

Advantage of 3D single reflection optics for small protein crystals and long unit cell analysis

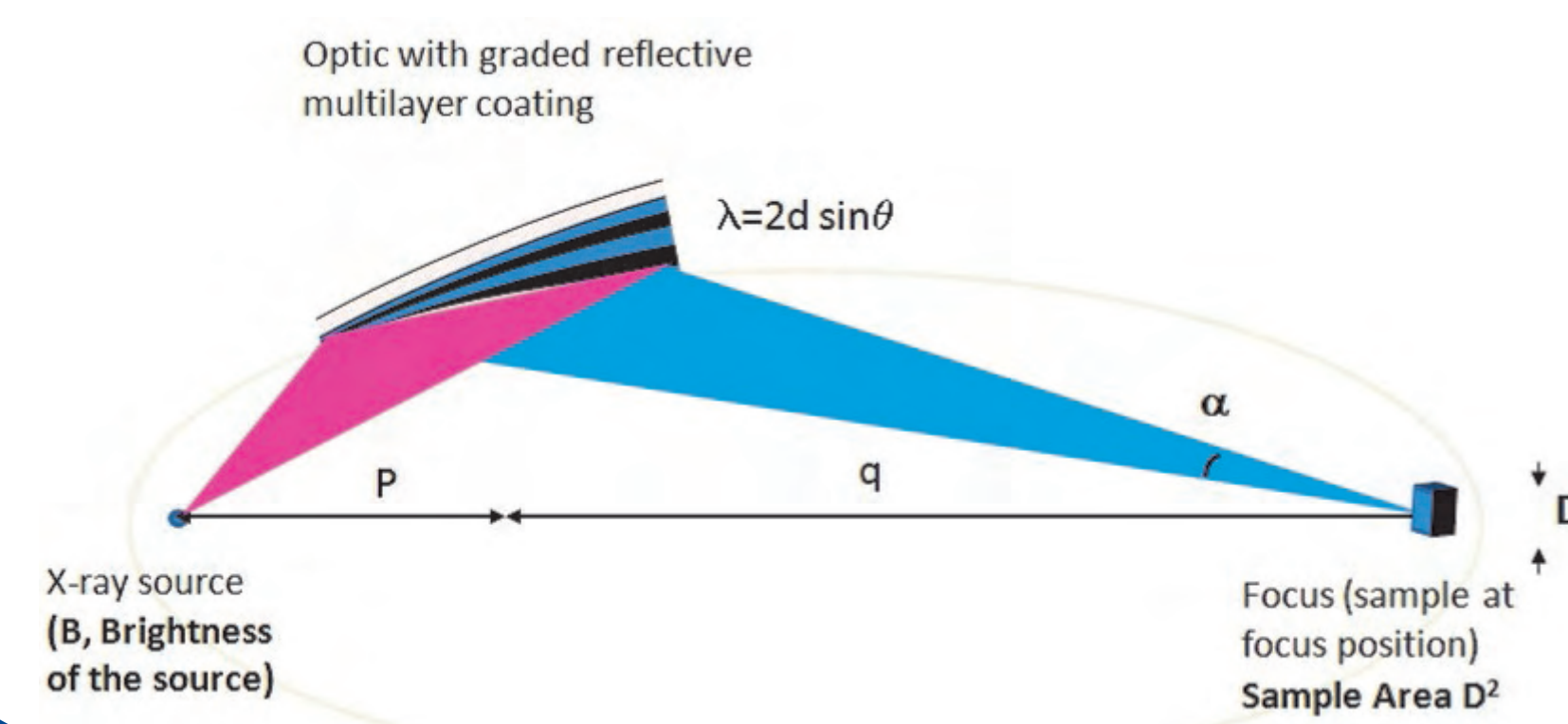


Reflecting Future Technology

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Focusing system description

Source-Optic-Sample efficiency



Useful Flux F within Sample Area :
 $F = B \times \alpha^2 \times D^2 \times \text{Eff}$

(for X-ray beam over-illuminating the sample)
 α^2 is optic convergence solid angle
D² is sample area
B is source brightness (ph/s/mm²/sr)
Eff is optic efficiency in the system configuration

