

Fast & Curious

Data collection strategies for HPC detectors

Hans Gildenast, Application Scientist

10.11.25

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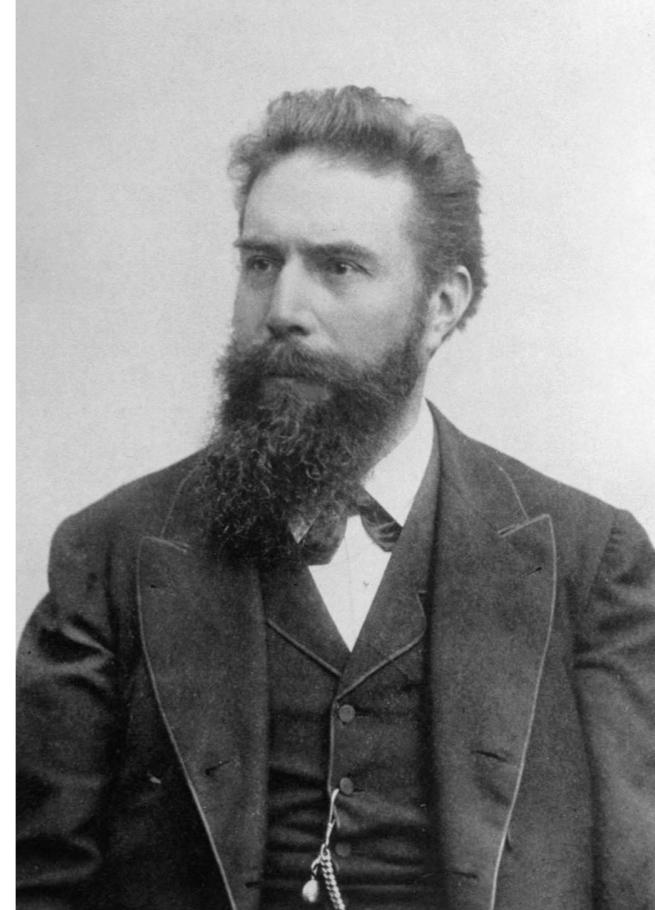
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What does it take to get good MX data?

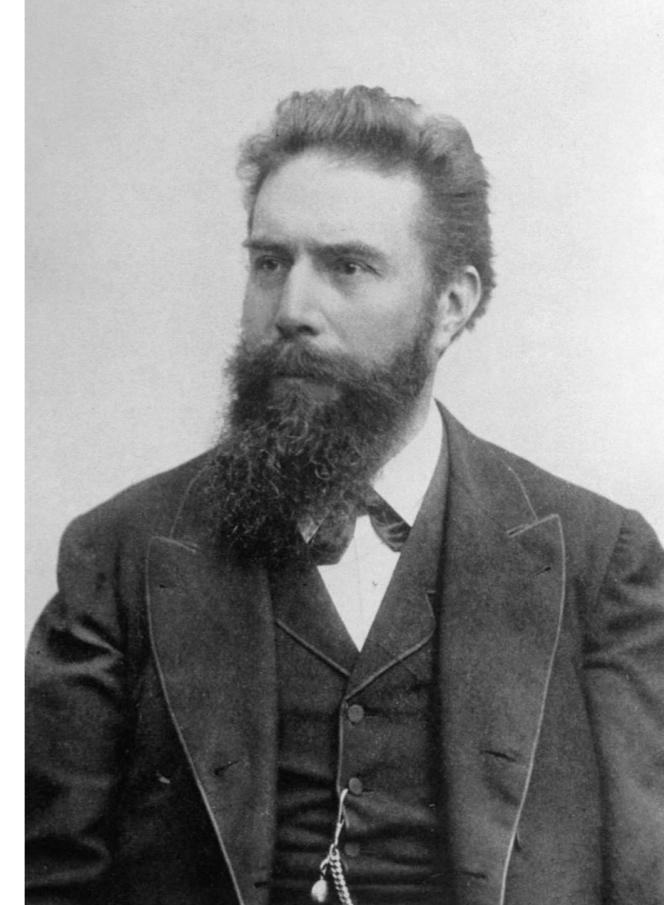
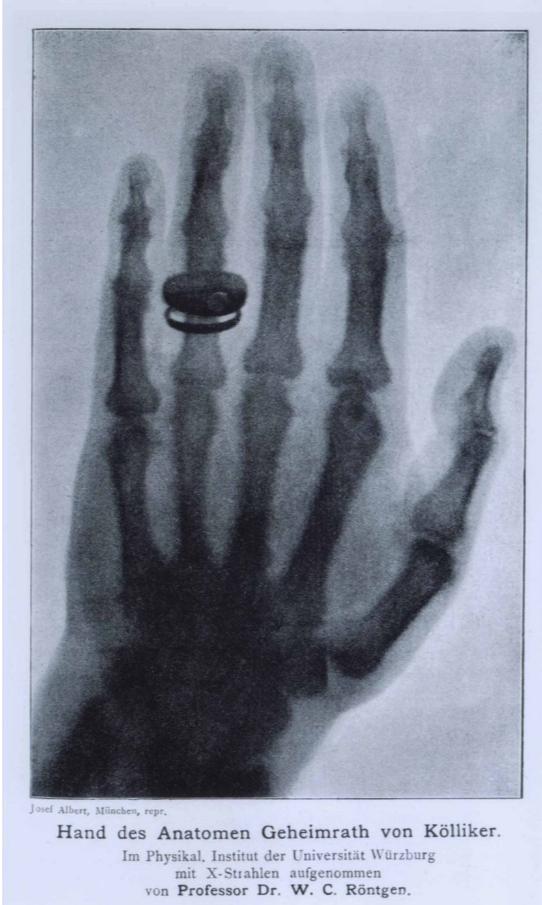
- low/no Radiation Damage
- Completeness
- Redundancy
- No Noise and Low Background
- Scattering
- An Excellent Detector



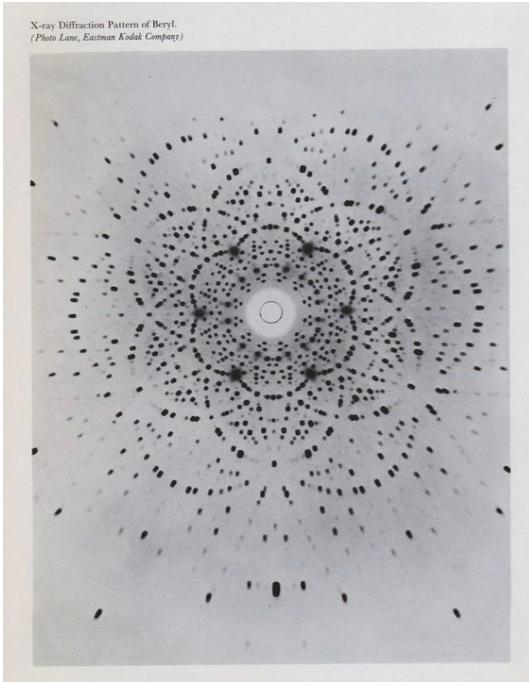
1895



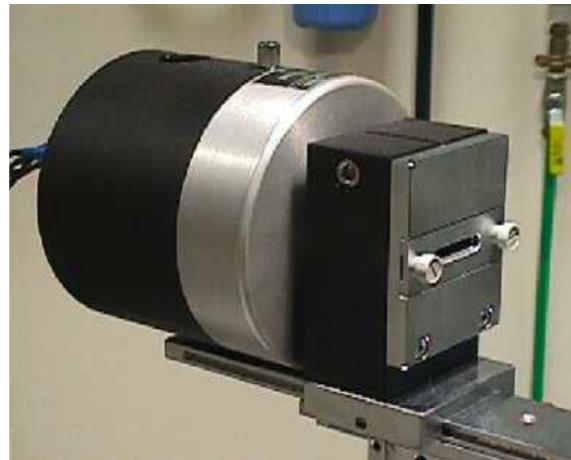
1895



History of X-ray Detection



X-ray film
1914-1940s



Point-detectors
1914-1990s

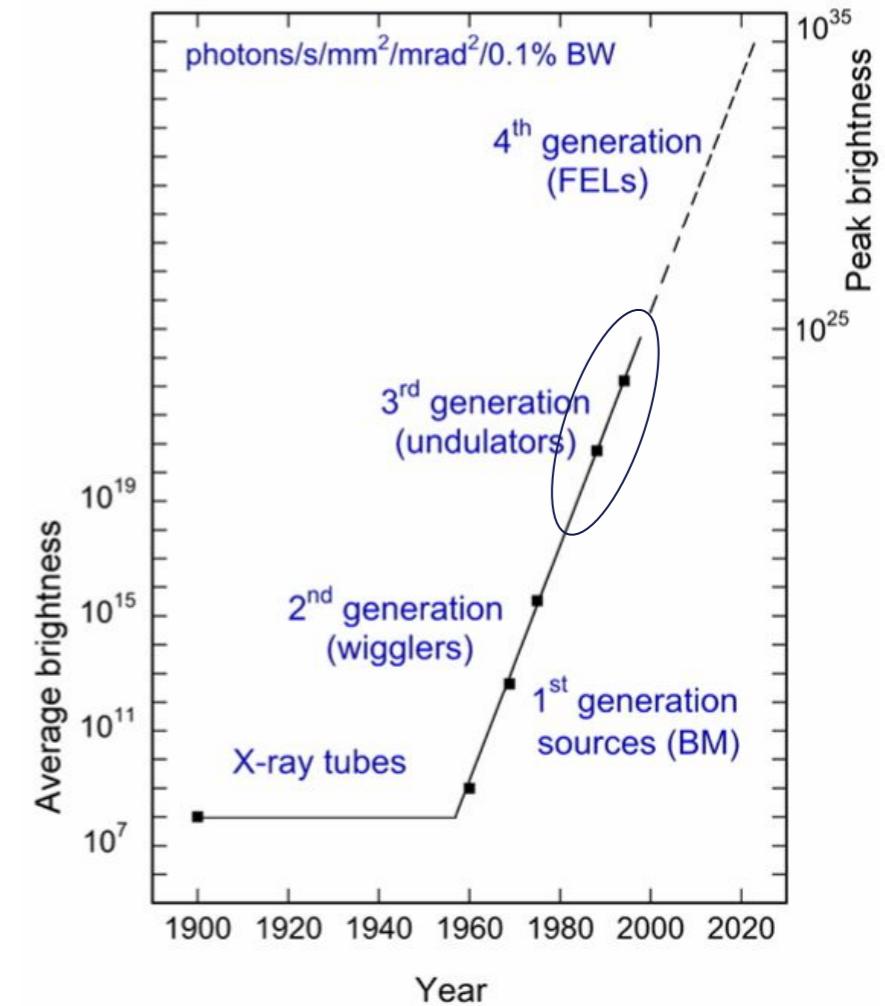
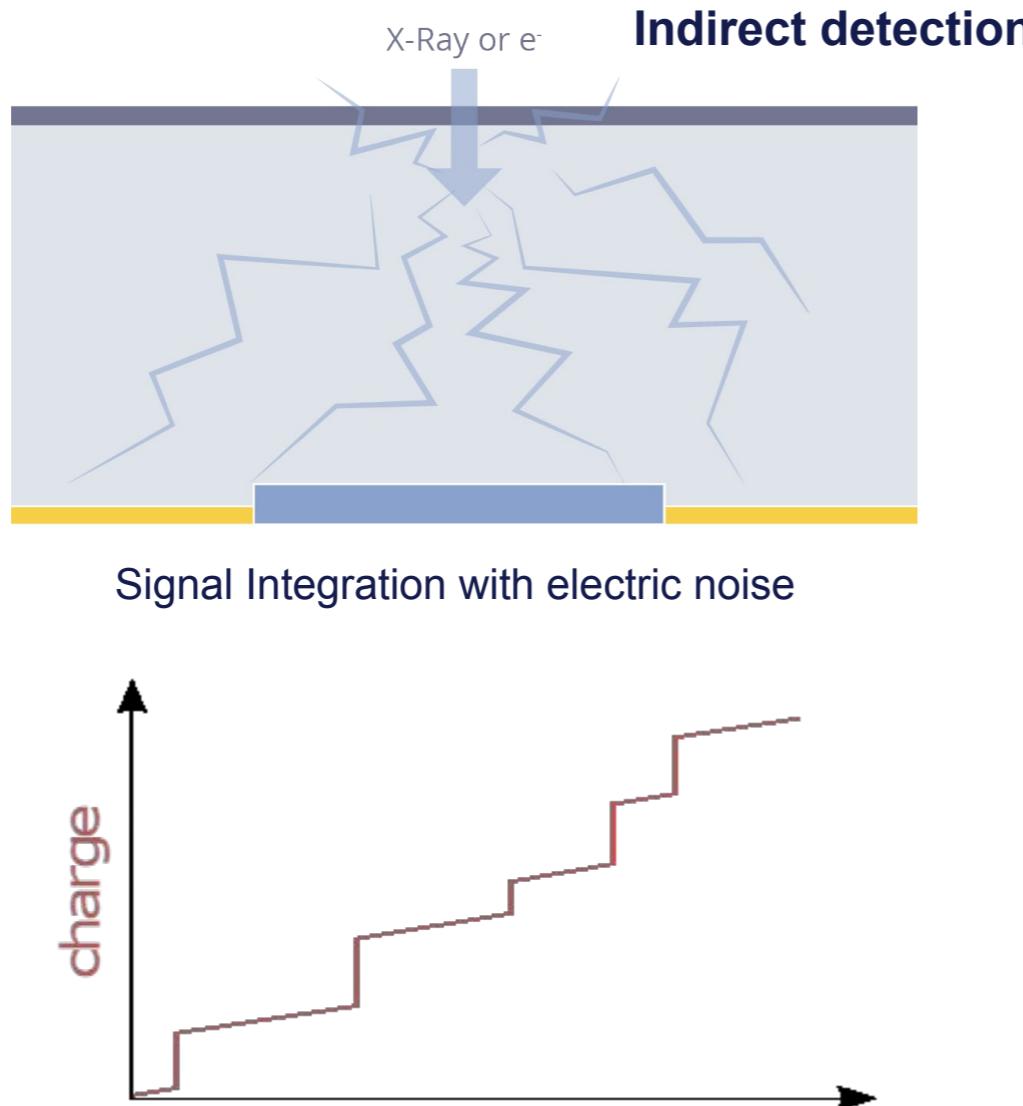


