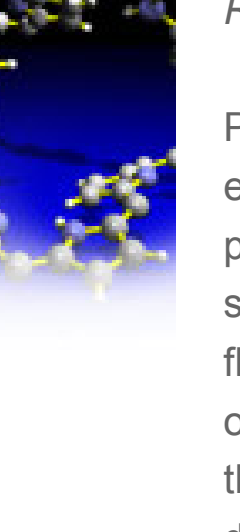
Polymetallic Sulfide Ore Analysis with Supermini200
Rigaku Corporation

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 >**

EDXRF Application Note

Sulfur and Chlorine in Activated Carbon
Applied Rigaku Technologies

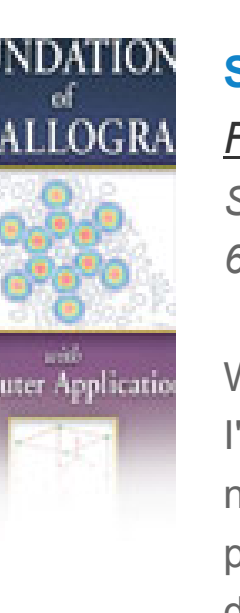
Sulfur and chlorine may occur naturally in charcoal and in the production and regeneration of activated carbon various solvents may be used, including sulfur-based and chlorine-based solvents. As the material is processed the sulfur and chlorine levels are monitored until they reach an acceptable content. 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

Narcotics Identification Using Handheld Raman
Rigaku Analytical Devices

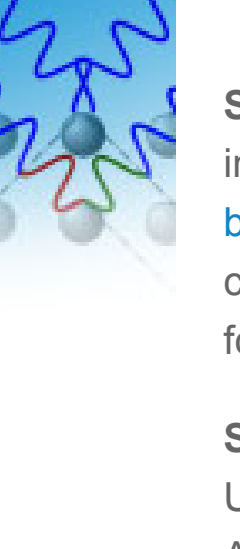
Mobile techniques for fast and accurate identification of illegal drugs and narcotics are in demand by several agencies involved in removing controlled substances from circulation. Raman spectroscopy is considered a confirmatory test under Category A by the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG), and may be used towards obtaining sufficient probable cause to hold suspects. **For more >**



SCX Application Note

Large meso-Pentafluorophenyl-Substituted Expanded Porphyrins
Rigaku Oxford Diffraction

Porphyrin analogs having five or more pyrrole rings are referred to as ring-extended porphyrins. They have been found to have a variety of interesting properties diverging from those of porphyrin. Whilst porphyrin has a planar structure, the ring extended porphyrins take on a twisted structure due to both their flexibility and by the presence of hydrogen bonds among NH groups. The flexibility of the structure increases with increasing ring size, meaning that structures of these large twisted compound are difficult to predict. Precise structure can only be determined by way of single crystal X-ray structure analysis. **For more >**



Scientific Book Review

Foundations of Crystallography with Computer Applications
Second Edition by Maureen M. Julian, Taylor and Francis, LLC, 2015, 680 pages, ISBN 9781466552913.

When I was handed this book at the ACA meeting this past July, I said to myself I've already done this. Nevertheless, I took the book and brought it home. I placed it next the first edition and immediately noticed it was nearly twice the thickness, 680 pages versus 368 pages, so I took both off the shelf and started looking for the differences. **For more >**

Material Analysis in the News

News for September 2015

September 1, 2015. New research conducted at Nanyang Technological University in Singapore and National Taiwan University demonstrates a molybdenum-nickel-based hydrogen evolution catalyst that can be deposited on a flexible, conductive carbon fiber cloth. Their synthesis for making the Ni-Mo-S/C catalyst is a straight-forward process that is biomolecule-assisted using L-cysteine as its sulfur source.

September 4, 2015. Researchers from Louisiana State University, Fudan University, the University of Florida and the Collaborative Innovation Center of Advanced Microstructures in Nanjing, China, conducted research on materials that separate into different regions through a process called electronic phase separation, which is poorly understood. Their research advances the understanding of how these materials can be manipulated.

September 4, 2015. An international team of scientists has developed what may be the first one-step process for making seamless carbon-based nanomaterials that possess superior thermal, electrical and mechanical properties in three dimensions. In early testing, a three-dimensional (3D) fiber-like supercapacitor made with the uninterrupted fibers of carbon nanotubes and graphene matched or bettered — by a factor of four — the reported record-high capacities for this type of device.

