

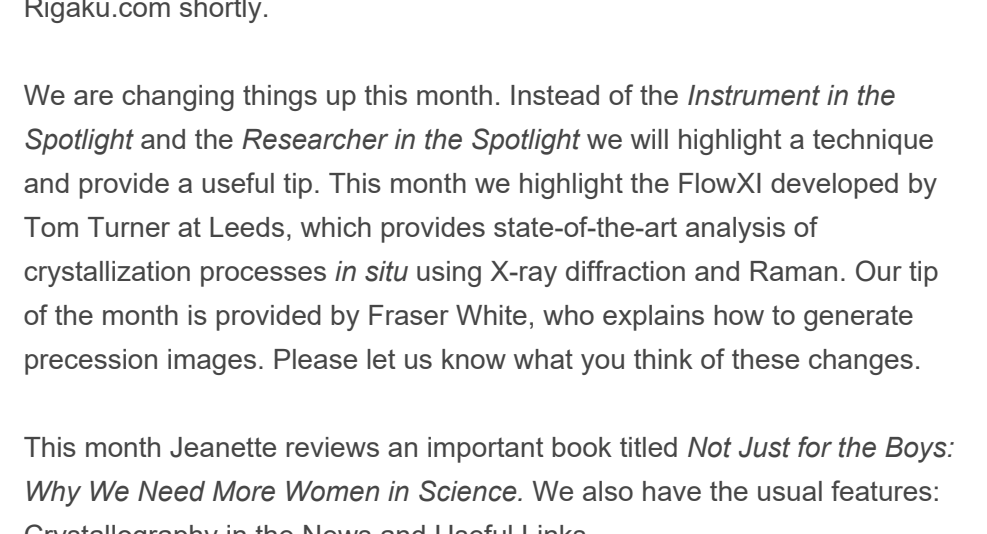
Volume 15, No. 9, September 2023

INTRODUCTION

For the first time in a few years, we held our annual European Users' Meeting in the UK. We had a strong turnout and an interesting program with a lot of innovative techniques and topics packed in.

The first day of our meeting was based around electron diffraction, with talks from invited speakers and NEDF staff to introduce the facility itself and the capabilities of electron diffraction in general.

After the coffee break, we took our guests to see the facilities in Warwick, both their existing XtaLAB Synergy X-ray diffractometers and their brand-new electron diffractometer, the XtaLAB Synergy-ED.



Despite the fantastic evening meal, merriment, and an unwelcome fire alarm at around 1:30 am everyone still managed to get back to the meeting room for 9 am the next day, where we had talks from our staff and more invited speakers.

Thanks to our speakers, and attendees for making this meeting possible and making it such a fun event. We are fortunate to have a community of fantastic users.

By popular demand, we have decided to run another Rigaku School for Practical Crystallography in January 2024. The dates are January 15-19 and January 22-26. A syllabus and registration information will appear at Rigaku.com shortly.

We are changing things up this month. Instead of the Instrument in the Spotlight and the Researcher in the Spotlight we will highlight a technique and provide a useful tip. This month we highlight the FlowXI developed by Tom Turner at Leeds, which provides state-of-the-art analysis of crystallization processes in situ using X-ray diffraction and Raman.

This month Jeanette reviews an important book titled Not Just for the Boys: Why We Need More Women in Science. We also have the usual features: Crystallography in the News and Useful Links.

Fraser White and Joe Ferrara

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 and electron diffraction, X-ray fluorescence and X-ray imaging.

UPCOMING EVENTS: 80th Pittsburgh Diffraction Conference, Pittsburgh, PA, October 15-17, 2023.

SERMACS 2023, Durham, NC, October 25-28, 2023.

31st Protein Structure Determination in Industry, Cambridge, UK, November 12-14, 2023.

Rayons X et Matière 2023, Bordeaux, France, November 21-24, 2023.

CRYSTALLOGRAPHY IN THE NEWS

September 6, 2023 Researchers from The Scripps Research Institute report the structures several transition state analogs of Pd catalysts that activate sp3 C-H bonds and arylate free alcohols.