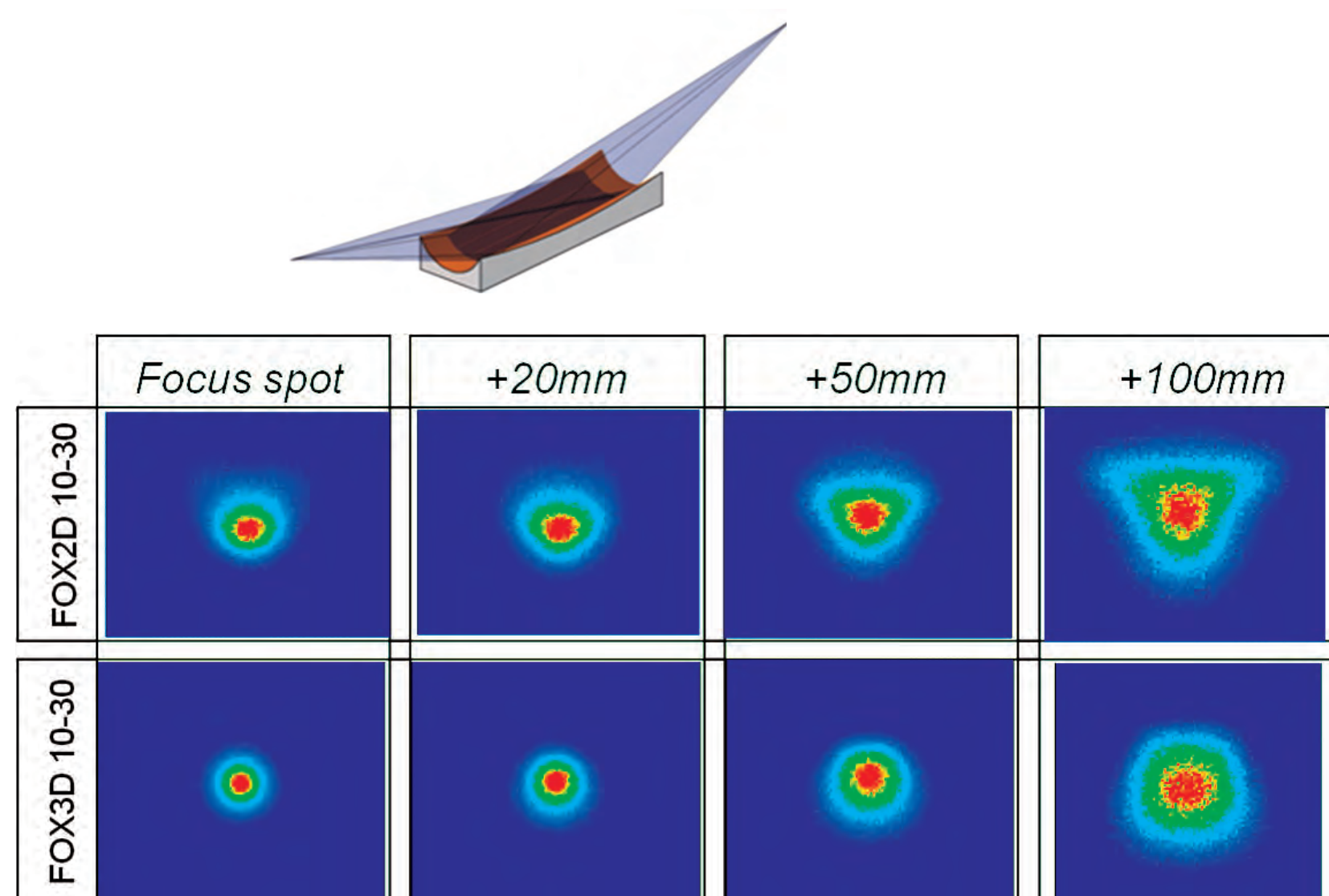
Best compromise is obtained with beam matching sample size