Image plates
1985-1990s

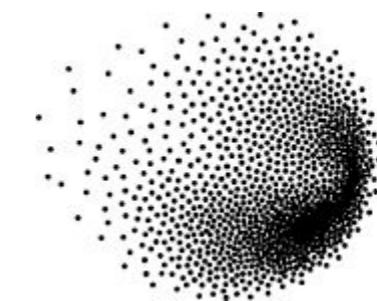
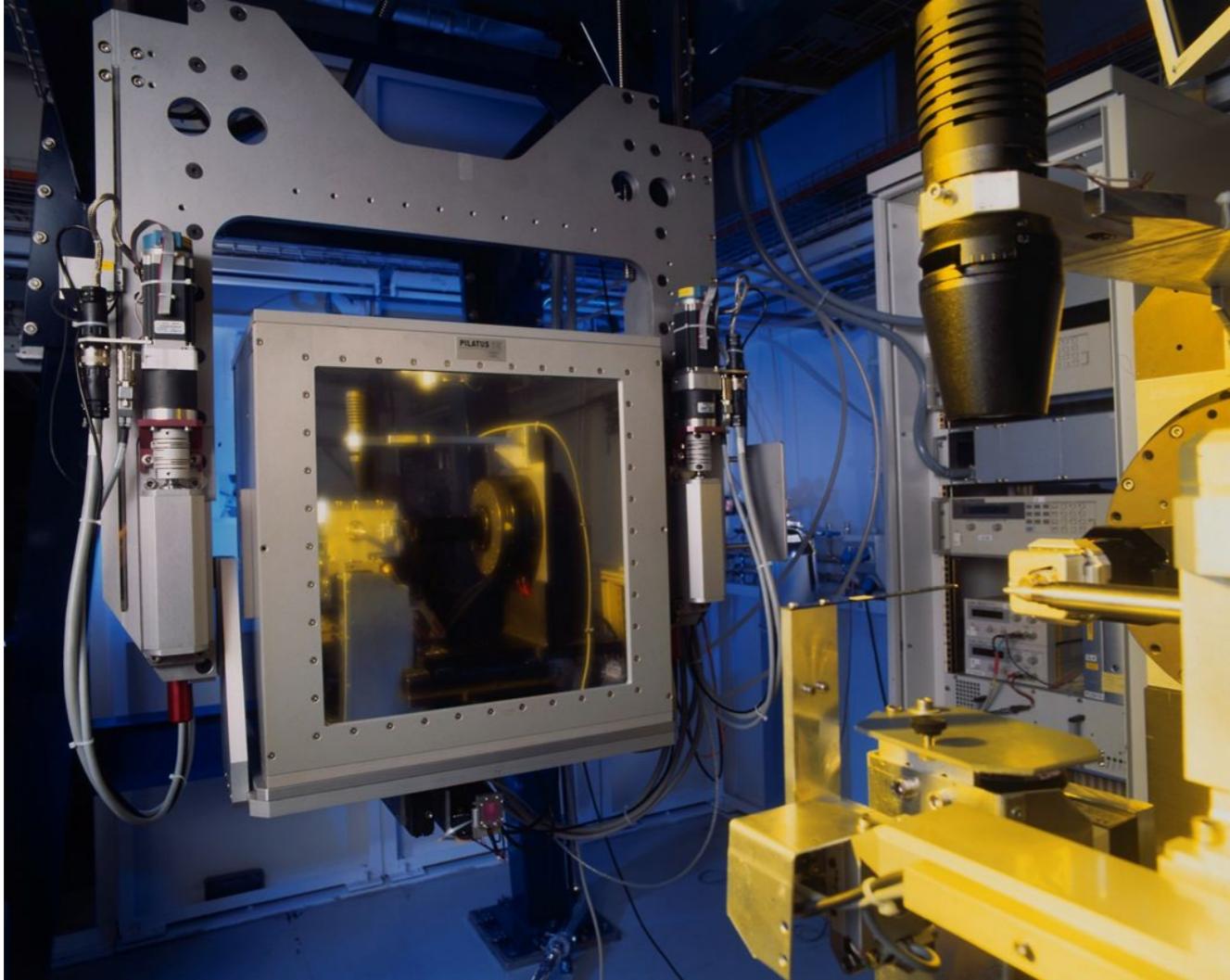


