

Protein Crystallography

FOX3D CU 14_39P

Abstract

Xenocs' FOX3D CU 14_39P was tested at Sanofi Aventis Vitry for single crystal diffraction application on several protein crystals.

Purpose of these tests was to validate the performance gain of this new technology compare our previous generation FOX2D.

Results confirm that the improved focussing properties and higher collection angle are translated into an enhanced intensity and improved signal to noise ratio comparing to the precedent FOX2D multilayer mirrors in particular for small and weakly diffracting crystals.

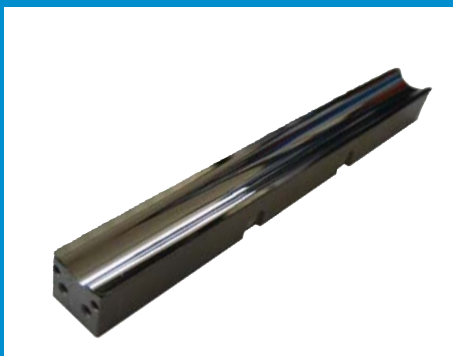


Fig. 1 : the FOX3D CU 14_39P X-ray optic

Comparative testing of FOX3D and FOX2D optics for protein crystallography on a 70 μm rotating anode generator

Data courtesy of Magali Mathieu and Valérie Steier, Sanofi-Aventis-Vitry, France

Introduction

The FOX3D CU 14_39P is a first 3D single reflection mirror from a Xenocs new product range. Benefiting of a novel technology, the FOX3D CU 14_39P boasts a large collection angle and produces a highly symmetric focal spot.

Dr. Magali Mathieu and Dr. Valérie Steier of Sanofi-Aventis in Vitry (France) compared the performance of a FOX3D CU 14_39P to that of a FOX2D mirror using crystals of different sizes. Both mirrors were installed on a rotating anode with a 70 μm source size. Three crystals were used :

- A) a large, well-diffracting crystal;
- B) a small, weakly diffracting crystal;
- C) a small, moderately diffracting crystal.

Experiment

The results obtained for crystal A, B and C are presented in the tables at page 2 and 3. A dataset is considered to be usable to a given resolution if Rmerge is below 0.35 and Mean (I/sd(I)) is greater than 2 for that resolution shell. The data were processed with Mosflm and scaled with Scala (CCP4 suite).

CRYSTAL A

Size : 300*300*10μm³ - MA345dtb slits : 1*1/0.8/0.8 - Distance : 175 mm -
Dphi/image : 1° - Exposure time : 3' - Space group : C2 - # collected images : 180

	FOX2DCU 12_38P			FOX3DCU 14_39P		
	Overall	InnerShell	OuterShell	Overall	InnerShell	OuterShell
Low resolution limit	28.99	28.99	2.14	24.43	24.43	2.14
High resolution limit	2.03	6.42	2.03	2.03	6.42	2.03
Rmerge	0.097	0.034	0.323	0.094	0.034	0.309
Rmeas (within I+/-)	0.115	0.041	0.386	0.112	0.041	0.369
Rmeas (all I+ & I-)	0.115	0.041	0.386	0.112	0.041	0.369
Rpim (within I+/-)	0.061	0.022	0.208	0.059	0.023	0.198
Rpim (all I+ & I-)	0.061	0.022	0.208	0.059	0.023	0.198
Fractional partial bias	0.028	-0.023	0.084	0.046	-0.015	0.109
Tot. # of observations	45688	1492	5699	45890	1477	5655
Total number unique	13511	470	1802	13556	463	1797
Mean(I)/sd(I)	16.6	57.9	3.5	17.1	62.6	3.5
Completeness	98.7	99.2	91.1	98.5	97.8	90.2
Multiplicity	3.4	3.2	3.2	3.4	3.2	3.1

Conclusion Crystal A : Data is of equivalent quality with both mirrors.