→ Optic magnification $M=q/p$

Superior focussing properties of FOX 3D optics

FOX 2D Optics

Toroidal substrate with multilayer optic



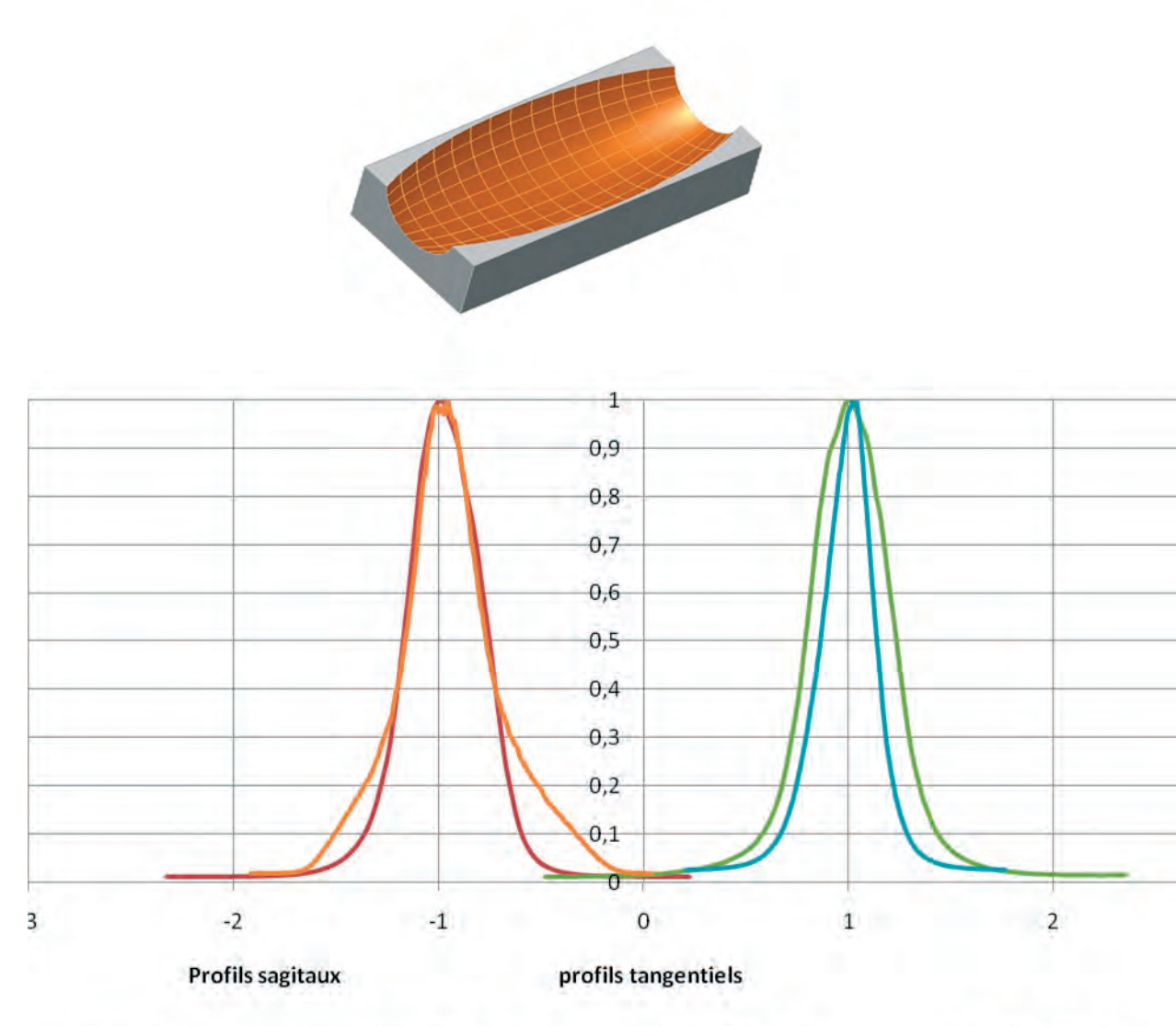
Comparison of the beam profile at different points along beam path for FOX3D and FOX2D optics (simulation)

Benefits:

- smaller spot size for equivalent magnification
- higher flux density
- shaper beam profile (leads to background reduction)