CCD/CMOS
1990s-2006

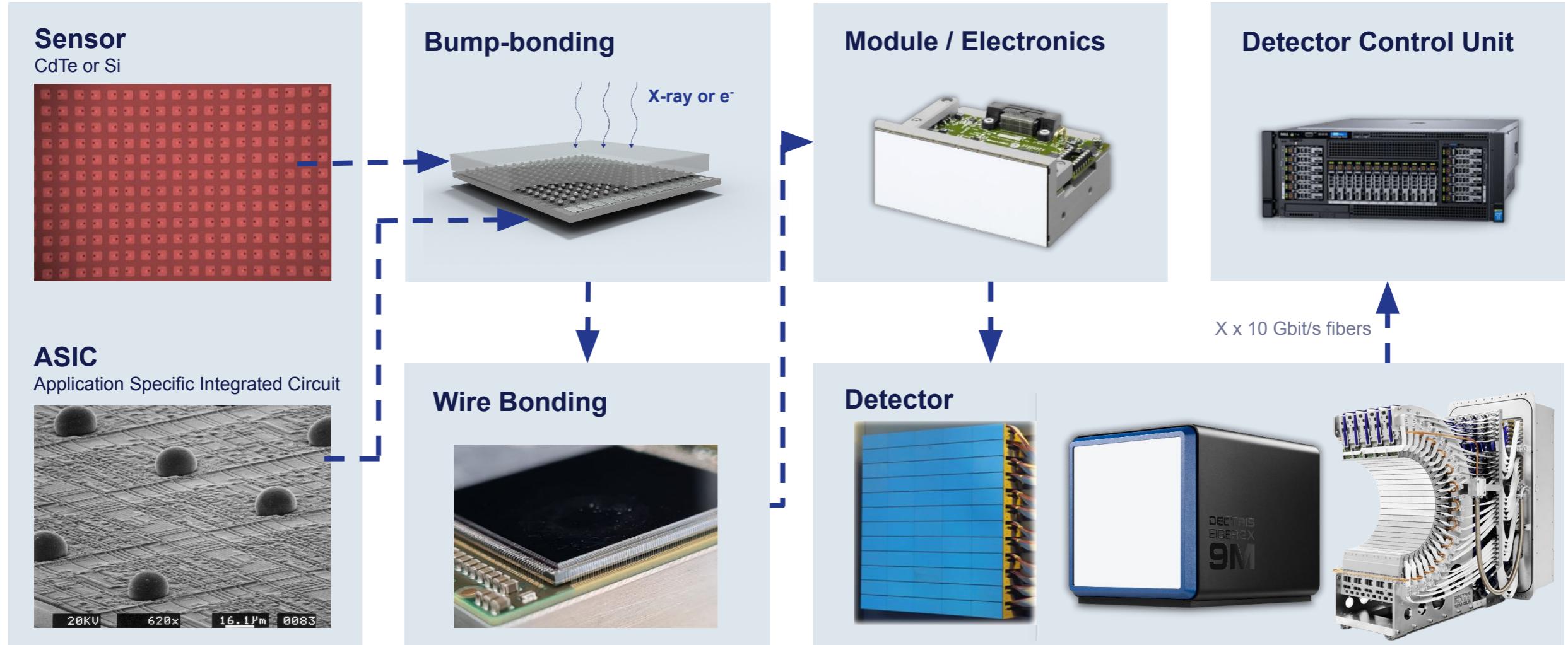
History of X-ray Detection



Hybrid Pixel Photon Counting X-ray Detectors

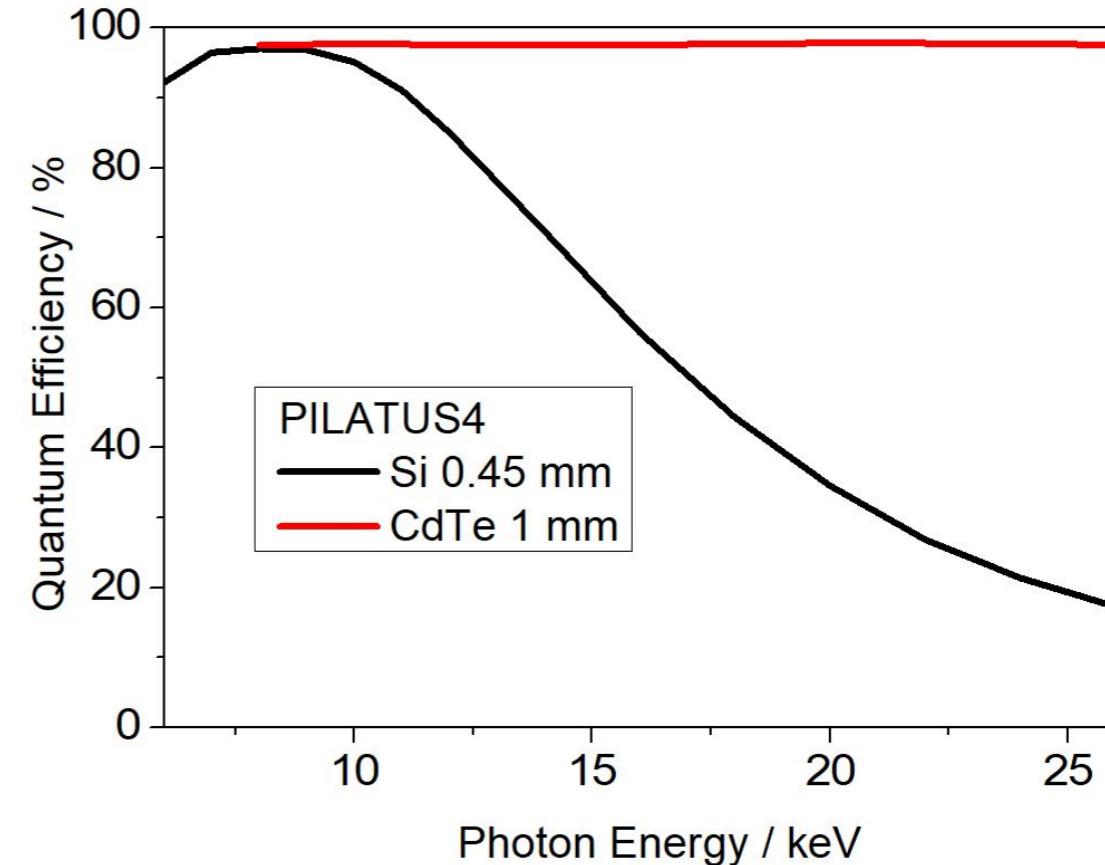
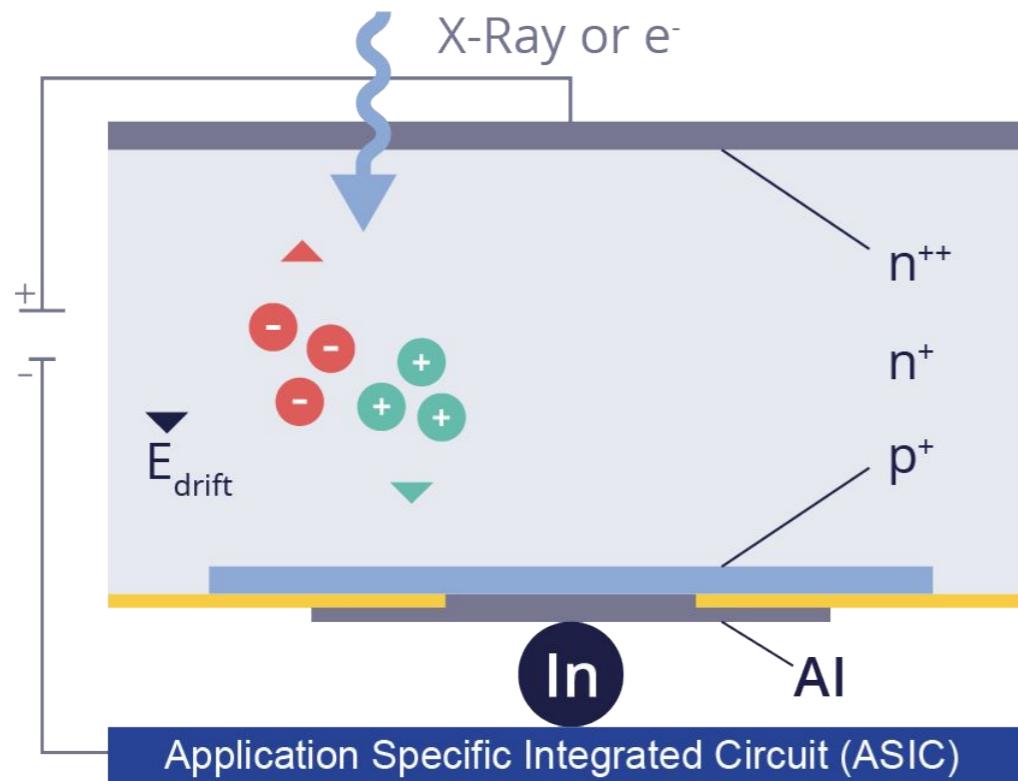


Hybrid Pixel Photon Counting X-ray Detectors



Hybrid Pixel Photon Counting X-ray Detectors

Direct detection

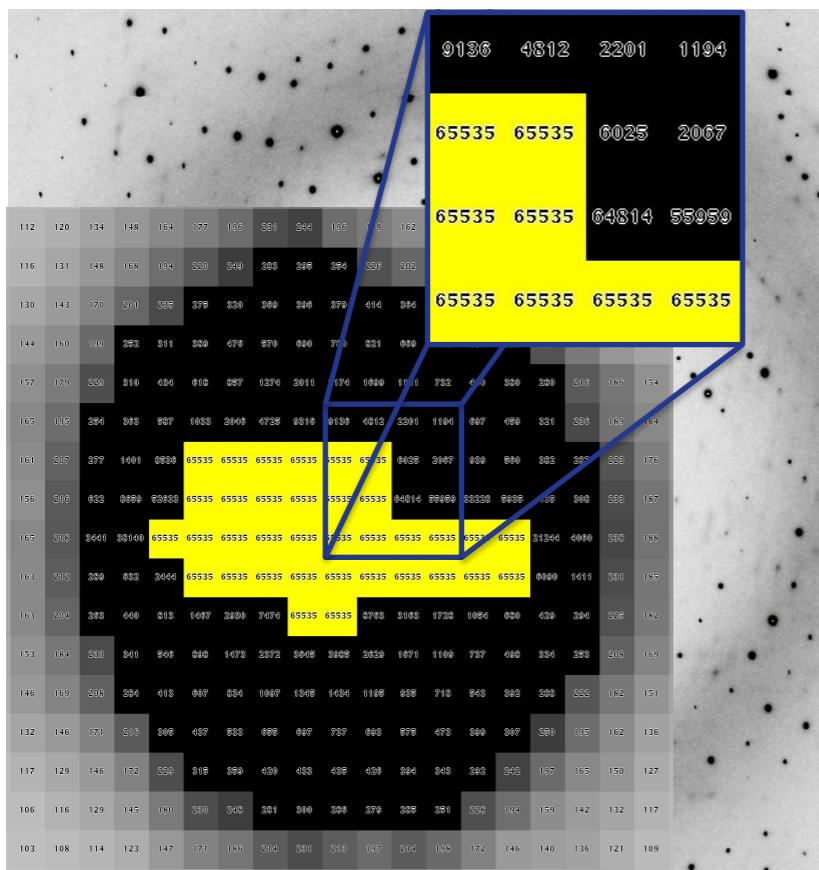


MX at high photon Energies: [Dickerson & Garman, J. Synchrotron Rad. 2019, 26, 922.](#)

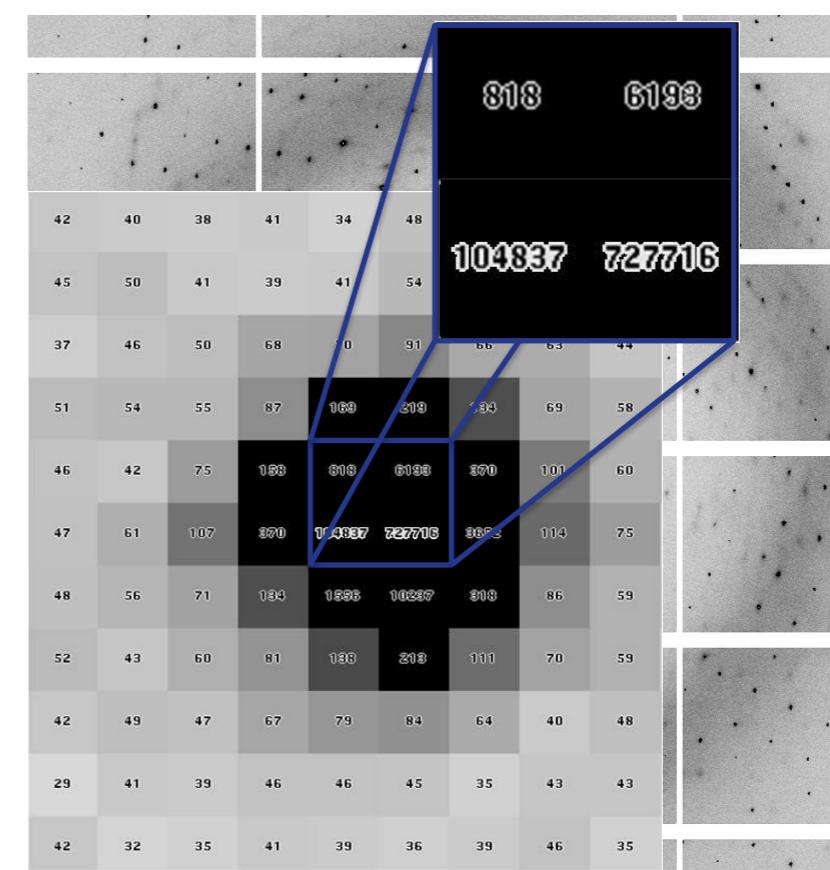
[Storm, Axford & Owen, IUCrJ 2021, 8, 896.](#)

Hybrid Pixel Photon Counting X-ray Detectors

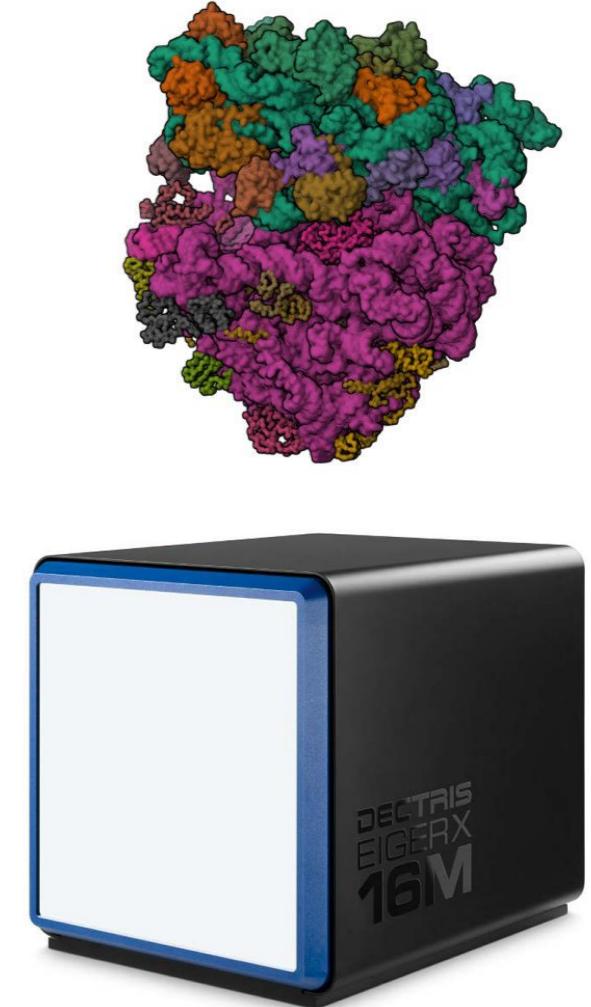
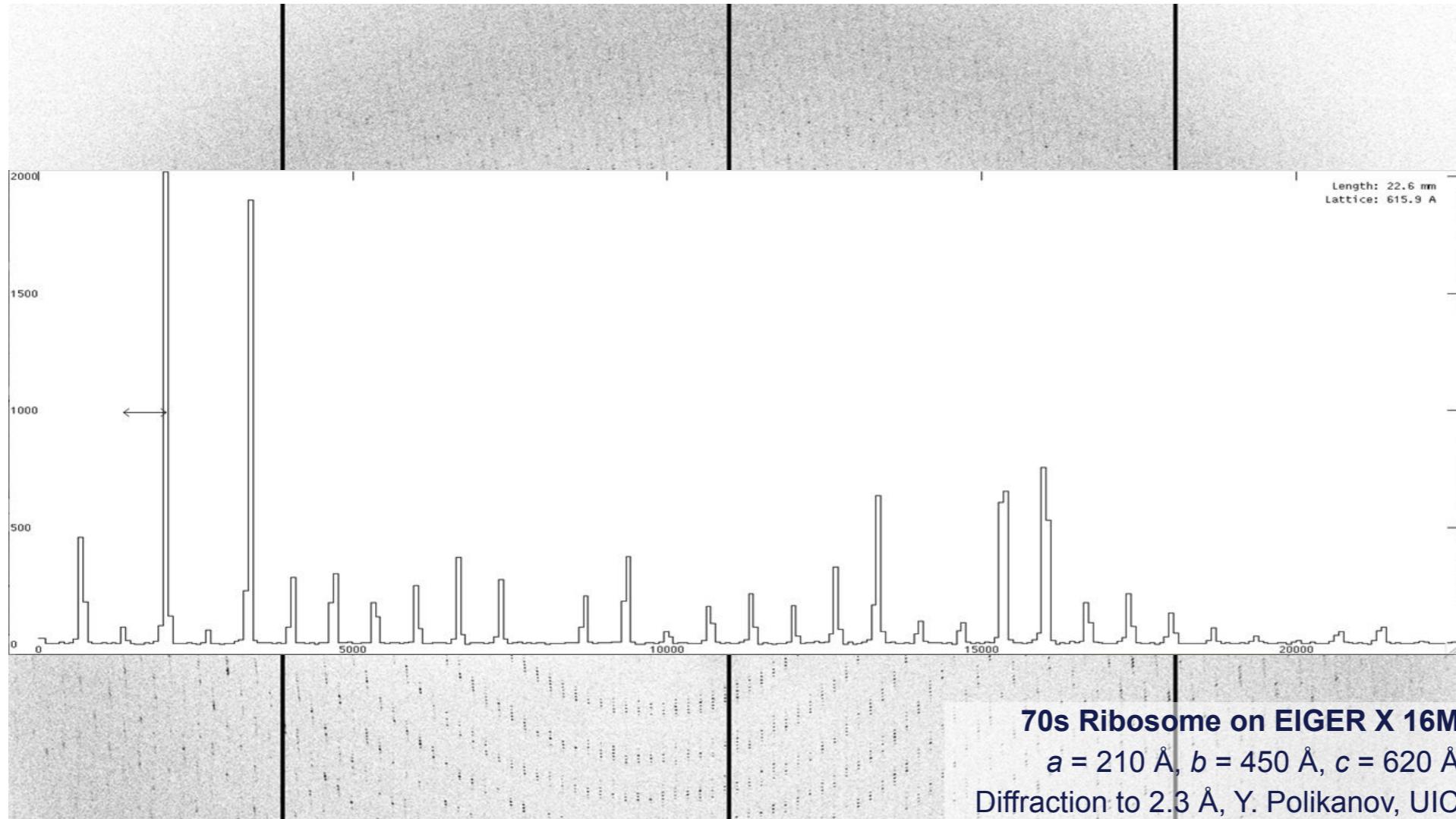
Indirect Detector CCD



