

Oral presentation

Can we increase throughput without compromising on quality?**M. Mazzorana¹, D. Aragão¹, N. Paterson¹, M. Williams¹, P. Romano¹, D. Hall¹, R. Flaig¹**

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With the advent of new and bright light sources, the appetite for extremely focused beams has grown, and is leading to the development of new and exciting capabilities for MX beamlines. Diamond Light Source, the UK National Synchrotron, has embraced this challenge by providing a suite of 7 MX instruments [1], and a number of ancillary laboratories for sample preparation and complementary techniques for integrative structural biology.

Among these instruments is I04 [2,3], a tuneable microfocus beamline which covers a wide range of beamsizes (5-100 μm) across the whole energy range (6-20 keV), thanks to a finely tuneable array of compound refractive lenses. I04 also features fast and reliable robotics, a state-of-the-art multi-axis goniometer and a large and high frame rate pixel array detector.

Constant improvement of control and data acquisition software, meticulous logistics and detailed post-collection auto-processing pipelines enormously increase the throughput of I04, without compromising on its versatility. Accurate and reproducible experiments are made possible thanks to the full integration of dose-driven data collection: precise measurements of flux and other beam parameters are provided in real time to the built-in Raddose3D calculator [4] to help design experiments to achieve optimal data quality by controlling the dose (and therefore radiation damage) based on experimental aim.

At its full potential, I04 can collect up to 32 samples per hour, including mounting, automated X-ray centering, and two full rotations (360 degrees each) at different crystal orientations. This experiment mode is available to all interactive users and can be serialized into data collection queues. To the extreme, it constitutes the core of unattended data collection, a ‘user-less’ mode which can be conveniently interleaved with the classical user mode, where full control of the beamline is given to the operator.

The versatility of uses maximises I04’s throughput, ensuring the best usage of beamtime: not only can multiple short sessions be scheduled throughout the day (allowing multiple users to obtain frequent and rapid information on their samples), but unattended data collection can drastically reduce the idle time between sessions and continue during unsocial hours or weekends.

Here we present the features that make of I04 a unique high-throughput micro- and variable- focus beamline, which combines efficient and automated operations with fully controlled bespoke experiments addressing different experimental aims to meet the needs of a wide variety of users.

[1] Mazzorana M., *et al.*, (2020). *Drug Discovery Today: Technologies*, **37**, 83-92.

[2] Flaig R.*et al.*, (2017). *Acta Cryst.* **A73**, a71.

[3] <https://www.diamond.ac.uk/Instruments/Mx/I04.html>.

[4] Bury C.S. *et al.* (2018). *Protein Sci.* **27**, 217–228.