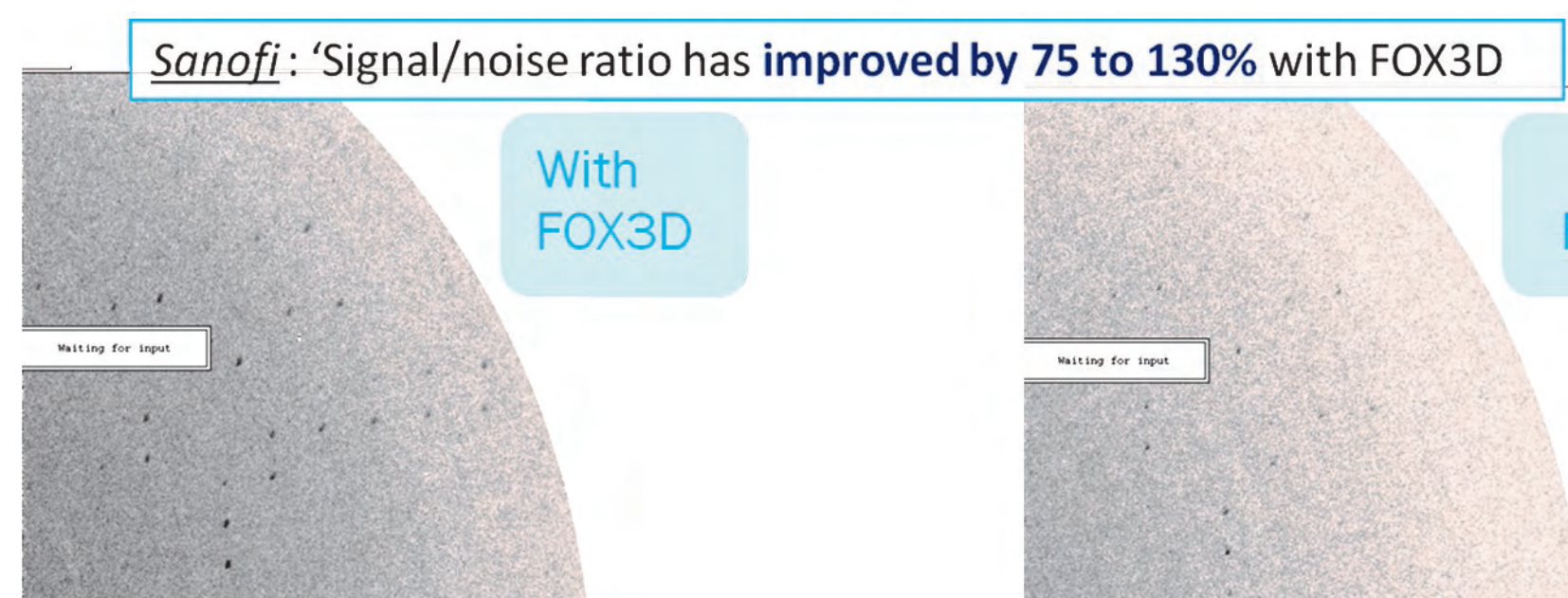
FOX 3D Optics

Aspheric substrate with multilayer optic



Intensity profiles FOX3D vs FOX2D

FOX3D Optics in small single crystal XRD



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

Test on a 100*60*60µm³ crystal
FOX 2D 12_38 and FOX 3D 14_39 comparison



Microfocus system (GeniX) for Protein Crystallography

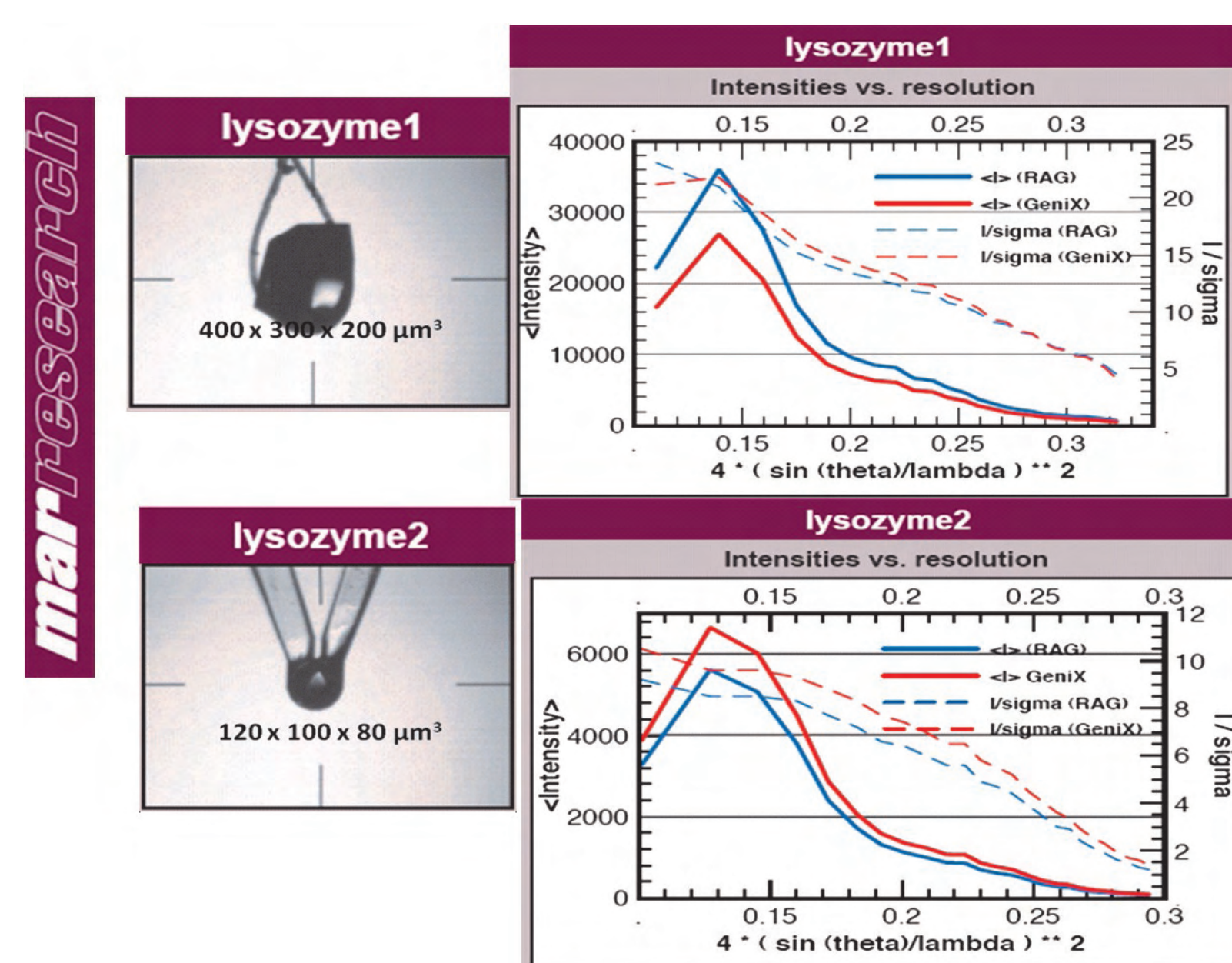
GeniX System

- Low Power (50W) /High brilliance microfocus source
- Efficiently coupled to X-ray multilayer optics

Configuration	GeniX	Optic	Flux (ph/s)	Divergence (mrad ²)	Spot size at focus
GeniX High Flux		FOX 2D 10_30	> 200 x 10 ⁶	4,8 x 4,8	230 µm FWHM
GeniX Very High Flux		FOX 3D 14_39	> 300 x 10 ⁶	5,3 x 5,3	190 µm FWHM

Comparative crystallographic data with a RAG

Comparative crystallographic results of a GeniX High Flux Generator and a RAG (200 µm, 2kW)