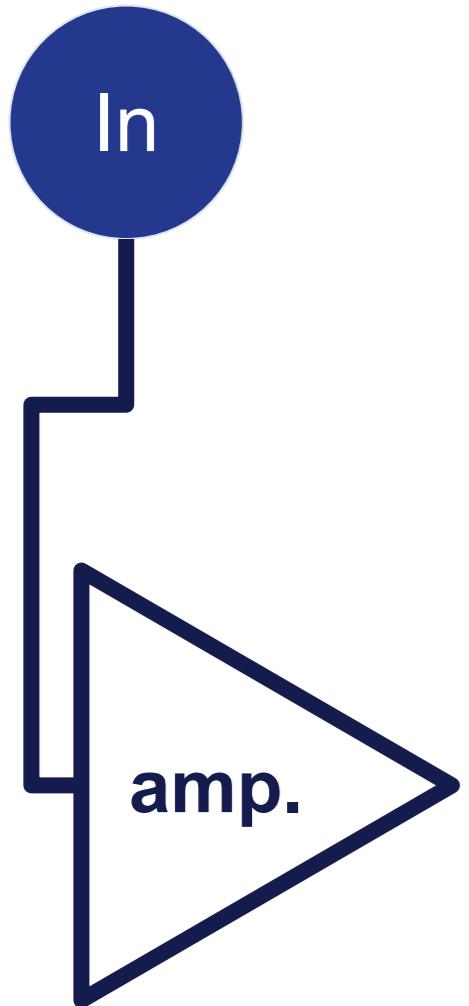
HPC detector PILATUS



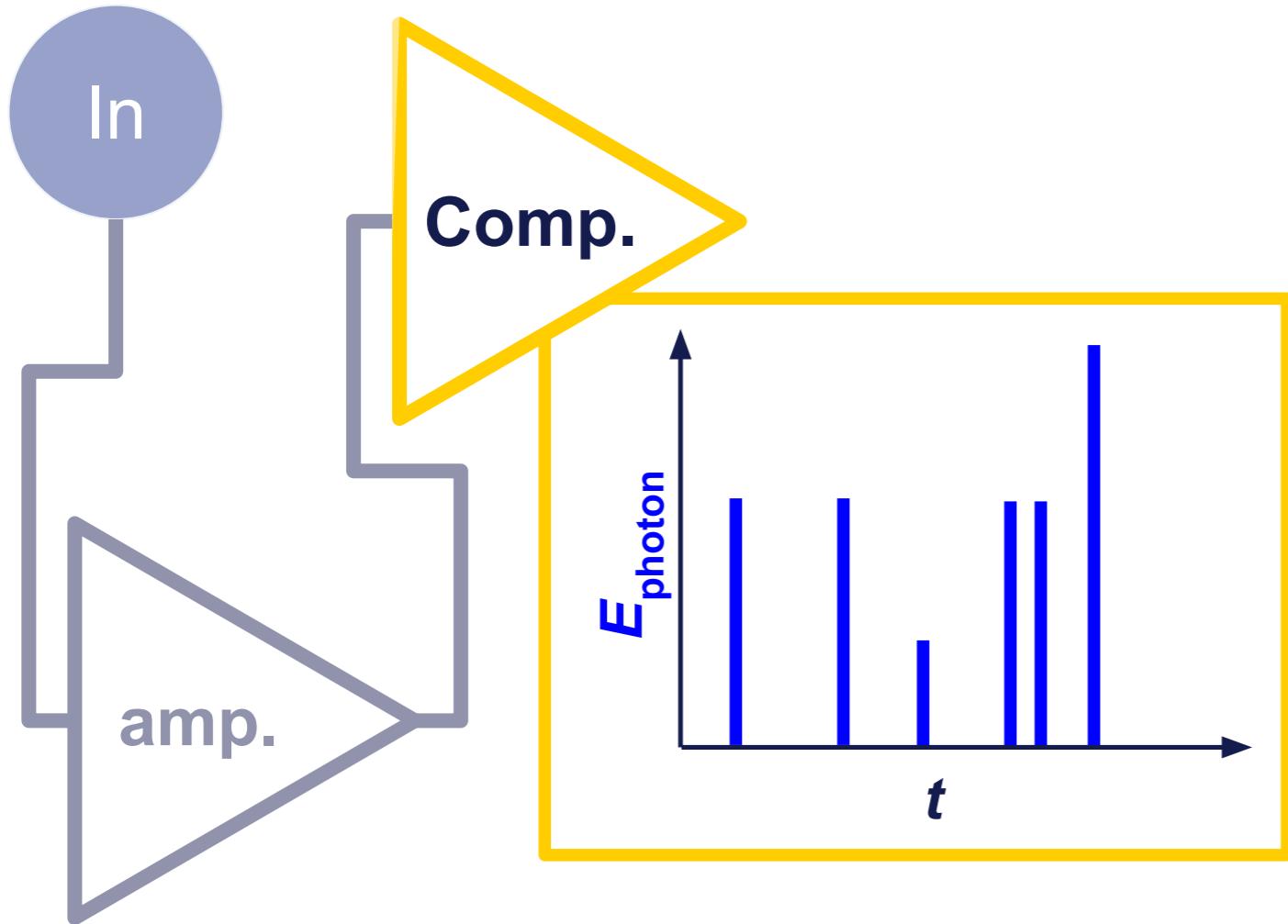
Hybrid Pixel Photon Counting X-ray Detectors



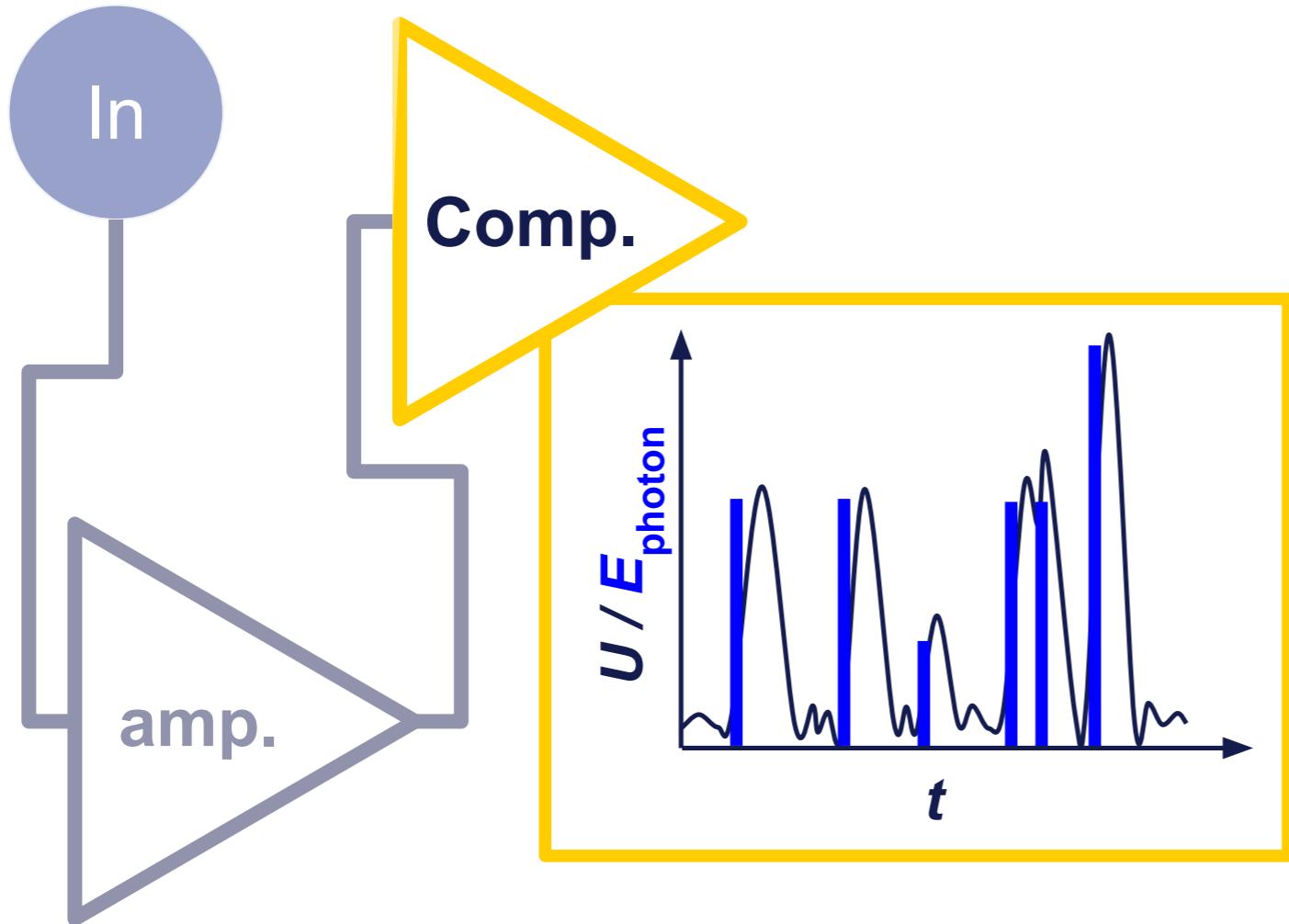
Hybrid Pixel Photon Counting X-ray Detectors