September 6, 2023 Scientists from China and the U.S. have characterized a Li-S battery cell in situ using a EC-TEM holder using both electron microscopy and electron diffraction.

September 8, 2023 Researchers from the Chinese Academy of Sciences and UC Berkeley have synthesized and characterized a stable Cu(III) complex.

September 8, 2023 Scientists from UC Berkeley, UC Davis and F. Hoffmann-La Roche have synthesized a novel Cu(II) complex that initiates cross-coupling reactions.

USEFUL LINKS

We have had an earthquake in Morocco, a flood in Libya, a fire in Maui and an ongoing war in Ukraine. With so much suffering, perhaps it is a good time to donate to larger relief organizations like the International Red Cross and Red Crescent Movement, so they can distribute relief as needed.

FOLLOW US ON TWITTER

To keep up to date on the latest news and events from Rigaku Oxford Diffraction, follow our Twitter feed.



JOIN US ON LINKEDIN

Our LinkedIn group shares information and fosters discussion about X-ray crystallography issues and SAXS topics. Connect with other research groups and receive updates on how they use these techniques in their own laboratories.



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 Diffraction's CrySAlisPro software for single crystal data processing.



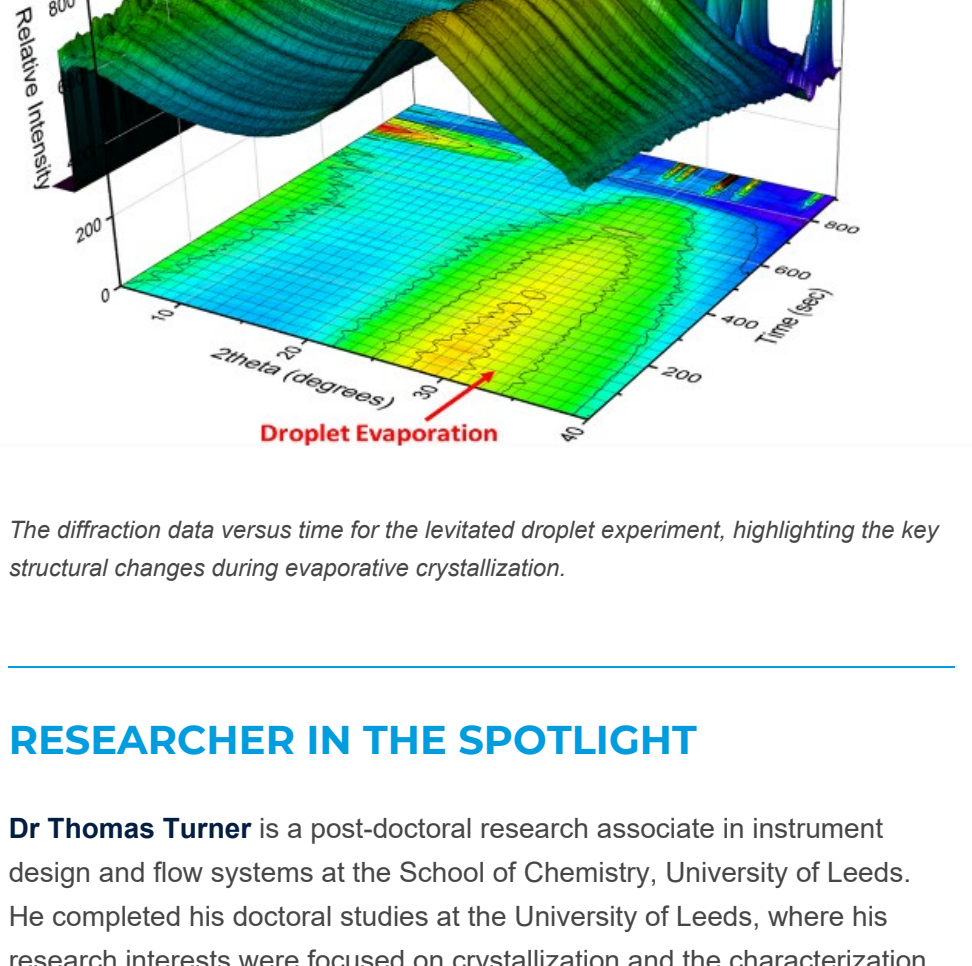
TECHNIQUE IN THE SPOTLIGHT

Flow crystallography

Flow crystallography is a technique where crystallization processes can be studied in situ by passing a crystallization mixture through an X-ray beam and detecting diffraction from crystals and crystallites.