→ The GeniX provides increased I/ sigma parameters due to a smaller spot size and high brilliance beam

→ The GeniX outperforms the RAG system in all aspects for the small crystal

FOX 3D and Montel optics efficiency

Multilayer optics coupling efficiency

Resulting flux outcome from the optic is a convolution of Source intensity distribution (S_s) and acceptance size (S_m) by the multilayer optic

S_m is a function of Δθ (width of Bragg reflection of the multilayer optic) and p (source-optic distance) and is

S_r is resulting from the convolution of both size distribution

Efficiency of the coupling is therefore expressed as (gaussian hypothesis)

$$C_e = \frac{S_m}{\sqrt{S_s^2 + \lambda m^2}}$$

Multilayer Optic Efficiency

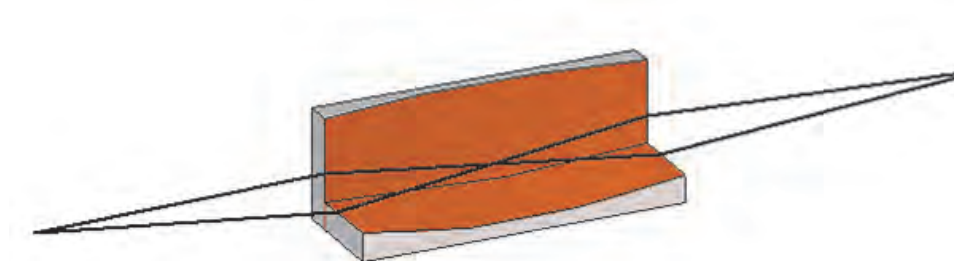
$$\text{Eff} = R * C_e$$

Comparative coupling efficiency: Montel VS FOX 3D

(simulation for source 70µm, source to optic p= 14cm, mirror length is 100 mm)

