Rigaku

Volume 13, No. 3, March 2021

WELCOME

I believe we are beginning to see the light at the end of the tunnel. I took my first business trip in months at the end of February. My wife traveled in early March. Life is slowly getting back to normal.

Nevertheless, we recognize that this summer will be much like last summer and, thus, we have started planning a fourth Rigaku School for Practical Crystallography. The tentative dates are June 7–11 and June 14–18. We will cover advanced topics in this school much as we did in December but over eight days, rather than five days. Details will be available on the Rigaku website in the coming weeks.

We have also begun planning for a workshop on high-pressure crystallography to be held in the first half of July. Please check rigaku.com for more details.

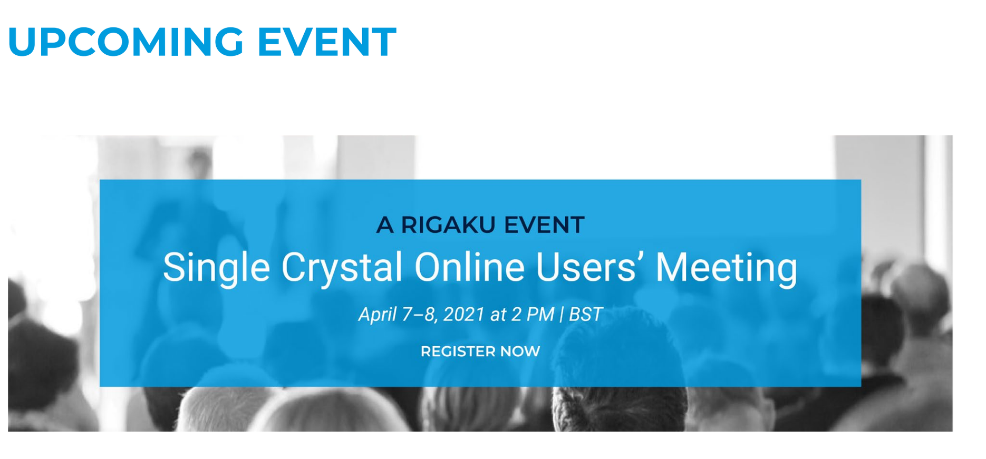
This month we are changing the format a little. Instead of "Product in the Spotlight," we have "What Can You Do with Your Synergy." This month we look at micro powder diffraction.

Our researcher of the month is Jared Allred from the University of Alabama, who is studying materials with functional properties. Our useful links and one of the videos focus on the pair distribution function (PDF) method. The second video is the winner of *Science Magazine's* "Dance Your Ph.D.*" contest.* This month's book review, *This Is How They Tell Me the World Ends*, will make you think hard about cybersecurity.

Stay positive, test negative and get vaccinated,

Joe

UPCOMING EVENT



We would like to invite you to join us for our Single Crystal Online Usersâ Meeting, to be held on April 7–8, 2021. The meeting will be held online via Zoom and will take place at 2 PM BST on both days to allow our users from across Europe and the Americas to attend. We intend to hold an additional meeting at a time more suitable for the Asia-Pacific region shortly afterward, so watch for another announcement soon.

We will have talks from our applications team, as well as from some of our customers. We aim to make our users' meetings a valuable educational experience for all those who attend, so if you'd like to learn more about your diffractometer, recent and upcoming developments and meet others in our community, please join us by registering at the link below.

REGISTER

CRYSTALLOGRAPHY IN THE NEWS

February 3, 2021: Researchers in Japan have demonstrated that a bowl-to-bowl inversion of a relatively small organic molecule with a bowl-shaped Ï-aromatic core generates ferroelectric dipole relaxation.

March 4, 2021: Researchers in Denmark, Germany and Switzerland have determined the structure of human glycine transporter 1 in complex with a benzoylpiperazine chemotype inhibitor at 3.4 Å resolution.

March 5, 2021: Researchers in the U.S. have used crystallography to identify a highly specific antibody to the most common TP53 mutation in complex with a common human leukocyte antigen-A (HLA-A) allele on the cell surface. This technique may help treat refractory cancers.

March 12, 2021: Scientists in China and Germany have synthesized a dimeric Ca^{+1} β-diketiminate that activates N_2, opening the possibility of catalytic chemistry with the *s*-block elements.