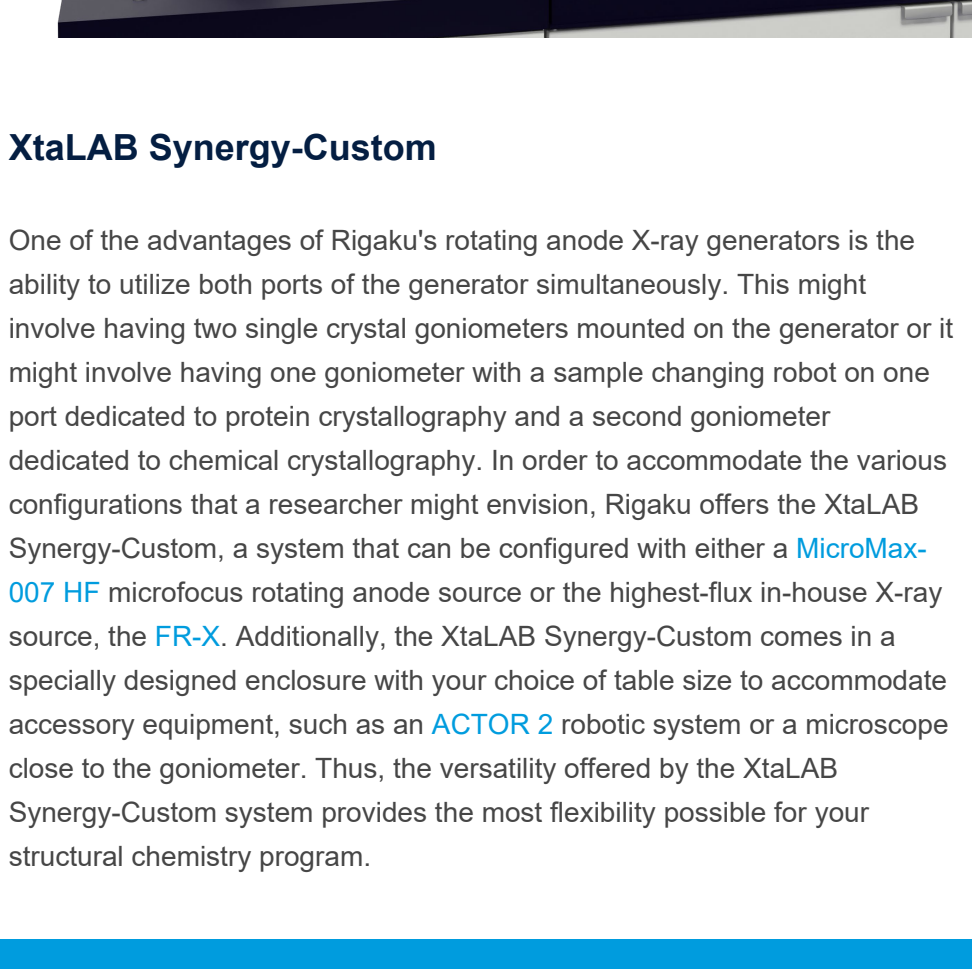
FlowXI is a new research facility at the University of Leeds that enables state-of-the-art analysis of crystallization processes in situ through combined Raman spectroscopy and powder X-ray diffraction.

The facility integrates a number of flow devices for studying crystallization processes, including a slurry recirculation loop for process reactors, droplet microfluidic devices, acoustic droplet levitator, variable humidity chamber and continuous flow crystallization devices.