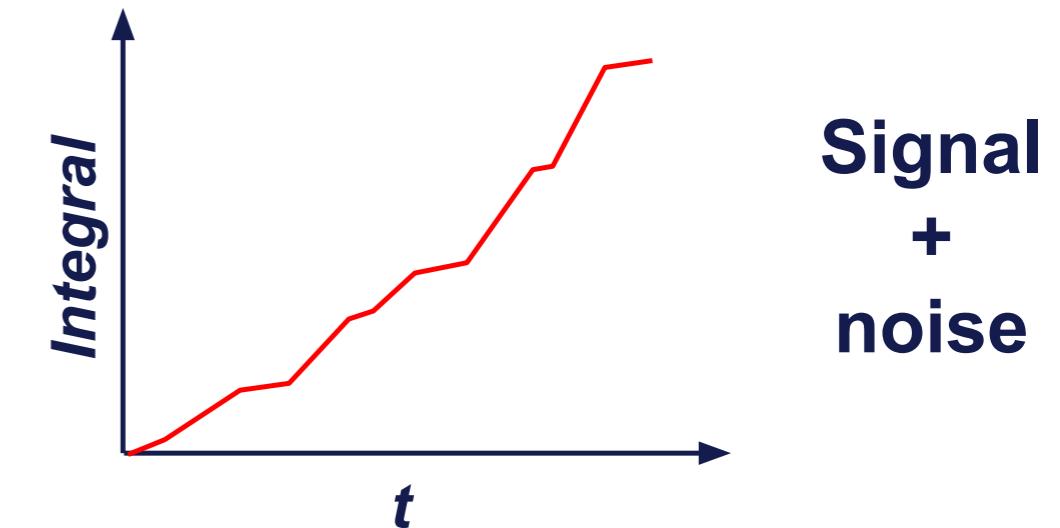
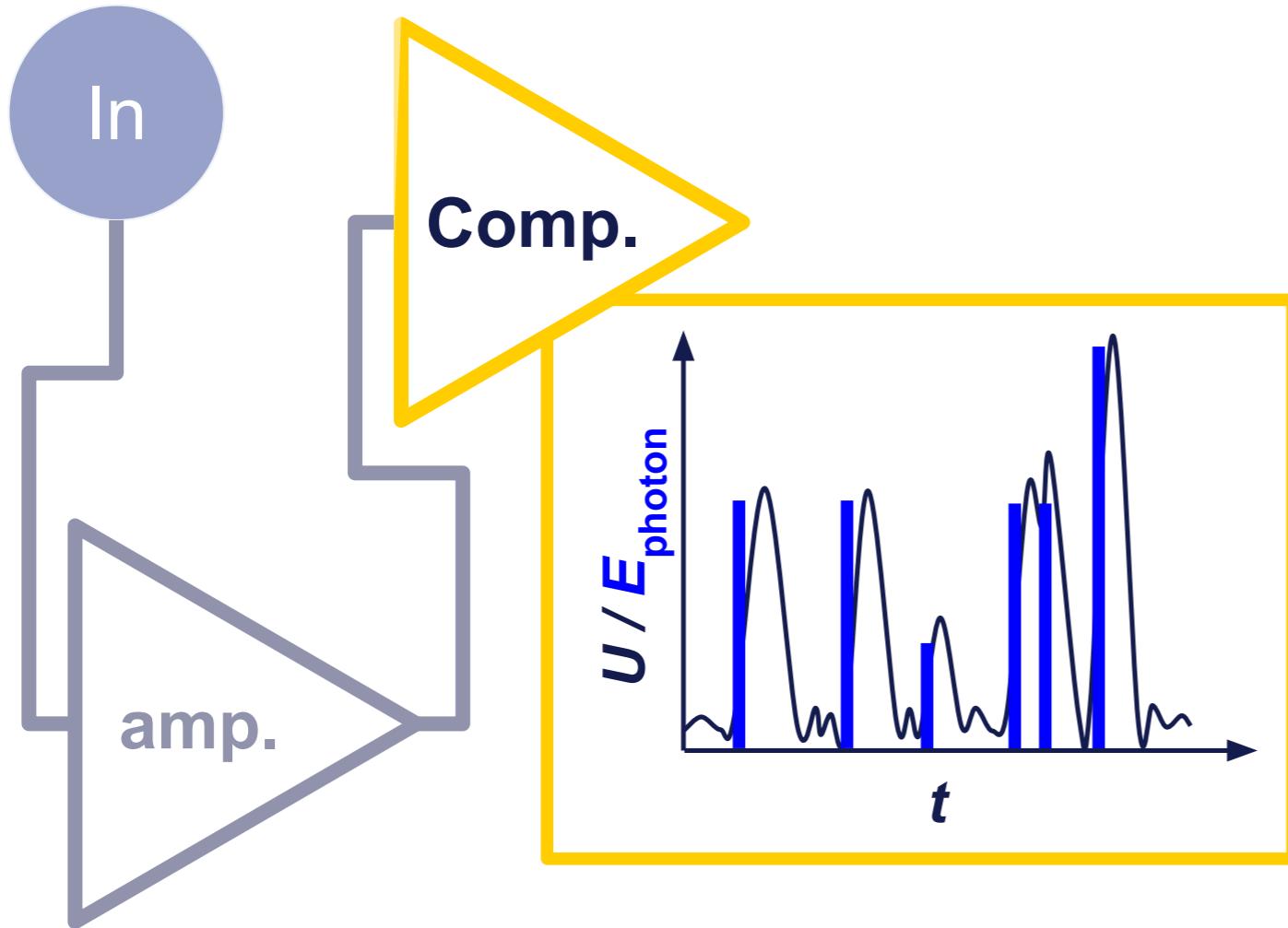
Hybrid Pixel Photon Counting X-ray Detectors



