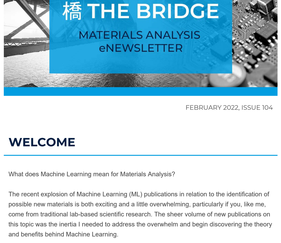

FEBRUARY 2022, ISSUE 104

WELCOME

What does Machine Learning mean for Materials Analysis?

The recent explosion of Machine Learning (ML) publications in relation to the identification of possible new materials is both exciting and a little overwhelming, particularly if you, like me, come from traditional lab-based scientific research. The sheer volume of new publications on this topic was the inertia I needed to address the overwhelm and begin discovering the theory and benefits behind Machine Learning.

It put me at ease to be reminded that in both biology and chemistry, big data and ML have been around for some time and are reflected in the popular sub-research topics of Bioinformatics and Computational Chemistry respectively.

But what about Materials Science?

Researchers are already using ML to discover functional band-gap materials for functional material applications such as light-emitting diodes (LEDs) or photovoltaics.

Batteries, topological insulators and superconductors are other areas where ML has been evaluated to find new materials with the required properties.

At Rigaku, we build the analytical instruments responsible for generating vast quantities of data needed to support ML. The importance of being able to collect accurate and precise measurements has not been overlooked, which is why we strive to build robust and reliable equipment to support this Artificial Intelligence.

In a 2021 review, the authors suggest that the "AI-based revolution is unlikely to stop, with many positive prospects for the near future focused on materials science." This is a future we eagerly anticipate at Rigaku.

FEATURED JOURNALS & REPORTS

Rigaku Journal
WINTER 2022, VOLUME 38, NO. 1

Thank you very much for reading the "Rigaku Journal"
Hikaru Shimura

For the past 70 years, since the founding of our company in 1951, our management philosophy has been to "contribute to the enhancement of humanity through scientific and technological development." By aligning ourselves with the enterprises and institutes pushing the boundaries of possibility over these seven decades, we have continuously expanded our portfolio of original technologies.
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Breaking the 1-μm Barrier with the Electron Diffractometer XtaLAB Synergy-ED
Sho Ito and Akihito Yamano

3D electron diffraction (3D ED)/Micro electron diffraction (MicroED) is a technique that can provide measurers with three-dimensional molecular structures from crystals of submicron order. However, 3D ED/Micro ED requires expertise in both electron microscopy and crystallography. Here, we introduce the newly developed electron diffractometer XtaLAB Synergy-ED specialized for 3D ED/MicroED experiments, its instrument...
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Powder X-ray Diffraction Basic Course Fourth Installment: Qualitative Analysis
Miki Kasari

An essential feature of the qualitative analysis of the powder X-ray diffraction (PXRD) method is that this provides information on the sample's crystal structure, which often affects the properties and functions of the material. The qualitative analysis by the PXRD method is a phase identification method based on the matching of known...
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Chemical State Analysis by X-ray Emission Spectroscopy
Hikari Takahara, Takashi Shoji and Yoshiaki Ito

X-ray emission spectroscopy (XES) is a chemical state analysis method. It is possible to show the change in a compound's bonding state profile by measuring fluorescent X-rays with high energy resolution. Recently, the XES method has been evaluated in the field of advanced materials such as battery materials and catalysts, and the...
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Wide-Angle X-ray Scattering Instrument NANOPIX-WE

In recent years, many countries have become increasingly concerned about environmental issues, and are accelerating their efforts to reduce their environmental impact by reducing dependence on fossil fuels (coal and oil) to achieve the carbon neutral. Developed countries and manufacturers are creating social policies and manufacturing strategies for low environmental load. Thus, the demand for advanced polymer materials...
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UPCOMING RIGAKU WEBINARS

CT Image Processing Virtual Workshop: Processing Images Using ImageJ
March 9, 2022 1 PM | CST

You have probably applied some form of image processing to your CT data, such as denoising or smoothing, before. Have you ever wondered how it works or what is different between different denoising techniques? In this workshop, we will review how these image processing techniques work and how to choose the right one. This is an interactive workshop. We will demonstrate some of the techniques using ImageJ. You can download the sample images and follow us through the process and ask questions.
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Thermal Analysis Technical Seminar: Thermal Analysis Of Biodegradable Plastics
March 17, 2022 12 AM | CDT

The seminar will focus on thermal analysis methods such as STA, HUM-STA, STA-MS and DSC on the thermal behavior of bio-based and petroleum based biodegradable plastics ranging from household goods to medical purposes for drug delivery, surgery, etc.
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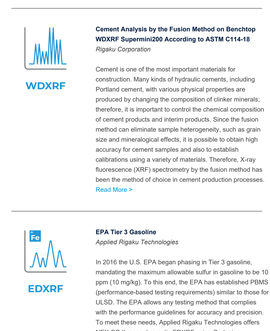
VIDEO OF THE MONTH



Machine-learning techniques used to accurately predict battery life

Kristen Severson from IBM Research in Cambridge, MA discusses the applications of machine learning in battery research.

FEATURED APPLICATION NOTES

XRD

Crystal Defect Analysis of a Single Crystal Substrate by X-ray Reflection Topography
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 XTOP high-sensitivity and high-resolution X-ray camera, is capable of obtaining high-resolution topographs like those measured with dedicated equipment.
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WDXRF

Cement Analysis by the Fusion Method on Benchtop WDXRF Supermini200 According to ASTM C114-18
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. Since the fusion method can eliminate sample heterogeneity, such as grain size and mineralogical effects, it is possible to obtain high accuracy for cement samples and also to establish calibrations using a variety of materials. Therefore, X-ray fluorescence (XRF) spectrometry by the fusion method has been the method of choice in cement production processes.
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EDXRF

EPA Tier 3 Gasoline
Applied Rigaku Technologies

In 2016 the U.S. EPA began phasing in Tier 3 gasoline, mandating the maximum allowable sulfur in gasoline to be 10 ppm (10 mg/kg). To this end, the EPA has established PBMS (performance-based testing requirements) similar to those for ULSD. The EPA allows any testing method that complies with the performance guidelines for accuracy and precision. To meet these needs, Applied Rigaku Technologies offers NEX CG II monochromatic ED XRF using Cartesian Geometry polarization. Ideal for ultra-low sulfur measurements such as Tier 3 gasoline and ULSD, NEX CG II is a multi-element analyzer capable of also measuring other applications throughout the petroleum industry. Powerful yet simple and intuitive to operate, the NEX CG II is an excellent tool for downstream analyses as well as midstream and upstream.
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MATERIALS ANALYSIS IN THE NEWS

February 10, 2022: The 3D body scanners made by MiLabs and recently acquired by Rigaku are featured in an article from *Innovation Origins*. The story describes how the founder and CEO of MiLabs created the fully integrated SPECT, PET and CT imaging technology and set up the business to become the success it is today.

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