X-ray diffractometer system with dual wavelength X-ray source

XtaLAB Synergy-DW

1. Choosing a diffractometer—navigating a minefield of technology and jargon

On average, laboratories look to replace their diffractometers every ten years due to new technology becoming available, research taking a new direction or the need to replace aging parts. Starting your own research group—or setting up a central facilities laboratory—often requires a diffractometer that will ensure that your highest quality publications are supported with the gold standard of analytical techniques: a single crystal X-ray structure.

Purchasing a new X-ray diffraction system can be a time-consuming and difficult process, where the user needs to rapidly become an expert in the latest technology. Since this is a decision only made infrequently, the task can be daunting, especially with all the jargon associated with the technology.

Common but significant concerns during the purchase of a system are to ensure that 1) your investment will meet your changing research requirements over the course of the next ten or more years, and 2) you have a reliable system that will not require significant maintenance downtime or costs.

Table 1. Commonly used X-ray detector jargon.

Term	Translation	Meaning
HPAD	Hybrid Pixel Array Detector	Photon counting detectors including PILATUS, EIGER and HyPix detectors
CPAD	Charge-integrating Pixel Array Detector	Integrating detectors with glass taper or stub; including CCDs and CMOS detectors

Rigaku understands these issues and has a solution that addresses these concerns. As there is no precise way to know which direction your research will take, why not have:

- one source capable of producing two wavelengths
- a high-flux source for even the most challenging small molecule or protein samples
- the latest technology HPAD detector
- a fully integrated system in a compact cabinet controlled by one user-friendly, powerful software program

In straightforward terms, the XtaLAB Synergy-DW diffractometer combines the increased flux of a rotating anode source with the flexibility of two different wavelengths, making it ideal for laboratories exploring a wide range of crystallographic research interests. The system is based on Rigaku's proven, low-maintenance MicroMax-007HF microfocus rotating anode. The target is constructed with two different source materials (Cu and Mo, for example) and is coupled with an auto-switching dual-wavelength optic, meaning that you can select between copper and molybdenum X-ray radiation at the click of a button.

The XtaLAB Synergy-DW offers up to 30× higher flux compared to the standard sealed tube sources, and utilizing only one generator means overall maintenance is reduced. Rounding out the XtaLAB Synergy-DW configuration is Rigaku's fast and efficient four-circle kappa goniometer, which is compatible with HPAD detectors, including the HyPix-6000HE.

At Rigaku, we like to refer to the XtaLAB Synergy-DW as the 'Swiss Army Knife' of diffractometers, as it is possible to gain high-quality data on a range of samples, from MOFs to macromolecules. No matter where your research leads you, this system will be ready.

2. Measurement example

One of the best ways to evaluate a system is to actually collect data on it to see how it performs on typical samples from your research lab. It is all too easy to become lost in the technical specifications and numbers of component parts when the data should speak for itself. Since we believe so emphatically in the superior performance of our systems, we welcome you to visit one of our application laboratories around the world for a demonstration using your own samples.

In order to show the versatility of the Synergy-DW we obtained a sample of a lithium iron hydroxide selenide superconductor[(1), (2)] from Dr. Daniel N. Woodruff of the University of Oxford. These crystals tends to be very small and are typically analyzed at a beamline. This particular sample was 0.01 mm $\times$0.02 mm$\times$0.03 mm, outlined on the loop in Fig. 1.

Fig. 1. The sample of a lithium iron hydroxide selenide superconductor on a loop.

A XtaLAB Synergy-DW running molybdenum radiation and equipped with a HyPix-6000HE was used to collect a data set on the above sample to

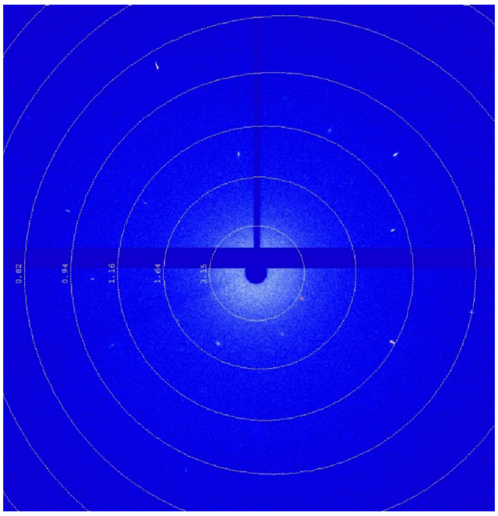

Fig. 2. Diffraction image of the lithium iron hydroxide selenide superconductor.

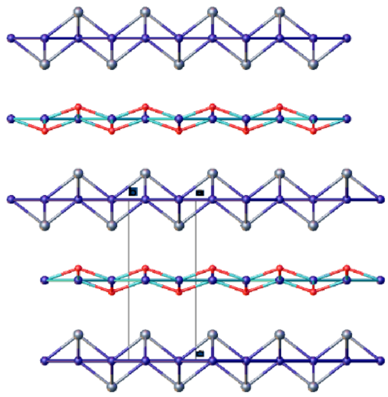

Fig. 3. The structure of the lithium iron hydroxide selenide superconductor.

IUCr resolution in a short 56 minutes (Fig. 2) with Rint=3.36% resulting in a structure with R1=3.0% (Fig. 3).

Reference

(1) H. Sun, D. N. Woodruff, S. J. Cassidy, G. M. Allcroft, S. J. Sedlmaier, A. L. Thompson, P. A. Bingham, S. D. Forder, S. Cartenet, N. Mary, S. Ramos, F. R. Foronda, B. H. Williams, X. Li, S. J. Blundell and S. J. Clarke: *Inorg. Chem.* **54** (2015), 1958–1964.

(2) D. N. Woodruff, F. Schild, C. V. Topping, S. J. Cassidy, J. N. Blandy, S. J. Blundell, A. L. Thompson and S. J. Clarke: *Inorg. Chem.* **55** (2016), 9886–9891.