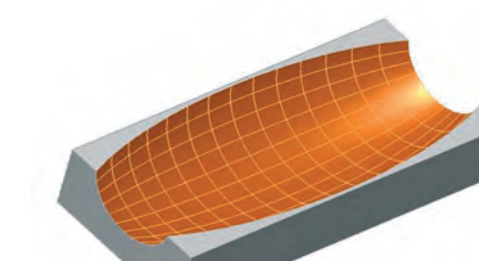
Montel Mirrors

Two reflection design



FOX 3D optics

Single reflection design

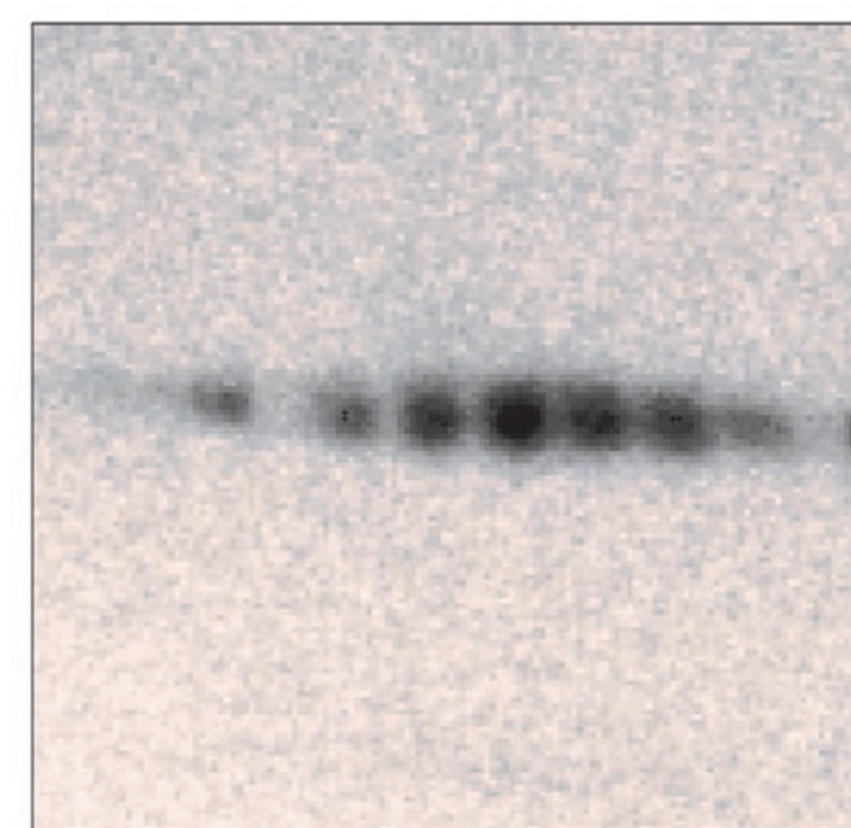


Mirror Type	Montel Mirrors	FOX 3D Mirrors
Optic Efficiency (Calculated over mirror length)	Eff = 42 %	Eff = 62 %

Single Reflection multilayer optics provide 50% higher flux compared to Montel mirrors for a similar optic geometry and a 70µm source

FOX 3D optics for long unit cells

- Resolving power (maximum unit cell) of FOX 3D 14_39 optics
A 220 Angströms unit cell edge resolved with a GeniX VHF (50 W, 50 µm source coupled to a FOX 3D 14_39 optic) on a MAR 345



Diffraction along a 220 Angströms Cell Axis
Crystal-to detector distance is set to 1.75 mm, enabling to resolve reflections along the closely spaced reciprocal cell axis at high resolution (1,9 Angströms).

