

Volume 16, No. 1, January 2024

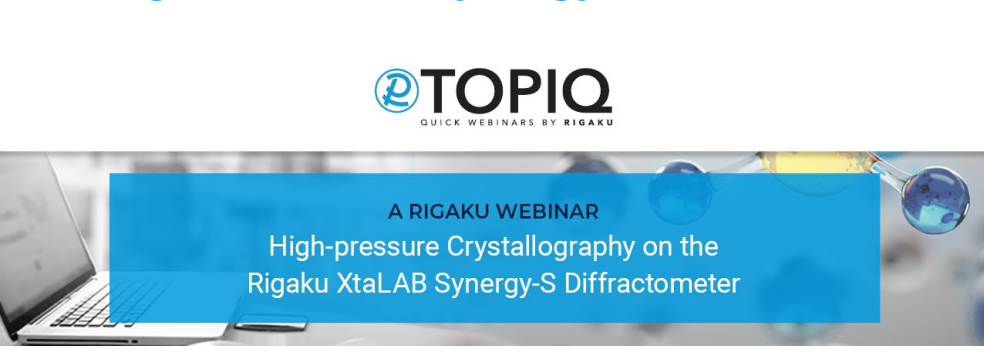
INTRODUCTION

The UK National Electron Diffraction Facility grand opening was held on January 16, 2024. In keeping with the tradition of naming the UK National Crystallographic Service's instruments after famous female crystallographers...



Left to right, front row: Simon Coles (Professor of Structural Chemistry and director of the Rigaku Polska Team)...

Last month marked a momentous occasion as we celebrated the illustrious career of Damian Kucharczyk, the visionary founder of KUMA Diffraction in 1993.



Adrian Jones presenting Damian with a retirement gift of a signed group photo of the Rigaku Polska Team.

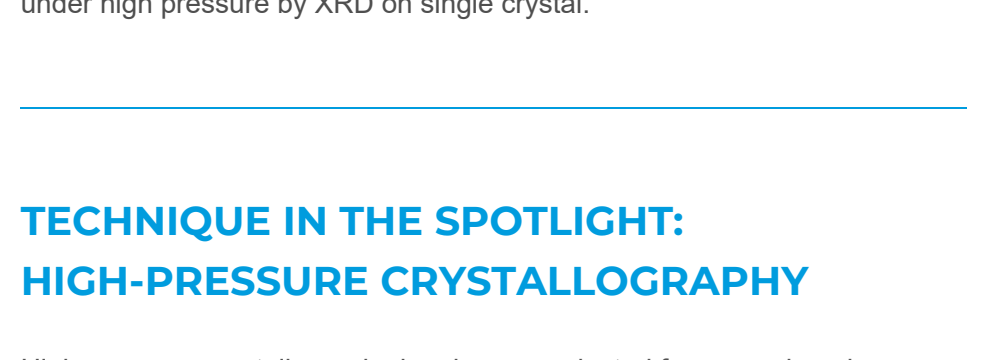
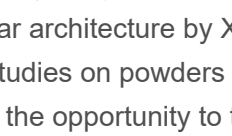
As Damian transitions into this new chapter of life, we extend our heartfelt wishes for a retirement filled with joy, fulfillment and the satisfaction of a legacy that will endure in the annals of crystallography.

This month we highlight the XtaLAB Synergy-S. Mark Del Campo provides the Tip of the Month and Jeanette reviews: Not Just for the Boys: Why We Need More Women in Science

Be safe,

Joe Ferrara and Mark Benson

TOPIQ | High-pressure Crystallography on the Rigaku XtaLAB Synergy-S Diffractometer



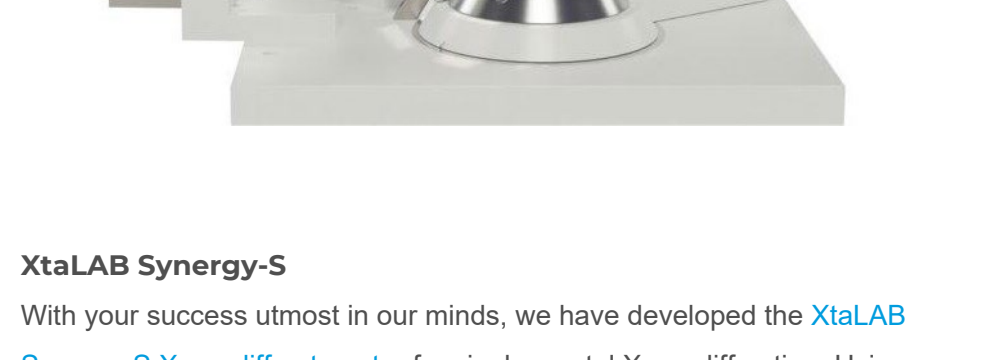
In this Webinar, the process of conducting a high-pressure crystallographic experiment on the XtaLAB Synergy-S will be explained and software features in CrysAlisPro relevant to the technique will be covered.

