Aspheric multilayer optics: New opportunities for laboratory X-ray diffraction and scattering applications

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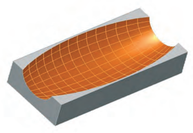
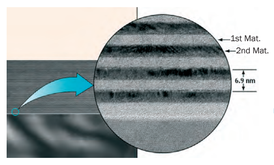
Xenocs®
Reflecting Future Technology

Increased collecting power

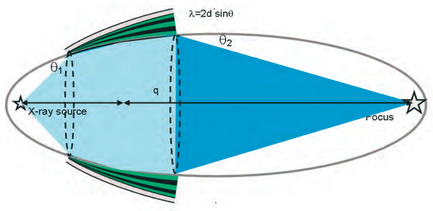
- Aspheric doubly curved surface
- Graded multilayer coatings



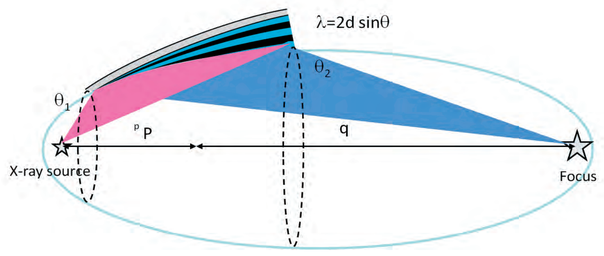
➔ larger collection angles
➔ single reflection optic



➔ high reflectivity
➔ tailored wavelength range

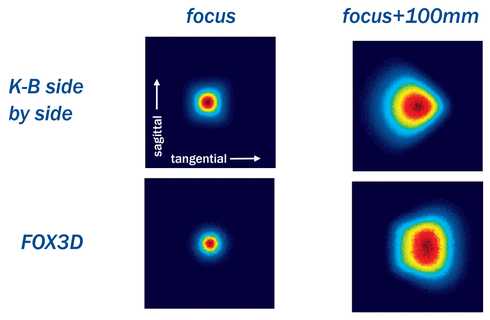


Increased collection angle in sagittal plane

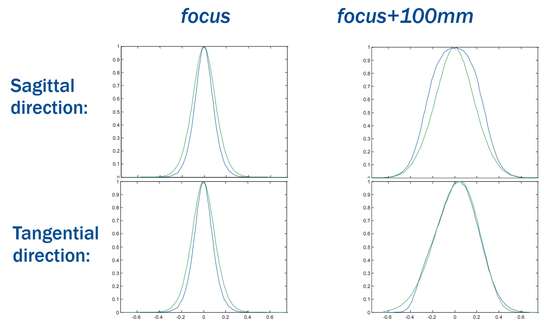


Increased collection angle in meridional plane

Superior focussing properties of 3D optics



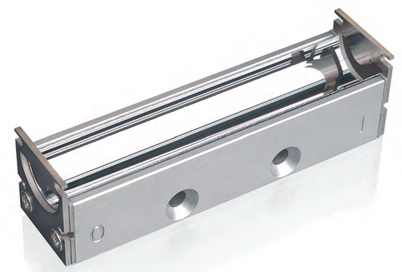
Comparison of the beam profile at typical positions along beam path for K-B side-by-side geometry and Xenocs FOX3D (simulation, 1.5x1.5mm)



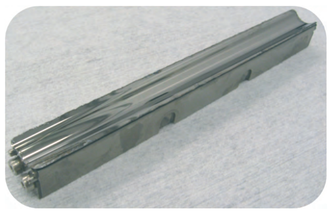
Intensity profiles KB vs FOX3D
Green line: KB
Blue line: FOX3D

Benefits:

- smaller spot size for equivalent magnification
- higher flux density
- sharper beam profile, reduced background reduction



FOX3D Optics for Protein Crystallography



- Flux Improvement by more than 2.5 in the diffracted spots
- Reduced Background

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

Crystal B: 300*60*5µm³	FOX2D CU 12_38P			FOX3D CU 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+/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+/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
Total no. 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

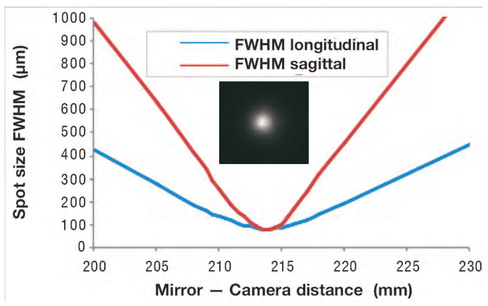
Data is significantly better on the FOX3DCU 14_39P. Signal/noise ratio has improved 40 to 67% depending on the resolution shell. Data usable to about 3.2A