→ FOX 3D 14_39 was used with 5,3 mradians divergence settings

→ A crystal with 220 Å was well resolved with the GeniX VHF system

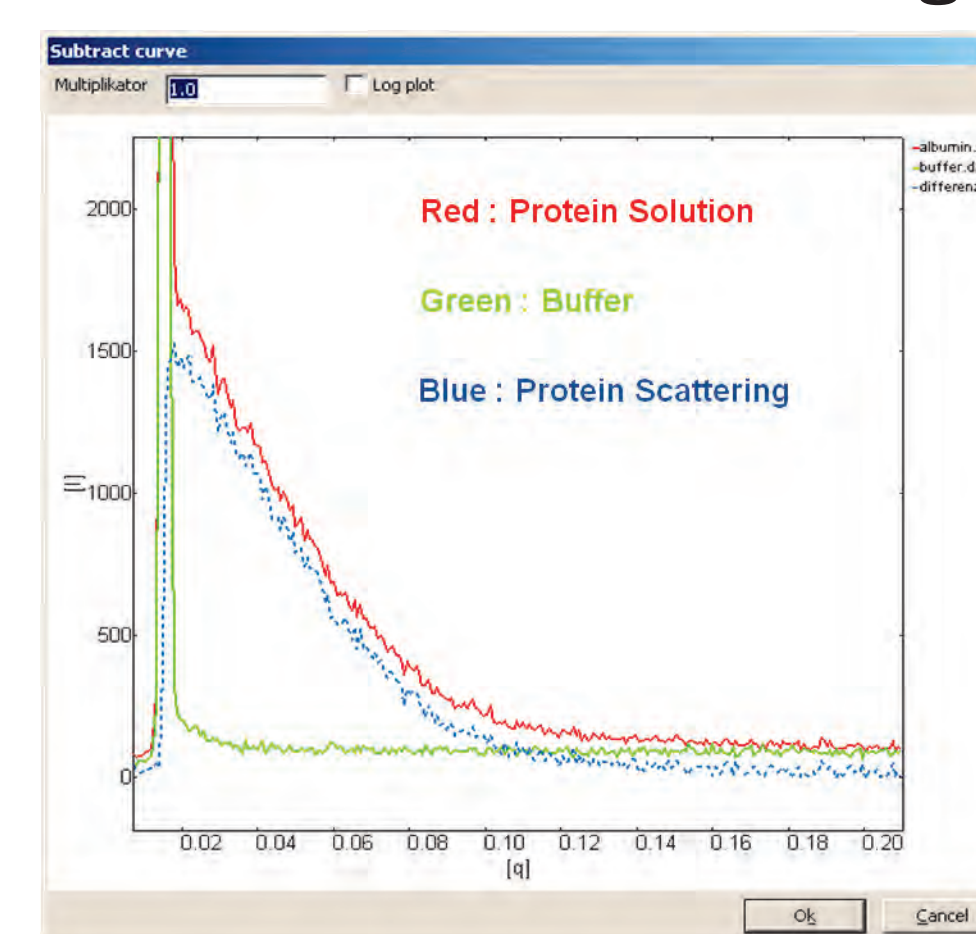
→ Longer unit cells (>300 Angströms) can be solved with optimized set-up (beam divergence)

Simulated resolving power (max unit cell) on a Micromax 007 HF RAG source

Configuration	Calculated Resolving Power (max unit cell)	Typical Flux [photons/sec]	Spot size at focus [µm FWHM]
FOX3D CU 14_39P optic (on a 1,2KW/70 µm source)	250 Angströms (max divergence : 5,3 mrad)	> 4.2 10 ⁹	210 µm FWHM
FOX3D CU 14_39P optic (on a 1,2KW/70 µm source)	>300 Angströms (reduced divergence)	> 1.3 10 ⁹	210 µm FWHM

GeniX with FOX 3D optics for protein solution SAXS

- Protein Solution Small Angle X-ray Scattering with a S3-Micro from Hecus



data courtesy of Hecus, X-ray Systems GmbH



Sample : BSA 33 mg/mL in buffer (PBS)
Measuring time : 30 min
Sample volume : < 10 µl
Program Hecus easySAXS

→ Data acquired by Hecus with S3-Micro SAXS equipment integrating a GeniX (50 W, 50 microns source coupled to FOX 3D long focusing optics)



■ FOX 3D single reflection optics provide improved focusing properties and higher intensity compared to other X-ray optics

■ FOX 3D 14_39 single reflection optic is optimised for protein crystallography in the laboratory enabling small crystal and long unit cell analysis

■ FOX 3D long focusing optics enable compact protein solution small angle scattering

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