Wednesday, March 7, 2024 at 09:00 CST

Time Zone Converter

REGISTER NOW

TOPIQ | Pump-multiprobe Photocrystallography on the XtaLAB Synergy-R system



In this Webinar we will describe a new setup, developed in collaboration between Cardiff University and Rigaku, that enables the collection of pump-probe Photocrystallography data down to a time-resolution of 10 ms.

Wednesday, January 31, 2024 at 09:00 CST

Time Zone Converter

Presenter

Dr. Lauren Hatcher, Cardiff University

REGISTER NOW

RESEARCHER IN THE SPOTLIGHT: LAURE VENDIER

Laure Vendier (INSA Toulouse engineer, physics engineering option, 1994), obtained her PhD in 1997 in the field of materials for electronics (thesis co-supervised by the INSA Toulouse and the Georgia Institute of Technology in Atlanta).

She was recruited at the CNRS in 1998 for an engineering position at CEMES within the X-ray diffraction department, and joined the LCC in 2003 to take responsibility for the laboratory's XRD platform.

Her main interests are crystallography on small molecules, more specifically the determination of molecular architecture by X-ray diffraction, on sensitive crystals, but also structural studies on powders and nanomaterials by X-ray diffraction.

TECHNIQUE IN THE SPOTLIGHT: HIGH-PRESSURE CRYSTALLOGRAPHY

High-pressure crystallography has been conducted for many decades now, with the origins of the modern method in approx. the 1970s. The method uses a device called a Diamond Anvil Cell (DAC) to isotropically compress a sample to pressures of up to 100 GPa whilst allowing X-rays to reach and diffract from the sample inside.

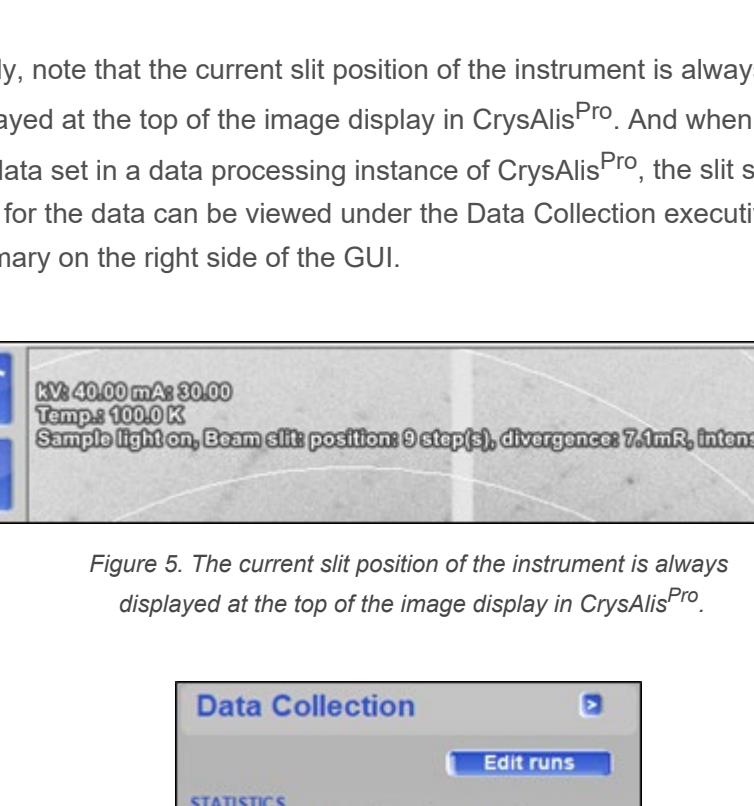
The application of pressure can bring structural changes, typically through the modification of intermolecular interactions, which in turn may bring about effects such as phase changes, amorphization, superconductivity, magnetism or polymerization, among others.

Conducting high-pressure experiments allows researchers to observe 3-dimensional structural changes at pressure, and is a valuable tool in materials science, pharmaceutical research and much more.

If you are interested in this technique and would like to know more, please join us for our webinar in March.

PRODUCT IN THE SPOTLIGHT

XtaLAB Synergy-S



With your success utmost in our minds, we have developed the XtaLAB Synergy-S X-ray diffractometer for single crystal X-ray diffraction. Using a combination of leading-edge components and user-inspired software tied together through a highly parallelized architecture...