Hybrid Pixel Photon Counting X-ray Detectors

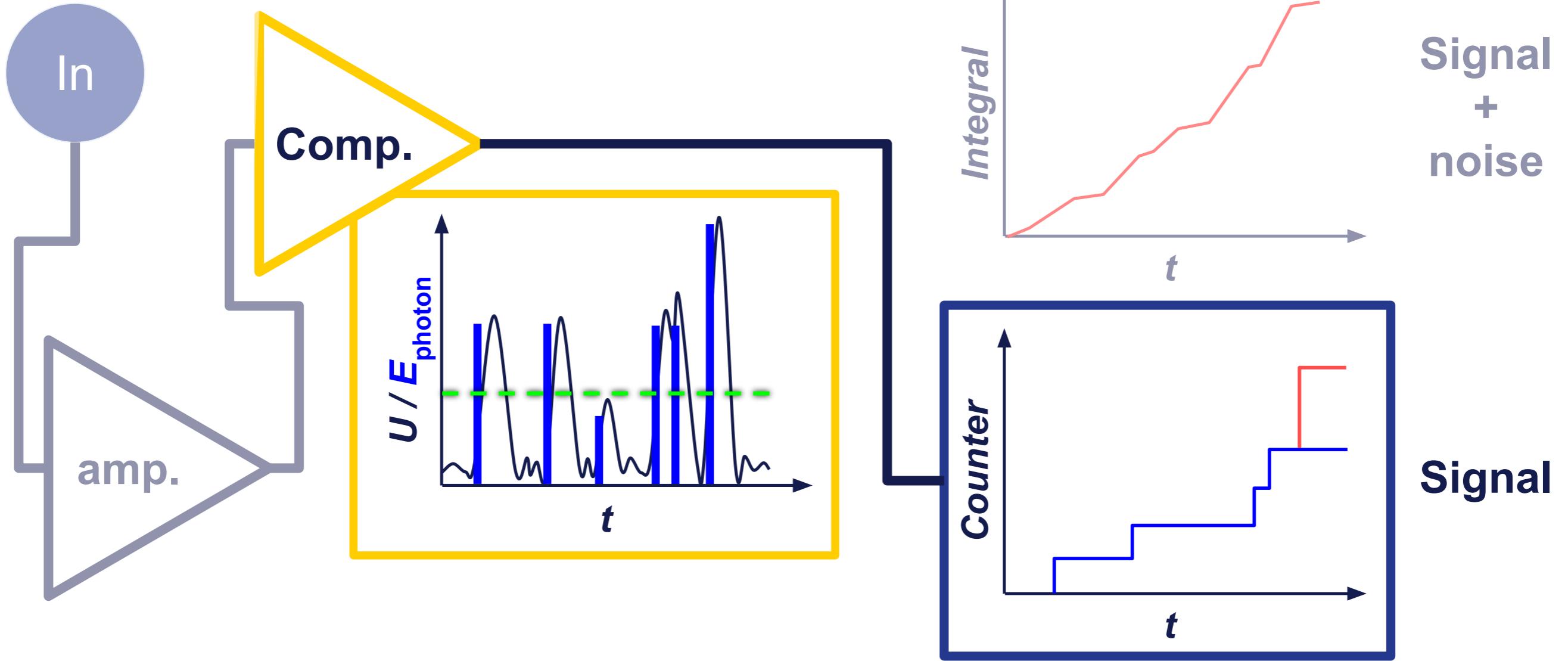


Hybrid Pixel Photon Counting X-ray Detectors

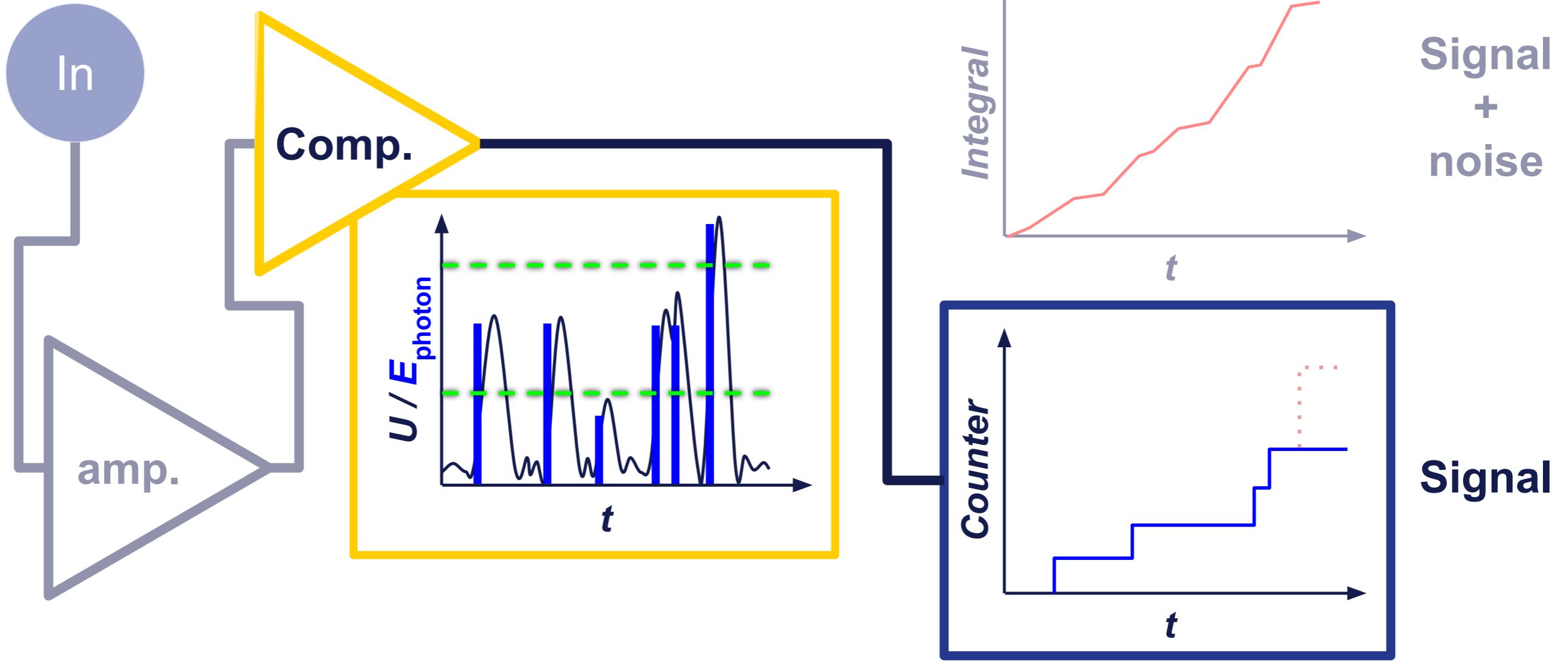


Signal
+
noise

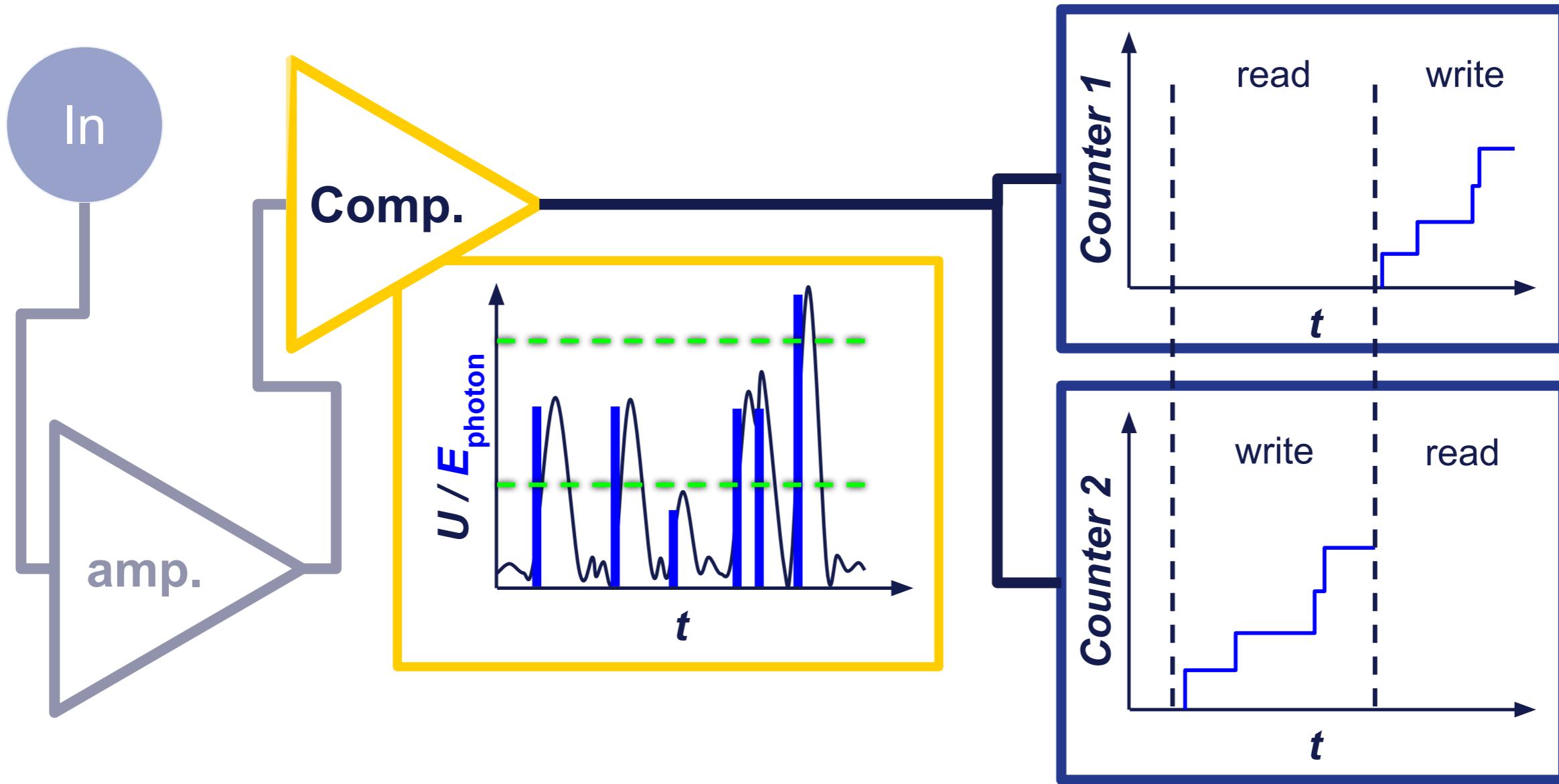
Hybrid Pixel Photon Counting X-ray Detectors



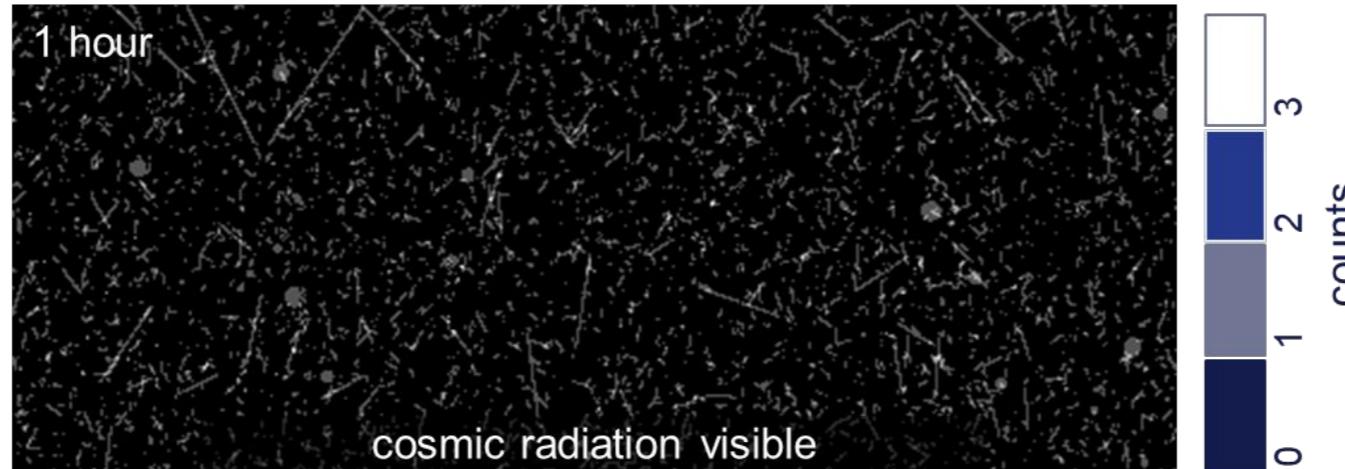
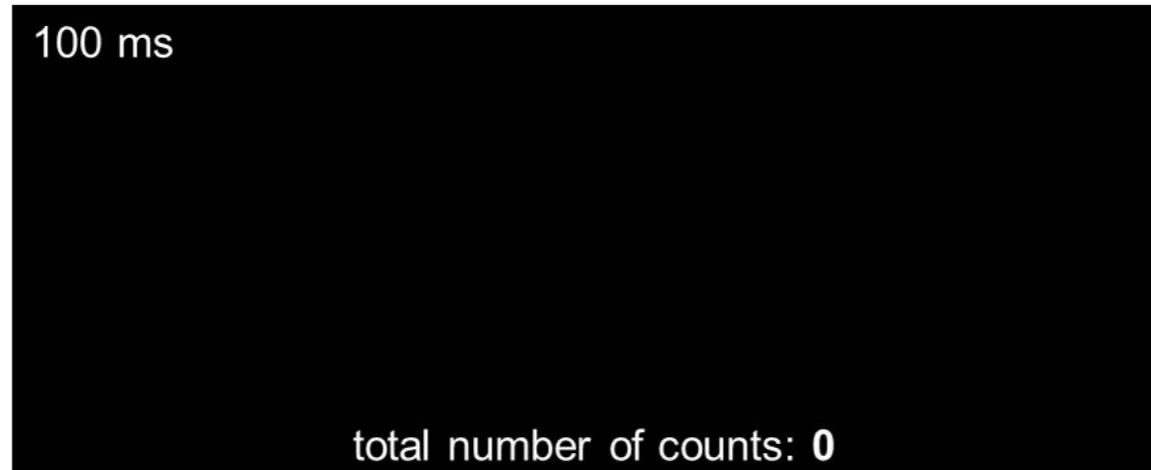
Hybrid Pixel Photon Counting X-ray Detectors



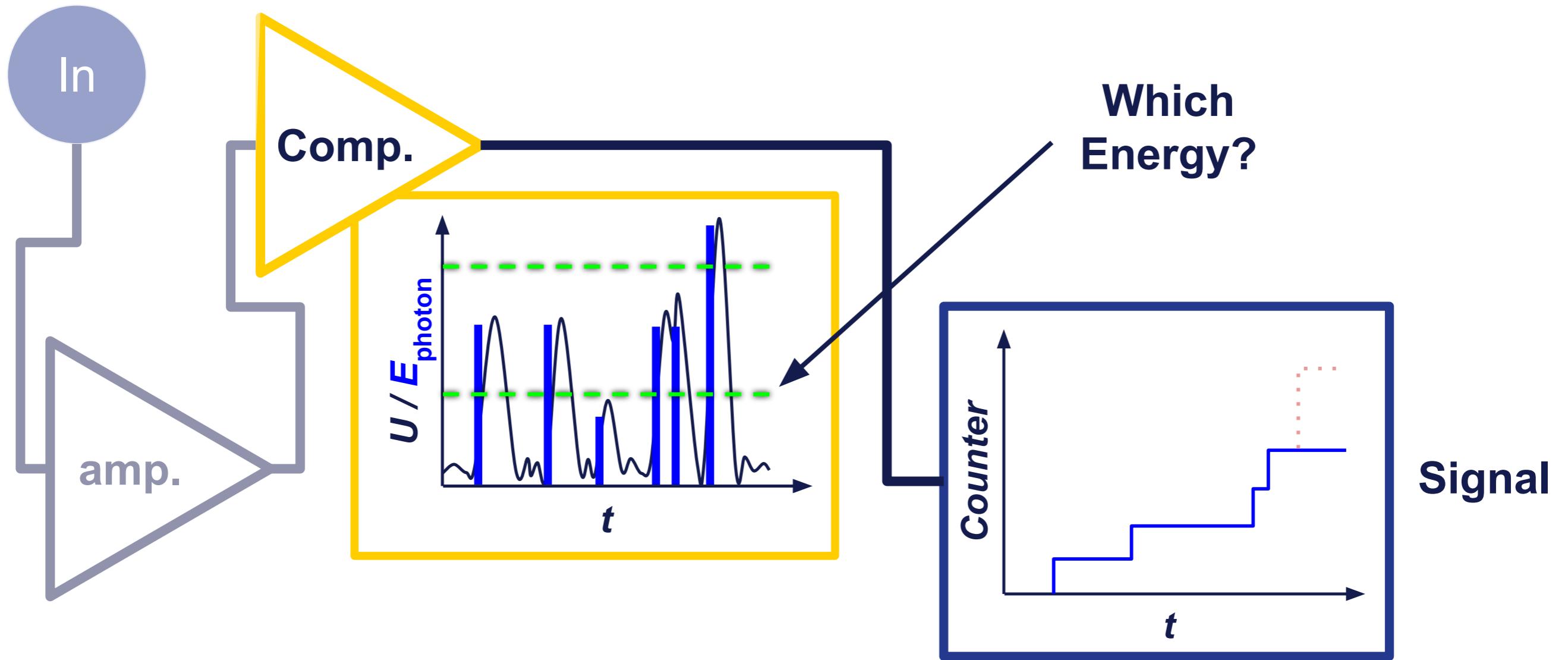
Hybrid Pixel Photon Counting X-ray Detectors



