

# Protein Crystallography

## FOX3D CU 14\_39P



Application Note n° AN-3D2

### Abstract

In early 2007, a direct comparison between a GeniX beam delivery system and a rotating anode generator using the same experimental conditions (same crystals, exposure times, detector, etc.) revealed that the GeniX system produces superior data with small crystals while the results for larger crystals are virtually identical.

In the current application note Dr. Claudio Klein from MARresearch compares the performance of the FOX2D CU 10\_30P optics to our latest model, the FOX3D CU 14\_39P optic, which features an optimized high precision ellipsoidal substrate and a state-of-the-art multilayer to achieve a beam with improved focusing properties and high flux density.

With the FOX3D optics we observe more than a 2-fold increase in diffraction as compared to the FOX2D optics, in particular when looking at small crystals. Hence the FOX3D CU 14\_39P optic pushes the performance of the GeniX beyond that of traditional rotating anode generators.

## Comparison of the GeniX 2D and GeniX 3D on a MAR345DTB for protein crystallography application

Data courtesy of Claudio Klein, Marresearch GmbH, Norderstedt, Germany

### Introduction

In this study, we have used a GeniX beam delivery system operated at 50kV/1mA (50 W), a mar345 image plate detector, and a mardtb goniometer system to compare the performance of two different types of optics:

- Xenocs FoX 2D Cu 10\_30P
- Xenocs FoX 3D Cu 14\_39P

The FoX 3D CU 14\_39P mirror features an optimized high precision ellipsoidal substrate and a state-of-the-art multilayer to deliver a beam with better focusing properties and higher flux density than the FoX 2D Cu 10\_30 optics.

Two crystals were used in this study:

- a large lysozyme crystal (~350µm in all dimensions)
- a mid-size lysozyme crystal (~180µm)

Table I : Technical Data of Optics

**Beam in focus :** Picture generated by the "Beam profile" method implemented in the mar345dtb program: the aperture of a pair of slits in front of an ionization chamber was set to 0.10 mm. The ionization chamber then scans an area of 0.5 x 0.5 mm across the beam. The resulting 2D image shows the distribution of intensities of the beam that travels through the small pinhole formed by the pair of slits.

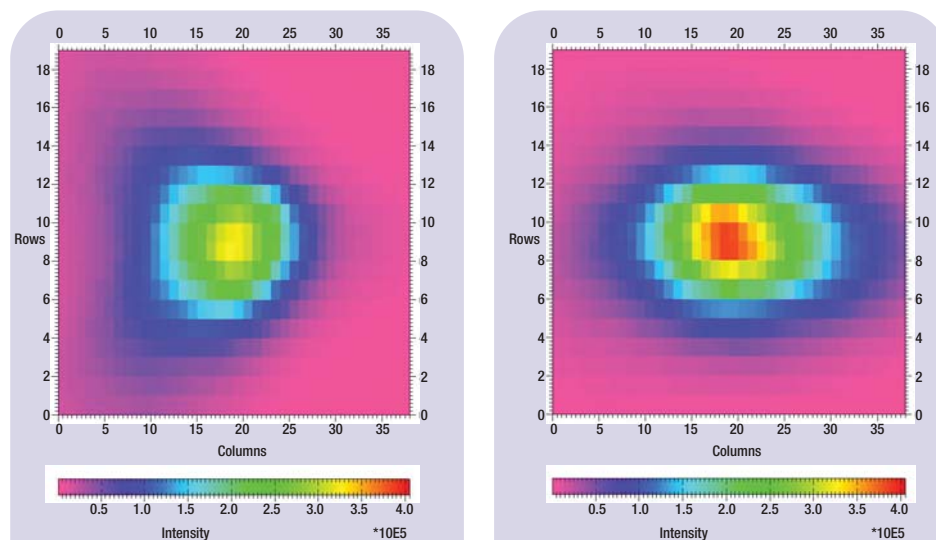
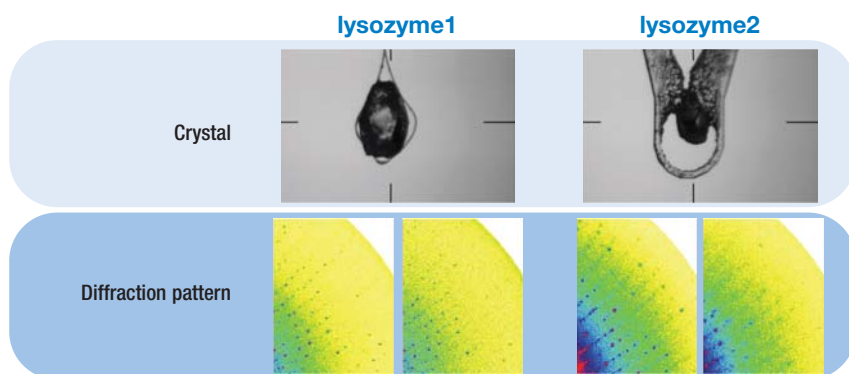


Fig. 1 : The marµX – a Turn-key System for X-ray Crystallography from MARresearch combining a GeniX beam delivery system, a MAR345 image plate detector and a marDTB goniometer system.

FOX2D CU 10_30 P		FOX3D CU 14_39 P	
10 cm	Distance source - optic center	14 cm	
30 cm	Distance optic center - focus	39 cm	
230 µm x 230 µm	Spot size in focus	190 µm x 190 µm	
> 2 x 10 <sup>8</sup> photons/sec	Typical flux	> 3 x 10 <sup>8</sup> photons/sec	
4.8 x 4.8 mrad <sup>2</sup>	Divergence	5.4 x 5.4 mrad <sup>2</sup>	

## Data collection & processing

The data for all crystals were collected on the same GeniX generator and the same mar345dtb detector system. When exchanging the mirrors, the beam was carefully realigned. Data were processed using mosflm & scala. The data set of the lysozyme1 crystal collected with the 3D optics suffered from an unstable cryo-cooler (variations of temperature of 20 deg.). This explains the higher R-factors despite much stronger intensities.