	FOX2DCU 12_38P			FOX3DCU 14_39P		
	Overall	InnerShell	OuterShell	Overall	InnerShell	OuterShell
Low resolution limit	42.41	42.41	3.27	24.49	24.49	3.27
High resolution limit	3.10	9.80	3.10	3.10	9.80	3.10
Rmerge	0.215	0.044	0.770	0.147	0.033	0.446
Rmeas (within I+/-)	0.251	0.051	0.899	0.174	0.039	0.525
Rmeas (all I+ & I-)	0.251	0.051	0.899	0.174	0.039	0.525
Rpim (within I+/-)	0.130	0.027	0.461	0.092	0.021	0.274
Rpim (all I+ & I-)	0.130	0.027	0.461	0.092	0.021	0.274
Fractional partial bias	-0.031	-0.007	-0.056	-0.038	-0.014	-0.023
Tot. # of observations	35098	1254	4222	32835	1025	3958
Total number unique	10121	348	1322	9800	320	1250
Mean(I)/sd(I)	8.3	51.8	1.7	13.9	78.4	2.4
Completeness	92.9	95.5	83.1	90.9	89.2	80.1
Multiplicity	3.5	3.6	3.2	3.4	3.2	3.2

CRYSTAL B

Size : 300*60*5 μm^3
 MA345dtb slits : 1*/0.8/0.8
 Distance : 250 mm
 Dphi/image : 1°
 Exposure time : 20'
 Space group : P21
 # collected images : 180



Data were processed only to 3.1Å and were usable to about 3.2Å. **Conclusion** : the data are significantly better on the FOX 3D CU 14_39P. Signal/noise ratio has improved 40 to 67% depending on the resolution shell.

	FOX2DCU 12_38P			FOX3DCU 14_39P		
	Overall	InnerShell	OuterShell	Overall	InnerShell	OuterShell
Low resolution limit	24.71	24.71	2.14	24.69	24.69	2.14
High resolution limit	2.03	6.42	2.03	2.03	6.42	2.03
Rmerge	0.275	0.081	1.095	0.128	0.045	0.455
Rmeas (within I+/-)	0.307	0.089	1.234	0.144	0.051	0.514
Rmeas (all I+ & I-)	0.307	0.089	1.234	0.144	0.051	0.514
Rpim (within I+/-)	0.133	0.037	0.555	0.064	0.023	0.233
Rpim (all I+ & I-)	0.133	0.037	0.555	0.064	0.023	0.233
Fractional partial bias	-0.046	-0.007	-0.259	-0.014	-0.007	-0.144
Tot. # of observations	91716	3003	11676	91220	2994	11383
Total number unique	18742	598	2603	19263	676	2529
Mean(I)/sd(I)	6.6	26.0	1.3	13.5	45.4	3.0
Completeness	96.1	88.4	92.1	98.3	98.1	89.4
Multiplicity	4.9	5.0	4.5	4.7	4.4	4.5

CRYSTAL C

Size : 100*60*60 μm^3
 MA345dtb slits : 1*/0.8/0.8
 Distance : 175 mm
 Dphi/image : 1°
 Exposure time : 5'
 Space group : I222
 # collected images : 120



The data were usable to 2.15Å. **Conclusion**: Signal/noise ratio has improved by 75 to 130% with FOX3D CU 14_39P.

In order to better illustrate the differences between the data obtained using the two mirrors, images of crystal C (with the same grayscale setting) taken using each optic are shown in Fig.2.

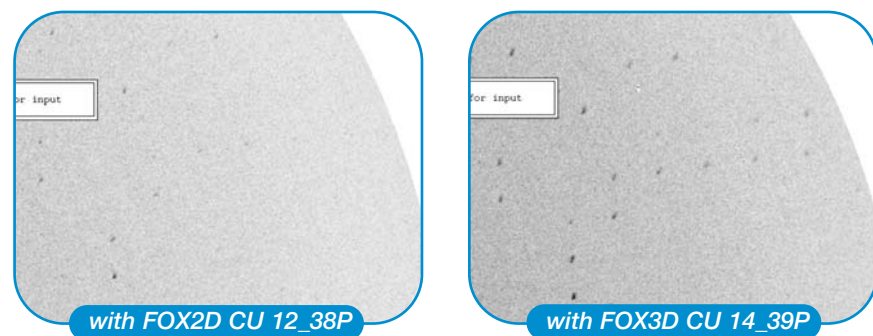


Fig. 2 : Diffraction images of Crystal C acquired using the FOX2D CU 12_38P optic (on the left) and the FOX3D CU 14_39P (on the right)

Conclusion

Both FOX2D CU 12_38P and FOX3D CU 14_39P mirrors provide good quality data for large, strongly-diffracting crystals. For medium to small size, moderately or weakly diffracting crystals, the enhanced collection angle and focusing properties of the FOX3D CU 14_39P lead to a significantly improved S/N ratio.

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