FlowXI Facility inside the X-ray enclosure probing the crystallization of Na2SO4 inside a 10 µl acoustically levitated droplet using combined Raman spectroscopy and X-ray diffraction.

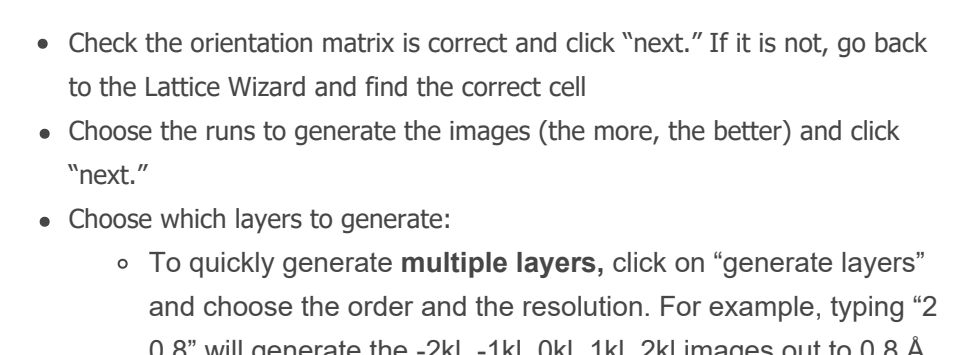
The facility has a state-of-the-art Rigaku XtaLAB Synergy Custom X-ray diffractometer with an ultrahigh-brightness source, optimized towards data collection from the weakest of diffracting samples.



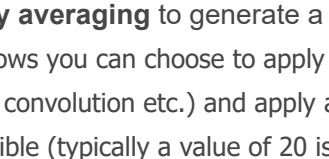
The diffraction data versus time for the levitated droplet experiment, highlighting the key structural changes during evaporative crystallization.

RESEARCHER IN THE SPOTLIGHT

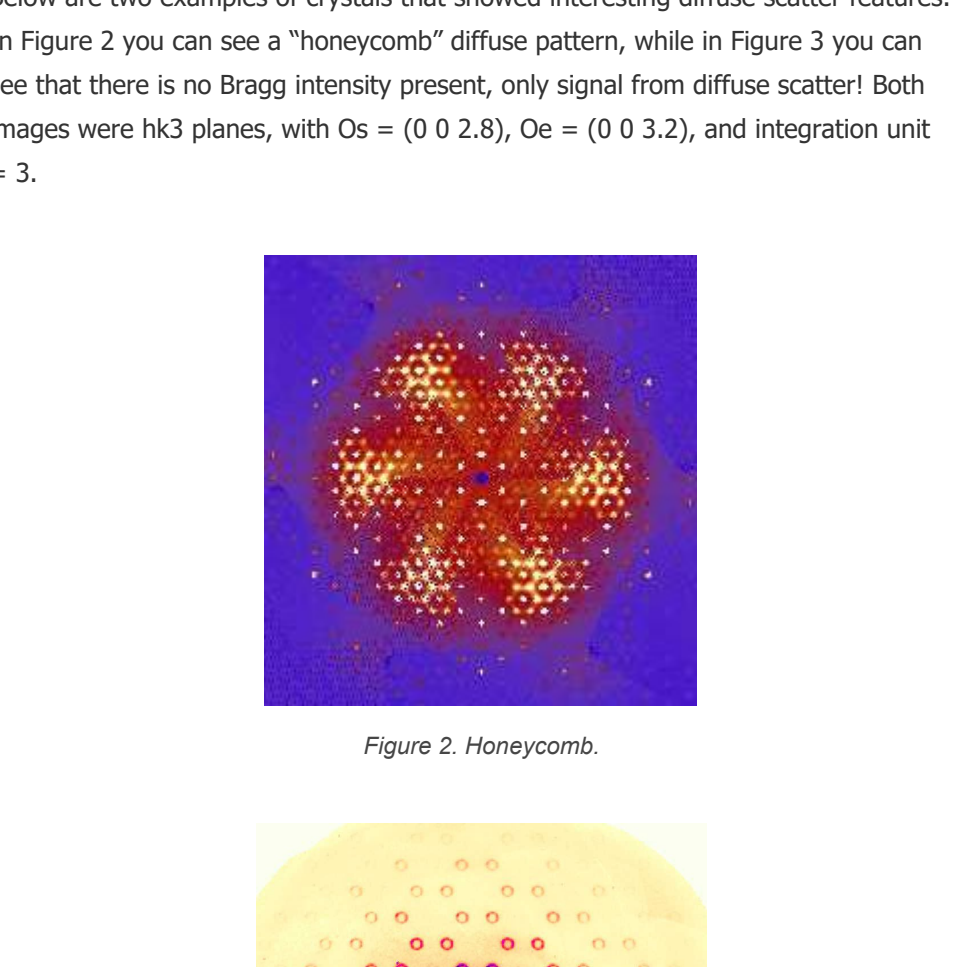
Dr Thomas Turner is a post-doctoral research associate in instrument design and flow systems at the School of Chemistry, University of Leeds. He completed his doctoral studies at the University of Leeds, where his research interests were focused on crystallization and the characterization of organic and pharmaceutical materials.