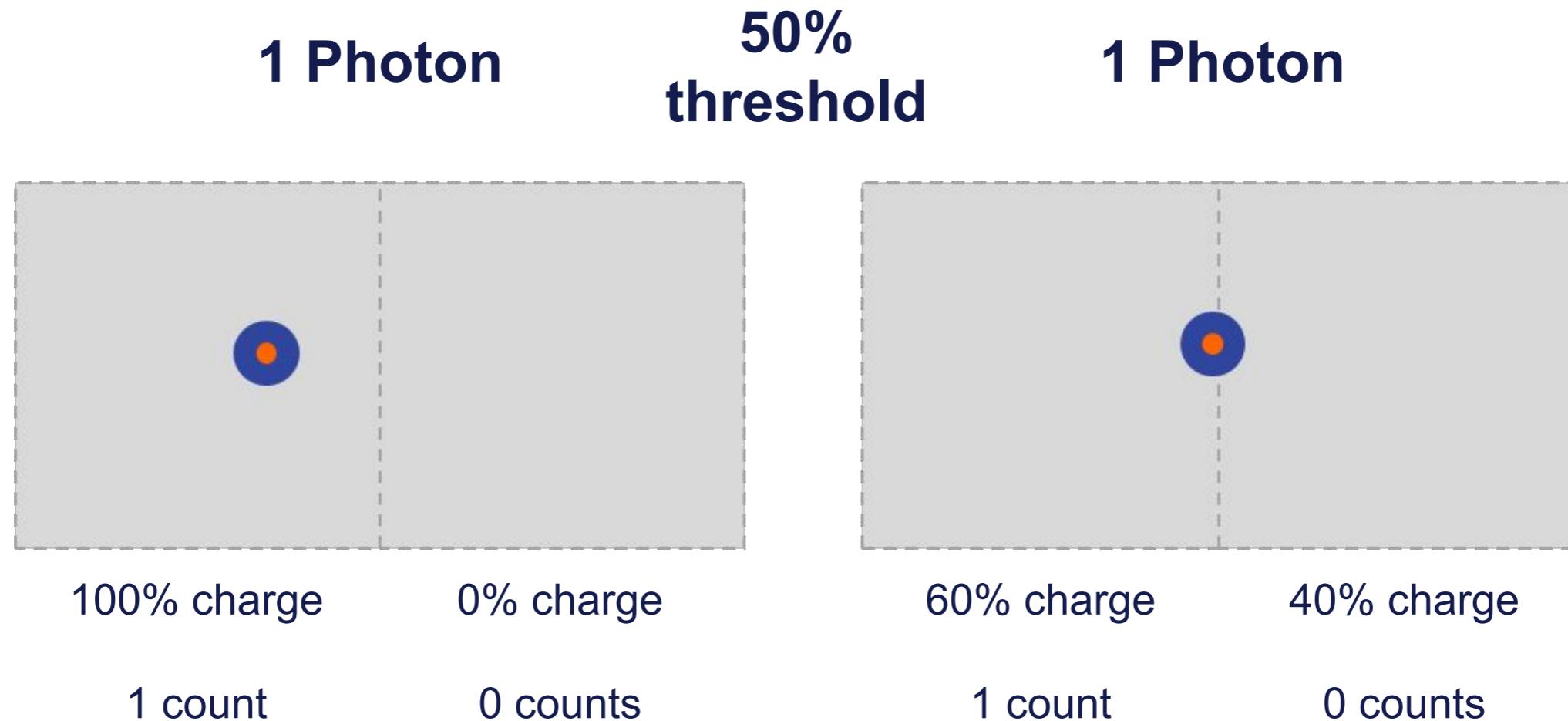
HPC Detectors - Zero Noise



Hybrid Pixel Photon Counting X-ray Detectors



Hybrid Pixel Photon Counting X-ray Detectors



EIGER2 & PILATUS4



Pixel ApparATUS (for the Swiss Light Source)



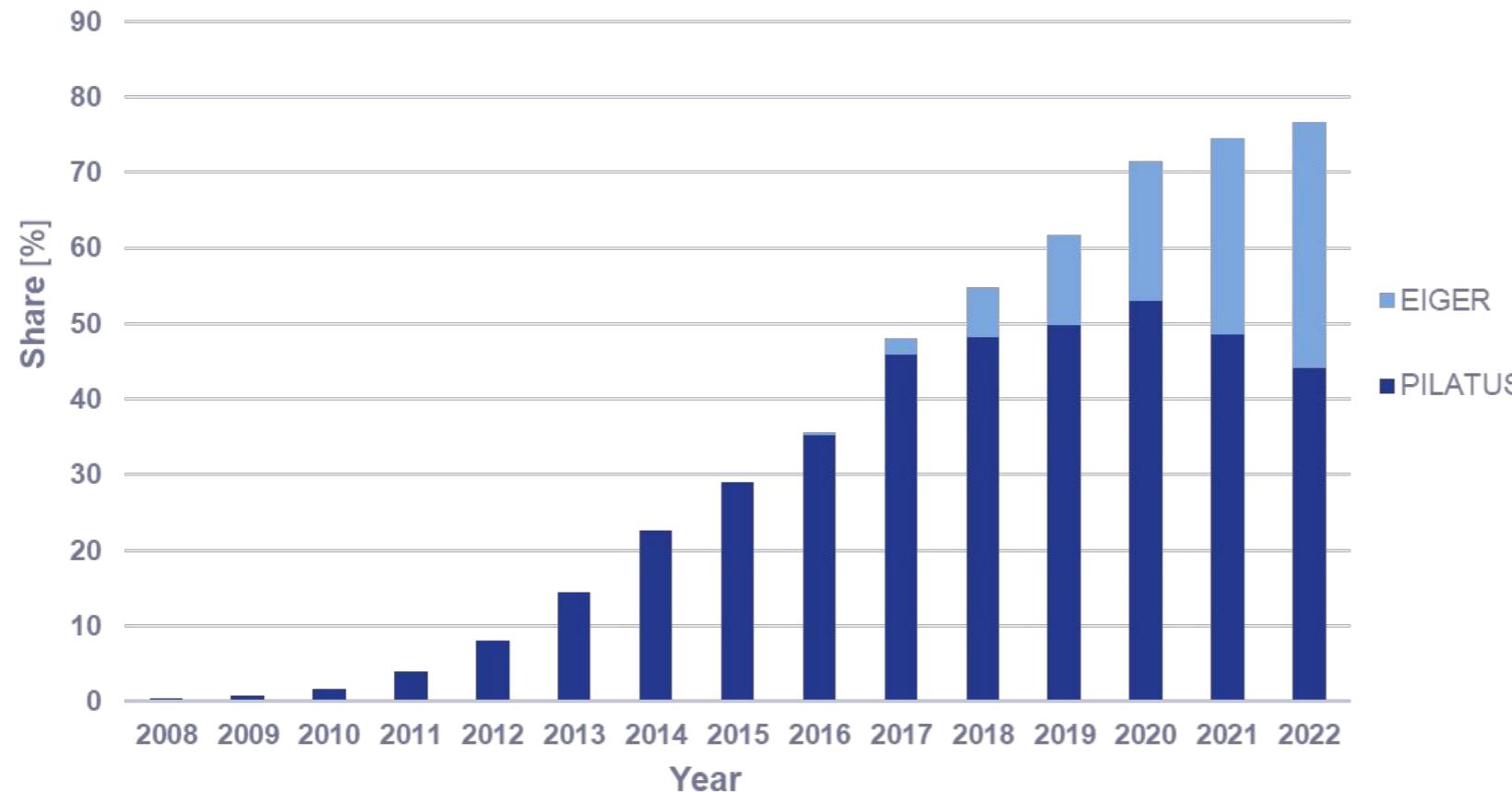
Extremely hIGh rate detEcToR

EIGER2 & PILATUS4

	EIGER 2	PILATUS4
Pixel size	75x75 μm	150x150 μm
Active Area		up to 31x32 cm
λ Range / \AA		2.0 - 0.3 (Si); 1.6 - 0.1 (CdTe)
Number of Energy Thresholds	2	4
max. framerate	1000 Hz	4000 Hz
Readout		continuous



HPC Detectors - Transforming Science

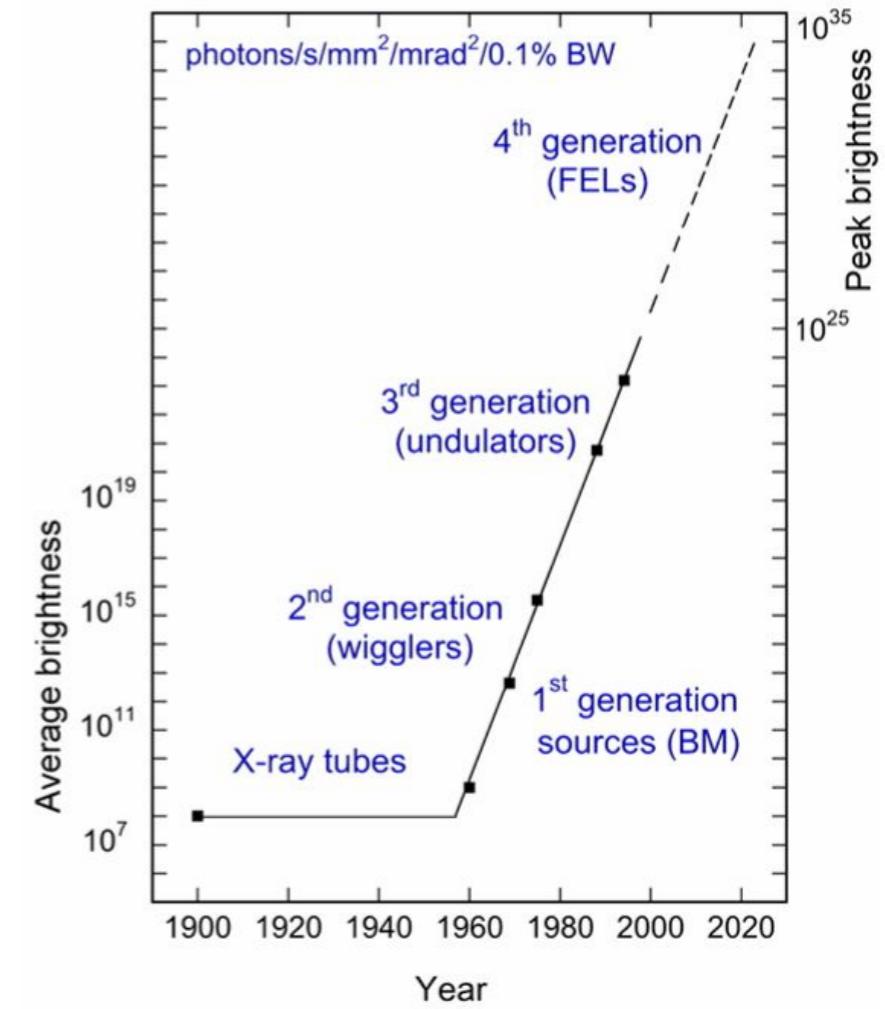
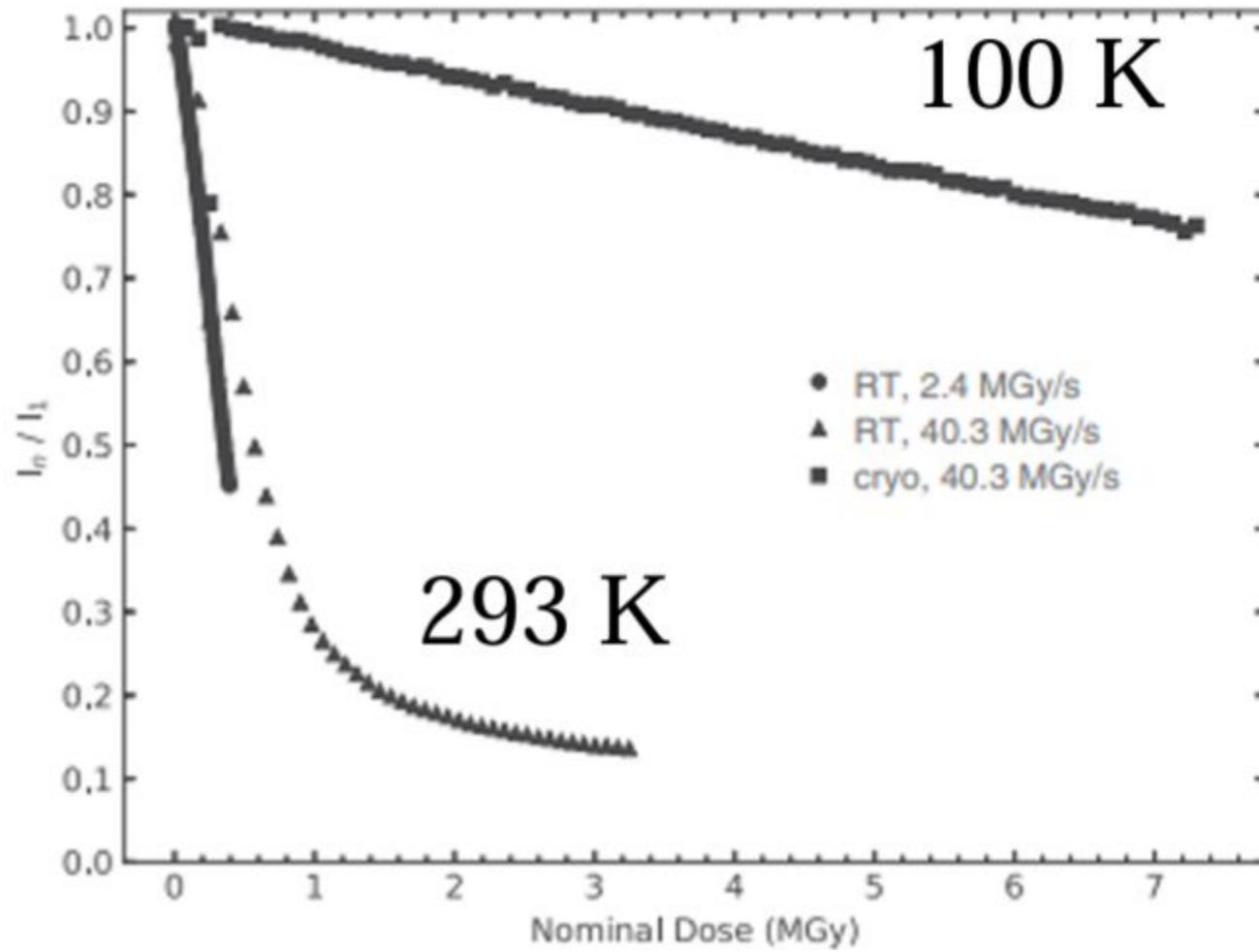


What does it take to get good MX data?