Space group	P 4 <sub>3</sub> 2 <sub>1</sub> 2	
Unit cell axes	a=79.1 b=79.1 c=37.9 Ang.	
High resolution limit	1.60 Ang.	2.0 Ang.
Mosaicity	0.30	0.90
Size of crystal	450µm x 300µm x 250µm	150µm x 170µm x 200 µm
Distance crystal-detector	100 mm	120 mm
Exposure time per image	90 sec	300 sec
Total no. of images	63	90
Delta-φ per image	1.0°	1.0°

Optics	3D	2D	3D	2D
Completeness all/ last shell	86.0 / 89.6 %	86.4 / 89.5 %	92.1 / 90.3	78.5 / 76.6
Multiplicity all/ last shell	5.3 / 5.1	5.3 / 5.1	6.4 / 5.5	5.7 / 5.4
Rsym all/ last shell	7.3 / 20.3 %	6.5 / 33.5	6.0 / 17.0	7.2 / 45.1
<Intensity> all/ last shell	9056 / 1071	2755 / 233	10134 / 1939	3298 / 300
I/σ all/ last shell	16.7 / 5.5	18.1 / 3.1	23.2 / 7.0	20.9 / 2.0

## Data comparison

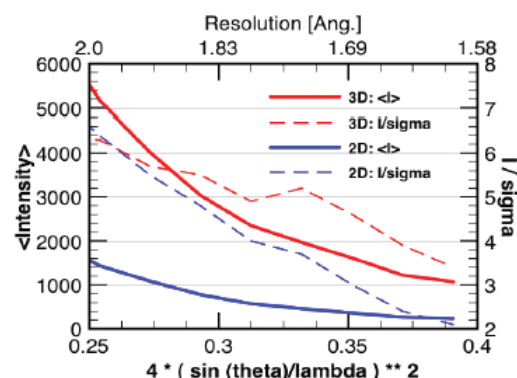
In the plots given in Fig. 2, the data collected with the 3D optic are drawn in red, the ones collected with the 2D optic are drawn in blue, respectively. The I/σ values (dotted lines) scale to the y-axis on the right hand side of the plot. For sake of clarity, for the well diffracting larger crystal only the high resolution ranges between 2.0 and 1.6 Ang. resolution are plotted.

For both the large crystal (lysozyme1) and the smaller crystal (lysozyme2) the 3D data show much larger net intensity values in all resolution shells than the 2D data. In particular at higher resolution, this also applies to I/σ-values. The difference of performance between the 3D and the 2D optic becomes more obvious when looking at the smaller crystal. Fig. 3 shows the ratio of the average net intensity of the diffraction data from both optics. For the large crystal we see a constant ratio of approx. 3 times more intensity up to 2 Ang. resolution. For higher resolution shells, the factor increases to 4.5. For the smaller crystal, the ratio is less linear, meaning that the smaller crystal benefits even more from the better beam quality of the 3D optic. In fact, a reasonable resolution limit for the chosen exposure time for the 2D optic was at about 2.2 Ang. while the data from the 3D optic extended to 1.9 Ang.

## Conclusion

The data collected here suggest that at least a two-fold increase in observed diffracted intensity can be expected from the FoX3D Cu 14\_39P optic as compared to the 2D optic. This increase translates in better I/σ ratios and possibly higher resolution. For smaller crystals, the performance difference is expected to further increase.

### lysozyme1



### lysozyme2

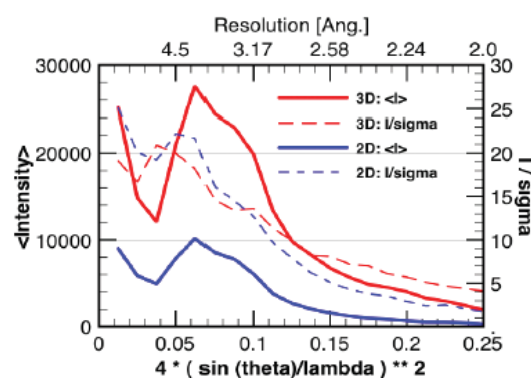


Fig. 2 : Intensities vs. resolution

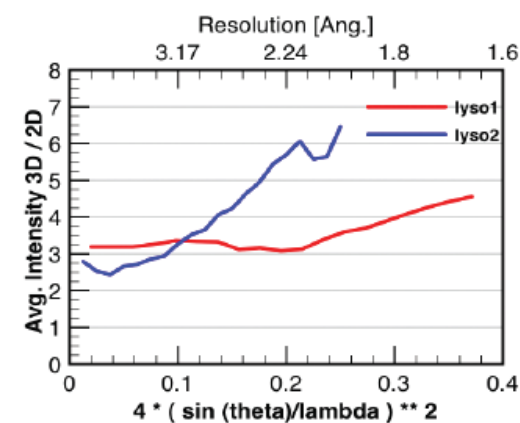


Fig. 3 : Ratio of the average net intensity of the diffraction data from both optics.

19 Rue François Blumet  
38360 Sassenage - France

Phone: +33 4 76 26 95 40  
Fax: +33 4 76 26 95 49

[www.xenocs.com](http://www.xenocs.com)  
[sales@xenocs.com](mailto:sales@xenocs.com)