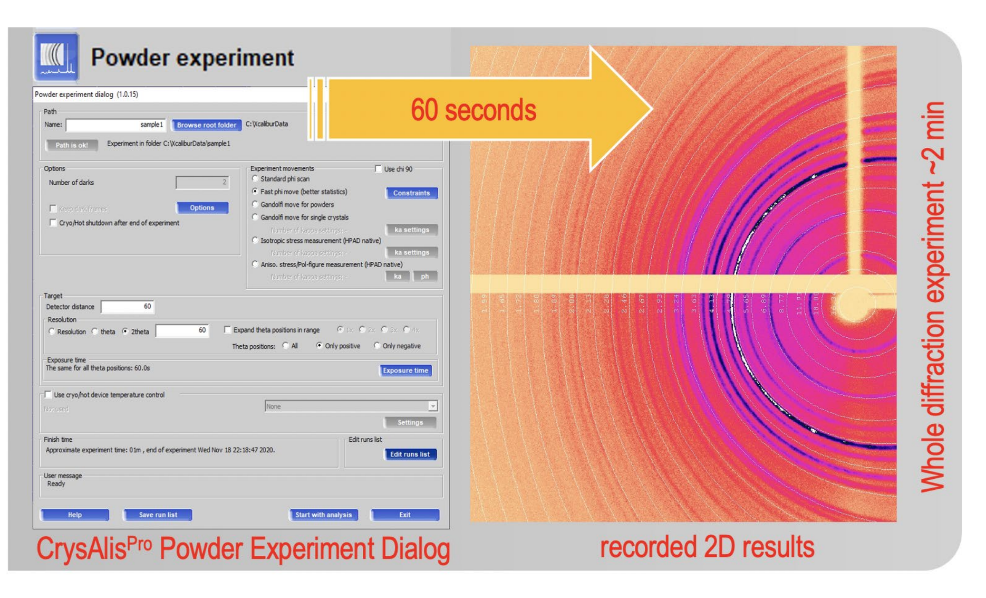
March 17, 2021: Researchers in China determined the structure of NLRP1 and 2:1 complex of NLRP1 and DPP9, helping to understand the mediation of innate immunity by NLRP1.

WHAT CAN YOU DO WITH YOUR SYNERGY?

Micro Powder Diffraction

Powder diffraction experiments are traditionally carried out with dedicated powder diffractometers. However, if only micrograms of material are available, the sample volume is too small to use standard powder diffractometers. The microfocus high-brilliance X-ray sources and high-performance detectors used in Rigaku Oxford Diffraction XtaLAB Synergy systems enable users to collect microdiffraction data without any configuration changes and with data collection times and quality on par with dedicated powder diffractometers.

XtaLAB Synergy single crystal diffractometers can even exceed the scope of usual powder instruments as they are regularly equipped with non-ambient temperature devices. The recording of high-quality powder diffraction data is furthermore supported by the automatic divergence control, accessible only for XtaLAB Synergy systems. By utilizing $CrysAlis^{Pro}$ and XtaLAB Synergy systems, single crystal dedicated laboratories can easily extend their range of samples to the polycrystalline phases.



The phase identification of organic polycrystalline materials can be achieved in a matter of minutes, without any time-consuming sample preparation or mounting techniques, with the help of the XtaLAB Synergy-S equipped with high-brilliance PhotonJet Cu Kα microfocus source and one our HyPix detectors.

Rigaku has recently released an application note entitled "Micro Powder Diffraction on XtaLAB Synergy Single Crystal Diffractometers." Drug development is one typical use-case for the measurement on micrograms of powder. Therefore, the characterization of Active Pharmaceutical Ingredients (APIs) is featured in this new application note. Such analysis can easily be adopted for research groups involved in the development of new API or functional materials.

READ MORE

RESEARCHER IN THE SPOTLIGHT

Jared Allred
Assistant Professor of Chemistry
University of Alabama

The Allred group specializes in the discovery and characterization of new inorganic materials with functional properties. Solid state devices are ubiquitous in energy and information technologies, but we often lack the chemical tools to control and manipulate the underlying charge and/or spin dynamics. This requires a fundamental understanding of how these emergent properties can be tied back to the local bonding environment.

They emphasize using state-ofâthe-art X-ray and neutron diffraction techniques to investigate the atomic positions both on the long-range averaged limit and the microscopic local scale in bulk solid-state compounds. They leverage what they learn to guide their synthesis efforts of future materials with desired properties.
Examples include:

Magnetic Materials: The long-range ordering of magnetic moments depends on the combination of competing interactions. Many facets of how this works are still not understood. What is known is that this complex interplay gives rise to the many different types of ordering that span various regimes of bondingâfrom localized to delocalized, ionic to covalent. One way to improve our understanding of these interactions is to tune material properties in order to stabilize unusual ground states. For example, one strategy is to tune across the boundary between localized and delocalized electronic states.