September 8, 2015. As part of a project funded by an Australian Research Council (ARC) discovery grant, Associate Professor Kenneth Sheedy, director of the Australian Centre for Ancient Numismatic Studies at Macquarie University (ACANS); Professor Damian Gore; and Dr Gil Davis used Energy Dispersive X-ray Fluorescence (EDXRF) Spectroscopy to evaluate the composition of approximately 1000 coins from archaic Athens (550 BC – 480 BC).

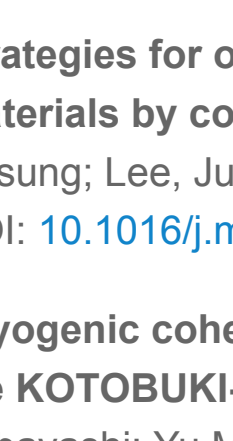
September 9, 2015. The Dirac cone, named after British physicist Paul Dirac, started as a concept in particle and high-energy physics and has recently became important in research in condensed matter physics and material science. It has since been found to describe aspects of graphene, a two dimensional form of carbon, suggesting the possibility of applications across various fields. Physicists at MIT have found another unusual phenomenon produced by the Dirac cone: it can spawn a phenomenon described as a "ring of exceptional points."

September 10, 2015. New research led by scientists from the Department of Energy's SLAC National Accelerator Laboratory and Stanford University shows how individual atoms move in trillionths of a second to form wrinkles on a three-atom-thick material. It was made possible with SLAC's instrument for ultrafast electron diffraction (UED).

September 11, 2015. The list of potential mechanisms that underlie an unusual metal-insulator transition has been narrowed by a team of scientists using a combination of X-ray techniques. This transition has ramifications for material design for electronics and sensors.

September 11, 2015. Using metallic osmium (Os) in experimentation, an international group of researchers have demonstrated, using X-ray diffraction, that ultra-high pressures cause core electrons to interplay, which results in experimentally observed anomalies in the compression behavior of the material.

September 14, 2015. Prof. Wladek Minor of the Department of Molecular Physiology and Biological Physics at the University of Virginia is working to overcome one of the greatest challenges in his field: the management of astounding amounts of raw data. Much of the older data – the raw X-ray diffraction results – is in danger of being lost, destroyed or forgotten. But Minor is changing that, and he's doing so with only $20,000 worth of hardware acquired with a National Institutes of Health grant.



Recent Scientific Papers of Interest

Papers for September 2015

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

2015 Atomic Spectrometry Update – a review of advances in X-ray fluorescence spectrometry and their applications. West, Margaret; Ellis, Andrew T.; Potts, Philip J.; Streli, Christina; Vanhoof, Christine; Wobrauschek, Peter. *Journal of Analytical Atomic Spectrometry*. Sep2015, Vol. 30 Issue 9, p1839-1889. 51p. DOI: 10.1039/c5ja90033f.

Strategies for overcoming limitations associated with fluorine determination in solid materials by conventional wavelength dispersive X-ray fluorescence spectrometry. An, Jinsung; Lee, Junseok; Yoon, Hye-On. *Microchemical Journal*. Sep2015, Vol. 122, p76-81. 6p. DOI: 10.1016/j.microc.2015.03.015.

Cryogenic coherent x-ray diffraction imaging for biological non-crystalline particles using the KOTOBUKI-1 diffraction apparatus at SACLA. Tomotaka Oroguchi; Yuki Sekiguchi; Amane Kobayashi; Yu Masaki; Asahi Fukuda; Saki Hashimoto; Masayoshi Nakasako; Yuichi Ichikawa; Hitoshi Kurumizaka; Mitsuhiro Shimizu; Yayoi Inui; Sachihiro Matsunaga; Takayuki Kato; Keiichi Namba; Keiichi Yamaguchi; Kazuo Kuwata; Hiroshi Kameda; Naoya Fukui; Yasushi Kawata; Takashi Kameshima. *Journal of Physics: B Atomic Molecular & Optical Physics*. 9/28/2015, Vol. 48 Issue 18, p1-1. 1p. DOI: 10.1088/0953-4075/48/18/184003.

Component analyses of urinary nanocrystallites of uric acid stone formers by combination of high-resolution transmission electron microscopy, fast Fourier transformation, energy dispersive X-ray spectroscopy, X-ray diffraction and Fourier transform. Xin-Yuan Sun; Jun-Fa Xue; Zhi-Yue Xia; Jian-Ming Ouyang. *IET Nanobiotechnology*. 2015, Vol. 9 Issue 3, p114-121. 8p. 3 Black and White Photographs, 2 Charts, 1 Graph. DOI: 10.1049/iet-nbt.2014.0017.