In some settings, there is a desire to share instrument resources across different research groups. The XtaLAB Synergy-S in a dual-source configuration is the perfect system to be shared between protein crystallographers and chemical crystallographers.

ACA SUMMER COURSE 2024

It is with great pleasure that the organizers of the ACA Summer Course announce the 2024 ACA Summer Course in Chemical Crystallography. The course will be held at Purdue University from June 23-30, 2024.

For international attendees requiring a visa to enter the United States: There have been increasingly long processing periods in recent years to obtain a B1 visa. If you are planning to apply for the course, please contact us as soon as possible.

TIP OF THE MONTH

Tip of the Month: Beam Slit (Divergence) Control

By Mark Del Campo

When using Cu radiation with a Rigaku VHF optic on a XtaLAB Synergy-S, -R, or -DW, diffraction spots can overlap in certain situations. For example, if a crystal is pseudo-merohedrally twinned then the spots from multiple lattices may overlap.

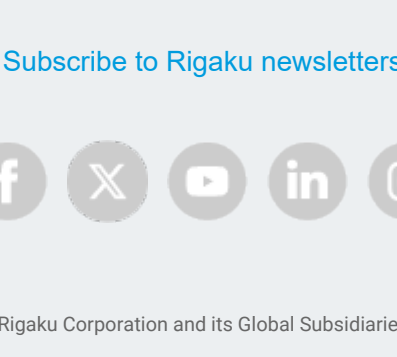
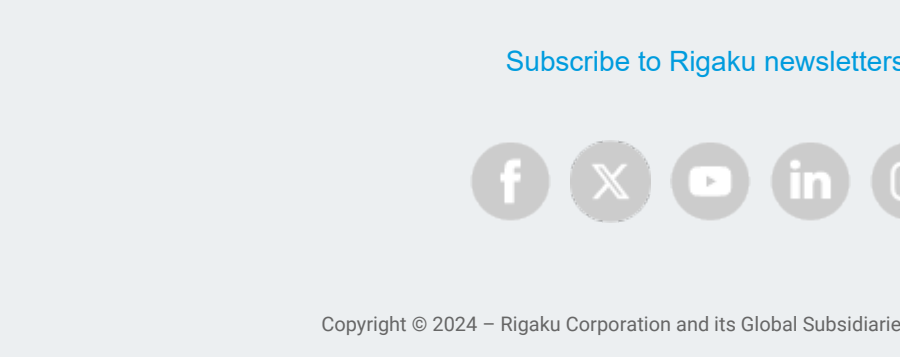


Figure 1. Access the Beam Slit Control.

For a XtaLAB Synergy-S or -R, this opens a Beam Slit Controller interface that shows the current motor position of the slit and the approximate divergence and relative beam intensity.



Figure 2. The XtaLAB Beam Slit Controller interface.



Figure 3. Beam Slit - Set Values Dialog.

For a XtaLAB Synergy-DW, the DW Beam Slit Controller interface is a little different in appearance, but similar in function. First, click on Init Beam Slit Control to connect to the slit and establish control.



Figure 4. The XtaLAB Synergy-DW Beam Slit Controller interface.

Be patient and remember that it may take several rounds of changing the beam divergence followed by a pre-experiment (screening) to establish an appropriate slit setting for a given crystal.

Finally, note that the current slit position of the instrument is always displayed at the top of the image display in CrysAlisPro. And when opening any data set in a data processing instance of CrysAlisPro, the slit setting used for the data can be viewed under the Data Collection executive summary on the right side of the GUI.



Figure 5. The current slit position of the instrument is always displayed at the top of the image display in CrysAlisPro.



Figure 6. The slit setting used for the data can be viewed under the Data Collection executive summary on the right side of the GUI.

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.

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.

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

UPCOMING WEBINAR: TOPIQ | Pump-multiprobe Photocrystallography on the XtaLAB Synergy-R system

Wednesday, January 31, 2024 at 09:00 CST

Presenter: Dr. Lauren Hatcher, Cardiff University

TOPIQ | High-pressure Crystallography on the Rigaku XtaLAB Synergy-S Diffractometer

Wednesday, March 7, 2024 at 09:00 CST

In this Webinar we will describe a new setup, developed in collaboration between Cardiff University and Rigaku, that enables the collection of pump-probe Photocrystallography data down to a time-resolution of 10 ms.

UPCOMING EVENTS: Pitcon 2024, ACS Spring 2024, 32nd Annual Meeting of the German Crystallographic Society (DGK)

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