Crystal C: 100*60*60µm³	FOX2D CU 12_38P			FOX3D CU 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+/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+/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
Total no. 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

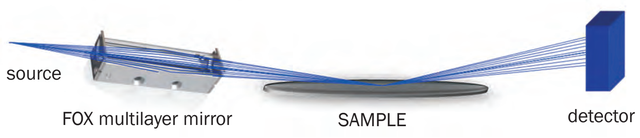
Signal/noise ratio has improved by 75 to 130% with FOX3DCU 14_39P Data usable to about 2.15A

Sanofi : 'Signal/noise ratio has **improved by 75 to 130%** with FOX3D

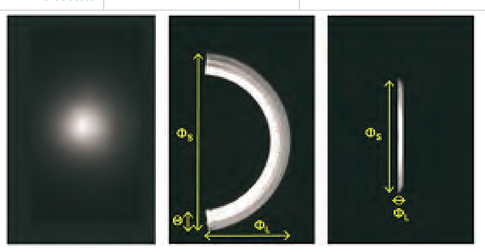
High Convergence FOX3D (XRR, microdiffraction)



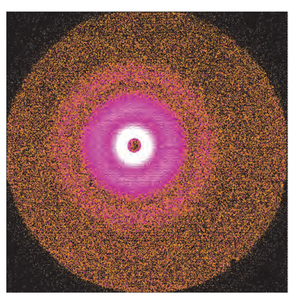
Focusing curves & CCD image of beam profile at focus (inset)

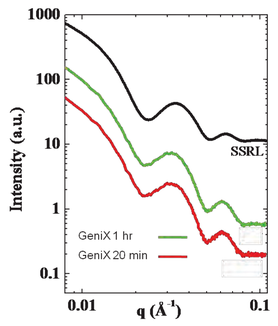


Beam configuration	Full Beam	Slit-limited Beam (customizable)
Typical flux	> 440 x 10^6 ph/s	> 26 x 10^6 ph/s
Beam convergence	ΦS ≥ 4 deg ΦL ≥ 2 deg Θ = 0.54 deg	ΦS = 2.6 deg ΦL = 0.05 deg
Spot size at focus FWHM	~80 µm	~80 µm



SAXS: GeniX Cu Low Divergence with FOX2D optic





Left) 2D SAXS data (20 minute exposure) obtained from a solution sample of micro-tubules (MT) at UCSB .
Right) Azimuthally averaged scattering data I(q) for MT compared to synchrotron data collected at beamline 4-2 at SSRL. Curves are shifted for clarity.

Key parameters of SAXS setup with GeniX

UCSB
Data courtesy of Dr. Youli Li, Univ. of California, Santa Barbara, USA.

Source-to-Sample Distance	1.8 meters
Sample-to-Detector Distance	1.7 meters
Detector	Bruker HI-STAR multiwire
Beam Collimation	3 sets of motorized slits
Qmin*	1.0x10^{-2} Å^{-1}
Beam Flux at sample*	1.4 x 10^7ph/s

** Note that a lower Qmin and higher flux can be obtained with further system optimisation.*

XENOCS supplies :

- innovative X-ray multilayer optics
- X-ray beam delivery solutions

Applications currently covered :

- Protein Crystallography
- Small Molecule
- SAXS
- High Resolution
- High pressure diffraction
- Powder diffraction
- Reflectometry
- And many others ...

X-ray beam characteristics of typical Xenocs solutions

	Applications	Typical Flux [photons/sec]	Focal Spot Size FWHM [µm²]	Divergence mrad²	Brightness 10^6 [mrad^{-2} mm^{-2} sec^{-1}]
FOX3D CU 14_39P optic (on a 1,2KW/70 µm source)	Proteomics	> 4.5 10^9	230 x 230	5.4 x 5.4	3000
FOX3D CU 21_21HC optic (on a 50W/50 µm source)	XRR Microdiffraction	> 440 10^6	80 x 80	70 x 8.7	113
GeniX CU VHF (50w/ 50µm source)	Proteomics	> 300 10^6	200 x 200	5.4 x 5.4	257
GeniX CU Low Divergence (50w/ 50µm source)	SAXS, WAXS	> 150 10^6	1500x1500	0.8 X 0.8	105

- **FOX3D solutions deliver optimal spot, flux and beam shapes**
- **FOX3D solutions preserve source brightness through the single reflection design**
- **FOX3D solutions enable larger collection angles : up to 4 degrees**

FOX3D optics combined with micro-focus sources deliver a higher flux and flux density onto your samples resulting in greatly improved signal to noise compared to traditional optics.

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