High temperature phase stability in $Li_{0.12}Na_{0.88}NbO_3$: A combined powder X-ray and neutron diffraction study. Mishra, S. K.; Krishna, P. S. R.; Shinde, A. B.; Jayakrishnan, V. B.; Mittal, R.; Sastry, P. U.; Chaplot, S. L. *Journal of Applied Physics*. 9/7/2015, Vol. 118 Issue 9, p094101-1-094101-7. 7p. DOI: 10.1063/1.4929645.

X-Ray fluorescence analysis of Ge–As–Se glasses using X-Ray and electron-beam excitation. Bordovsky, G.; Marchenko, A.; Seregin, P.; Bobokhuzhaev, K. *Inorganic Materials*. Sep2015, Vol. 51 Issue 9, p939-943. 5p. DOI: 10.1134/S0020168515080063.

Development and validation of X-ray diffraction method for quantitative determination of crystallinity in warfarin sodium products. Siddiqui, Akhtar; Rahman, Ziyaur; Korang-Yeboah, Maxwell; Khan, Mansoor A. *International Journal of Pharmaceutics*. Sep2015, Vol. 493 Issue 1/2, p1-6. 6p. DOI: 10.1016/j.ijpharm.2015.07.051.

Influence of content of pressure-transmitting medium on structural evolution of heulandite: Single-crystal X-ray diffraction study. Seryotkin, Yurii V. *Microporous & Mesoporous Materials*. Sep2015, Vol. 214, p127-135. 9p. DOI: 10.1016/j.micromeso.2015.05.015.

Modal mineralogy of CI and CI-like chondrites by X-ray diffraction. King, A.J.; Schofield, P.F.; Howard, K.T.; Russell, S.S. *Geochimica et Cosmochimica Acta*. Sep2015, Vol. 165, p148-160. 13p. DOI: 10.1016/j.gca.2015.05.038.

***In situ* X-ray diffraction characterisation of $Fe_{0.5}TiOPO_4$ and $Cu_{0.5}TiOPO_4$ as electrode material for sodium-ion batteries.** Bleith, Peter; Kaiser, Hermann; Novák, Petr; Villevieille, Claire. *Electrochimica Acta*. Sep2015, Vol. 176, p18-21. 4p. DOI: 10.1016/j.electacta.2015.06.105.

A study of X-ray multiple diffraction by means of section topography. Kohn, V. G.; Smirnova, I. A. *Acta Crystallographica. Section A, Foundations & Advances*. Sep2015, Vol. 71 Issue 5, p519-525. 7p. DOI: 10.1107/S2053273315012176.

***DIOPTAS*: a program for reduction of two-dimensional X-ray diffraction data and data exploration.** Prescher, Clemens; Prakapenka, Vitali B. *High Pressure Research*. Sep2015, Vol. 35 Issue 3, p223-230. 8p. DOI: 10.1080/08957959.2015.1059835.

Microscopic structure of methanol–water mixtures: Synchrotron X-ray diffraction experiments and molecular dynamics simulations over the entire composition range. Galicia-Andrés, Edgaár; Pusztai, László; Temleitner, László; Pizio, Orest. *Journal of Molecular Liquids*. Sep2015, Vol. 209, p586-595. 10p. DOI: 10.1016/j.molliq.2015.06.045.

Evaluation of Residual Stresses Relaxation by Post Weld Heat Treatment Using Contour Method and X-ray Diffraction Method. Xie, P.; Zhao, H.; Wu, B.; Gong, S. *Experimental Mechanics*. Sep2015, Vol. 55 Issue 7, p1329-1337. 9p. DOI: 10.1007/s11340-015-0040-2.

Measurement uncertainty in Total Reflection X-ray Fluorescence. Floor, G.H.; Queralt, I.; Hidalgo, M.; Marguí, E. *Spectrochimica Acta Part B*. Sep2015, Vol. 111, p30-37. 8p. DOI: 10.1016/j.sab.2015.06.015.

Quantitative evaluation of the broadening of x-ray diffraction, Raman, and photoluminescence lines by dislocation-induced strain in heteroepitaxial GaN films. Vladimir M Kaganer; Bernd Jenichen; Manfred Ramsteiner; Uwe Jahn; Christian Hauswald; Frank Grosse; Sergio Fernández-Garrido; Oliver Brandt. *Journal of Physics: D Applied Physics*. 9/30/2015, Vol. 48 Issue 38, p1-1. 1p. DOI: 10.1088/0022-3727/48/38/385105.