Multiferroic Materials: Sometimes magnetism is only one part of a rich tapestry of interconnected properties. Multiferroics are materials that exhibit multiple primary types of ferroic ordering, such as ferromagnetism or ferroelectricity. In many cases the way these parameters are coupled is obscured by details of the electronic or nuclear structure. Emerging diffraction technologies provide new avenues for teasing out the important parameters. These materials can be used in the next generation of sensor technologies, which depend on a combination of multiple order parameters—*e.g.,* orbitals, spins, charge—that couple in a controllable manner.

BOOK REVIEW

This Is How They Tell Me the World Ends: The Cyber-Weapons Arms Race
By Nicole Perlroth
ISBN: 978-1-63557-605-4

This Is How They Tell Me the World Ends is a gripping, nightmare-inducing deep dive into the high-stakes world of cybersecurity. Perlroth, who has covered cybersecurity, or, as it is known to insiders, information security or infosec, for *The New York Times* for the better part of a decade, is uniquely qualified to explain the intricacies of such a complicated, multi-faceted field. Perhaps the most horrifying, yet unsurprising, takeaway from her book is the realization that far-reaching and all-encompassing cyberattacks that can shut down an entire country are not a fear of the future, but one of the present, and even the past.

Perlroth starts with a description of such an attack on Ukraine. In 2017, Russian hackers implemented a series of escalating attacks designed to immobilize the entire country's online infrastructure, including shutting down the power grids. The attacks coincided with the anniversary of Ukraine's independence from Russia and were a brutal warning from the former mother country: come back, or we will make you. As Perlroth points out, though the digital onslaught was devastating, it could have been worse. The only saving grace was Ukraine's relative technological naivete—especially compared to a country like the United States, where finding anything not connected to the infamous Internet of Things is like finding a needle in the ocean. If an attack of a similar nature were perpetuated in the United States, one can only assume the aftermath would be exponentially more devastating.

The world of cybersecurity and internet hackers is a convoluted and cryptic one, as any reader might expect. Perlroth makes a valiant effort to disentangle the web of government agencies, independent contractors, ill-reputed hackers, and corporate security giants. *This Is How They Tell Me the World Ends* is not told in a clear, chronological order, and it isn't a cut-and-dry history of cybersecurity. As Perlroth herself explains, the concept of a "hacker" as someone who infiltrates computer firewalls and holds peopleâs data and devices for ransom is a relatively new one. One could argue several of history's innovators, such as Benjamin Franklin or Rosalind Franklin, "hacked" electricity and DNA respectively. Instead, the book is a series of anecdotes, carefully collected, vetted and reported by Perlroth.

One common thread throughout these anecdotal narratives is the concept of a "zero-day," a software bug that exposes the vulnerabilities of a user's device, giving a hacker complete and unfettered access to everything a user does, stores and shares on it. Such bugs sell for thousands—and sometimes even millions—of dollars. Perlroth elucidates numerous examples of zero-day bugs, including interviews with the very people who created them. Some of her sources are hackers and some of them former government employees, but they all seem to have one thing in common: a concern that cyberattacks are not simply going to become more widespread and destructive, but that they already are. Literally anything that connects to the internet can be hacked. Some attacks can even reach offline devices that are not currently connected. The great and powerful tools are all out there, and they are not being used responsibly.

Perlroth ends the book with a series of critical recommendations for government agencies and individuals to stay ahead of cyberattacks, both now and in the future. Many of the suggestions feel like they ought to be common sense but, sadly, that is not the case.

Jeanette S. Ferrara, MFA

RIGAKU TOPIQ WEBINARS

Rigaku has developed a series of 20–30 minute webinars that cover a broad range of topics in the fields of X-ray diffraction, X-ray fluorescence and X-ray imaging. You can register here and also watch recordings if you cannot attend live sessions.