THOMAS WILL be presenting a new TOPIQ webinar for us on November 15 at 4PM CEST entitled "Flow-XI: A New UK Facility for the Analysis of Crystallisation in Flow Systems."



PRODUCT IN THE SPOTLIGHT



XtaLAB Synergy-Custom

One of the advantages of Rigaku's rotating anode X-ray generators is the ability to utilize both ports of the generator simultaneously. This might involve having two single crystal goniometers mounted on the generator or it might involve having one goniometer with a sample changing robot on one port dedicated to protein crystallography and a second goniometer dedicated to chemical crystallography.

TIP OF THE MONTH

Generating Standard and Integrative Precession Images

What are they?

Reconstructed precession images (also called unwrapped images) allow you to create any plane of reciprocal space using all the relevant frames from the data collection. Integrative precession images allow you to take a larger slice of reciprocal space to better identify certain features.

Why should I use them?

Precession images are very useful for visualizing the crystallinity of your sample. They may help show weaker peaks due to twinning, superstructure or incommensurate behavior as well as diffuse scatter. Integrative layers can be particularly useful for studying diffuse scatter, as you can choose a thicker slice of reciprocal space with which to create a composite image.

How do I make them?

- Click on the Unwarping button on the Lattice Wizard window (Figure 1).



Figure 1. Unwarp access.

- Check the orientation matrix is correct and click "next." If it is not, go back to the Lattice Wizard and find the correct cell
Choose the runs to generate the images (the more, the better) and click "next."
Choose which layers to generate:
To quickly generate multiple layers, click on "generate layers" and choose the order and the resolution.
To generate a single layer, click on "New layer", choose "One pixel layer" for a standard precession image then choose the origin (O) and the two vectors (L1 & L2), as well as the output name for the image.



Figure 2. Honeycomb.



Figure 3. Diffuse rings.

BOOK REVIEW



Review: Not Just for the Boys: Why We Need More Women in Science by Athene Donald ISBN 9780192893406

Athene Donald's Not Just for the Boys: Why We Need More Women in Science is a concise but compelling read for anyone and everyone. It's a book for women who have pursued a career in science, regardless of where they are in that career.

As a Professor Emerita of Experimental Physics at the University of Cambridge, Donald certainly has her own breadth of experience navigating science and academia as a woman. While she does draw on that experience, much of Not Just for the Boys includes numerous anecdotes and personal stories from women across scientific disciplines.

Donald begins with a chapter entitled "What's the Problem?" in which she outlines and addresses the issues at hand—namely, after decades of initiatives to increase the number of women in science and the fact that the population of the world is roughly 50% women, women do not account for 50% of scientists.

Donald argues that science, like any field, benefits from the diversity of those pursuing it. She acknowledges that, as a white woman, she still garners certain privileges not afforded to colleagues of color, particularly women of color.

Review by Jeanette S. Ferrara, MFA

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