

## Advances in Crystallographic Hardware for Structural Biology

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### Introduction

The number of life science investigators utilizing crystallography in their research increases every year. Synchrotrons are an invaluable resource for structural work but not everyone has unlimited access to a beamline. In-house diffraction systems complement synchrotron access and can provide increased productivity in the home lab. In recent years, the performance and versatility of in-house systems has greatly improved. The enhanced performance allows data collection on demanding projects such as sulfur SAD phasing or microcrystalline samples. The systems are also perfect for fast sample characterization when preparing for beamline trips. The addition of automation components allows for increased throughput and remote operation.

### MICROSTAR with MX Optics

Bruker AXS has recently introduced the MICROSTAR MX™ (Figure 1) combining the popular MICROSTAR rotating anode generator with our new HELIOS MX multilayer optic. The HELIOS MX has a higher reflectivity than our previous generation mirror resulting in a 2X intensity increase. The focused spot at the sample is also 30% smaller than before, around 160 μm. Since most crystals tend to range between 75-180 μm in size, the MX spot is a better match during data collection helping to reduce background scatter while maximizing diffracted intensities. The flux generated by the MICROSTAR MX is similar to that found at second generation bending magnet beamlines (Figure 2).

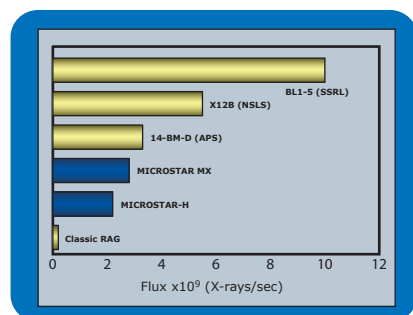


Figure 2. Flux through a 200 μm pinhole (X-rays/sec)



Figure 1. MICROSTAR MX

- Ultra-high intensity, more than  $1.5 \times 10^{11}$  X-rays/sec-mm<sup>2</sup>
- Optimized 160 μm beam minimizes air scatter
- True circular beam profile gives superior performance for long unit cells
- Advanced design for lowest cost-of-ownership

### BRUNO II robotic sample handler

BRUNO II is a robotic sample handling system for automated sample characterization and data collection (Figure 3). The storage Dewar holds uni-pucks for sample storage and transfer making it compatible with the vast majority of beamline robots. The BRUNO II software has a client/server architecture which allows for remote operation as well as advanced tools for sample characterization and data organization.

- Holds 5 uni-pucks, 80 samples
- Pin-in orientation reduces ice accumulation on samples
- Closed Dewar design minimizes ice formation and extends run time
- Dual gripper design simplifies sample handling



Figure 3. BRUNO II robotic sample handler

### I<sub>μ</sub>S source with QUAZAR optics

The I<sub>μ</sub>S is a microfocus sealed tube source similar in design to a standard x-ray tube except that the focused spot on the metal target is very small (< 50 μm). As a result, the I<sub>μ</sub>S produces a very bright beam even though it consumes only 30 W of power much lower than the standard 5-6 kW setting for a conventional rotating anode. The air-cooled source does not require routine maintenance such as filament or seal replacements so the operational costs are very low. When combined with QUAZAR multilayer optics, the intensity measured from the I<sub>μ</sub>S is higher than that normally expected for a conventional RAG (Figure 5). The QUAZAR optics which have been designed specifically for the I<sub>μ</sub>S, have two configurations which help to customize the beam characteristics to the type of samples normally screened. The standard QUAZAR has a larger beam and higher flux for samples that typically have dimensions greater than 150 μm. For much smaller crystals, the QUAZAR MX delivers a much smaller, higher intensity beam.



Figure 4. I<sub>μ</sub>S sealed-tube source and QUAZAR optic

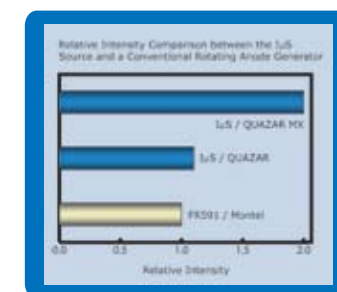


Figure 5. Intensity comparison

### Conclusions

Due to the types of projects pursued in structural biology labs today, it is necessary to expand the capabilities of home-lab systems. Higher intensity rotating anode generators and very low maintenance microfocus sources enable more of this work to be completed in-house.