RIGAKU REAGENTS

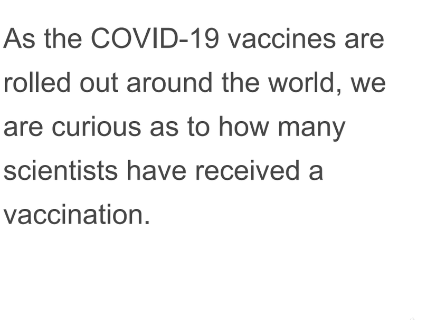
Wizard Classic:

Rigaku Reagents' Wizard Classic screens were designed to increase the probability of producing crystals during the coarse screening crystallization trials of biological macromolecules. Wizard Classic screens offer a large range of crystallants, buffers, and salts, covering a broad range of crystallization space, at pH levels from pH 4.5 to pH 10.5. They are proven to be a highly effective starting point for screening, with non-repeating formulations. Each of these screens is offered in either a 96 deep well block plate format or in 10 ml tubes.

SHOP HERE

SURVEY OF THE MONTH

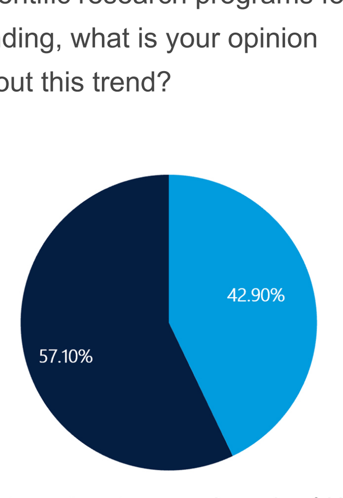
As the COVID-19 vaccines are rolled out around the world, we are curious as to how many scientists have received a vaccination.



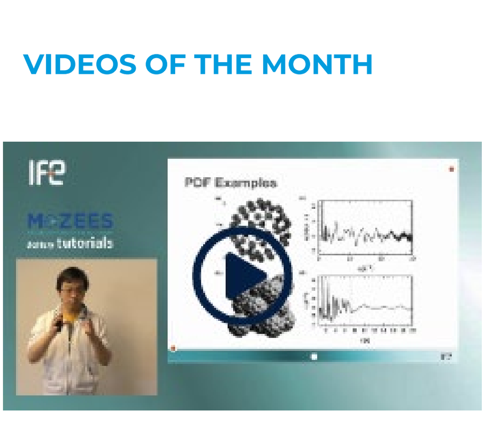
TAKE THE SURVEY

LAST ISSUE'S SURVEY RESULTS

There has been a recent increase in space exploration around the world. Since space exploration is an expensive activity that competes with other scientific research programs for funding, what is your opinion about this trend?


42.90%
57.10%
Science is science and we should be investing everywhere we can.
I volunteer to be on the first space craft to Mars.
Space exploration is interesting, but science that addresses real problems that face humans should have a higher priority.

VIDEOS OF THE MONTH



Pair Distribution Function

A video tutorial from MoZEES (Research Centre for Mobility Zero Emission Energy Systems) and Institutt For Energiteknikk (IFE). While Bragg diffraction is well known for providing average structure information, synchrotron or neutron sources enable wider and better access to local structure information hidden in the scattering signal by calculating the pair distribution function. Highly suitable for studying amorphous materials!

***Science Magazine*'s Annual "Dance Your Ph.D." Contest**

You may never look at clouds the same way again. A video created by three atmospheric science graduate students at the University of Helsinki features an original rap song and choreography explaining how groups of atoms stick together to form the billowy shapes in our sky. And it has just won *Science*'s annual "Dance Your Ph.D." contest.

USEFUL LINKS

Total Scattering and Atomic Pair Distribution Function Analysis: Overview and Applications

View the complete PDF presentation

S.J.L. Billinge
Department of Applied Physics and Applied Mathematics
Columbia University,
CMPMS, Brookhaven National Laboratory

Atomic Pair Distribution Function (PDF) Analysis

View the complete PDF presentation

2018 Neutron and X-ray Scattering School
Katharine Page
Diffraction Group
Neutron Scattering Division
Oak Ridge National Laboratory

JOIN US ON LINKEDIN

Our LinkedIn group shares information and fosters discussion about X-ray crystallography and SAXS topics. Connect with other research groups and receive updates on how they use these techniques in their own laboratories. You can also catch up on the latest newsletter or *Rigaku Journal* issue. We also hope that you will share information about your own research and laboratory groups.

JOIN HERE

RIGAKU X-RAY FORUM

At rigakuxrayforum.com you can find discussions about software, general crystallography issues and more. It's also the place to download the latest version of Rigaku Oxford Diffractionâs $CrysAlis^{Pro}$ software for single crystal data processing.

JOIN HERE

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