- low/no Radiation Damage
- Completeness
- Redundancy
- No Noise and Low Background
- Scattering
- An Excellent Detector 

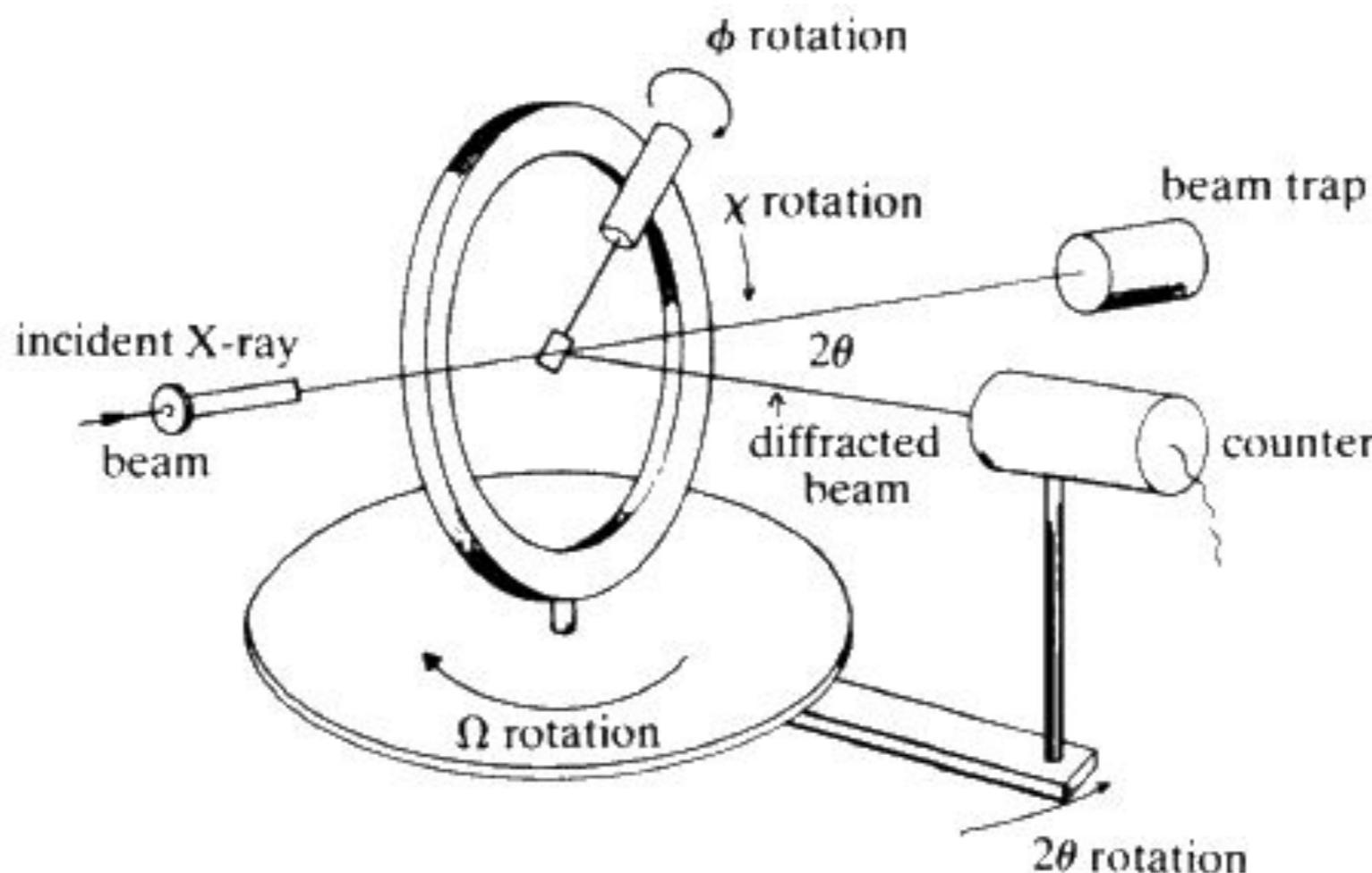


Radiation Damage Control



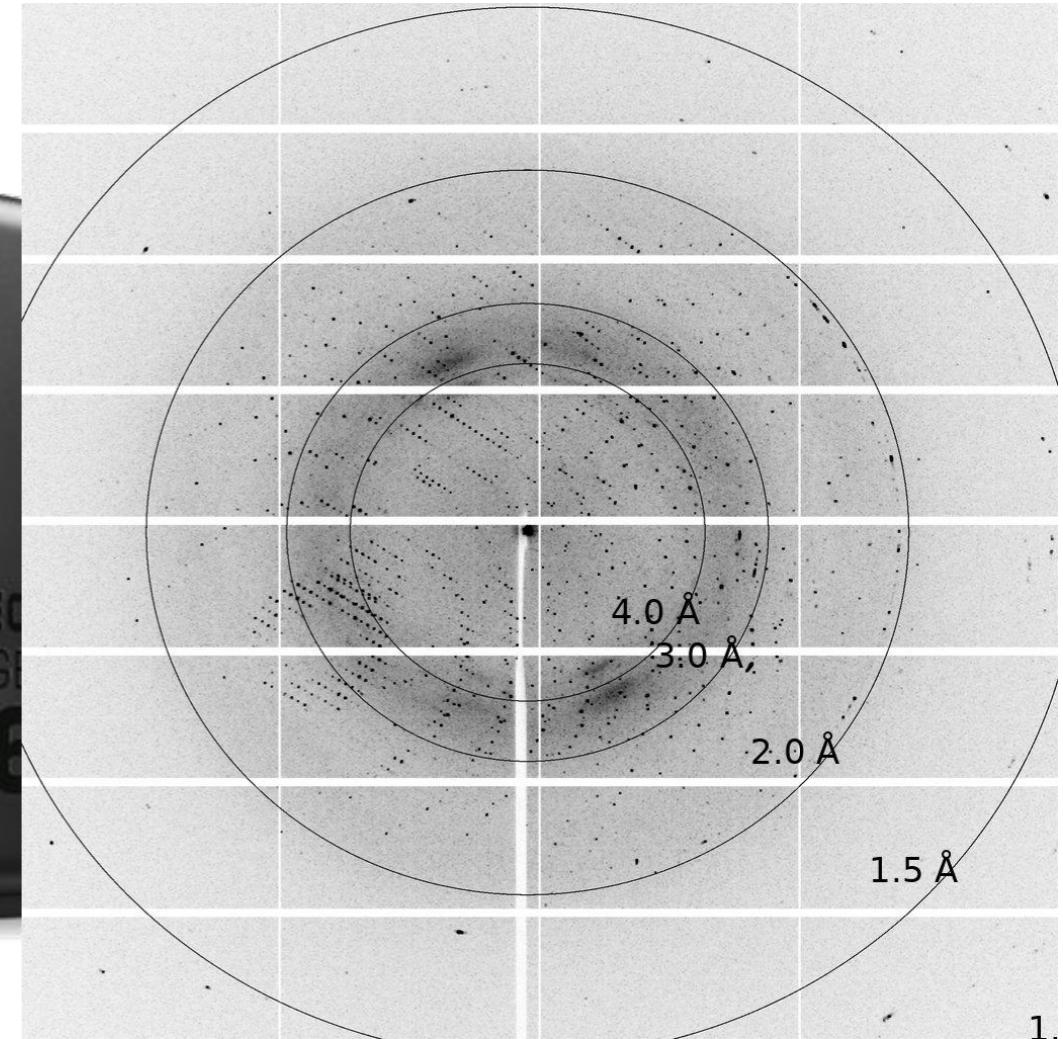
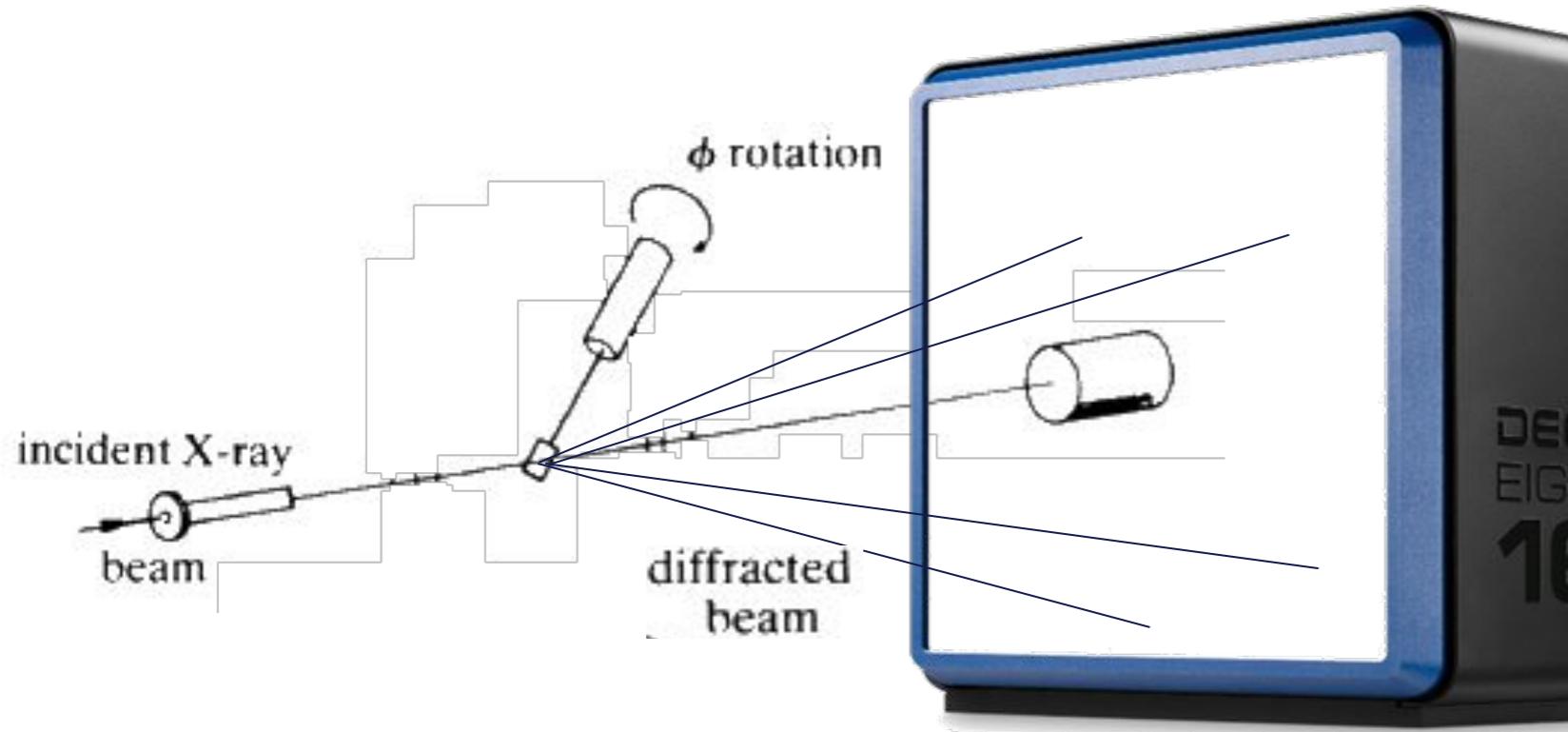
E. Gaman CCP4 school 2024.

Completeness



Z. Daughter, *ACTA Cryst D* 1999, 55, 1703.

Completeness



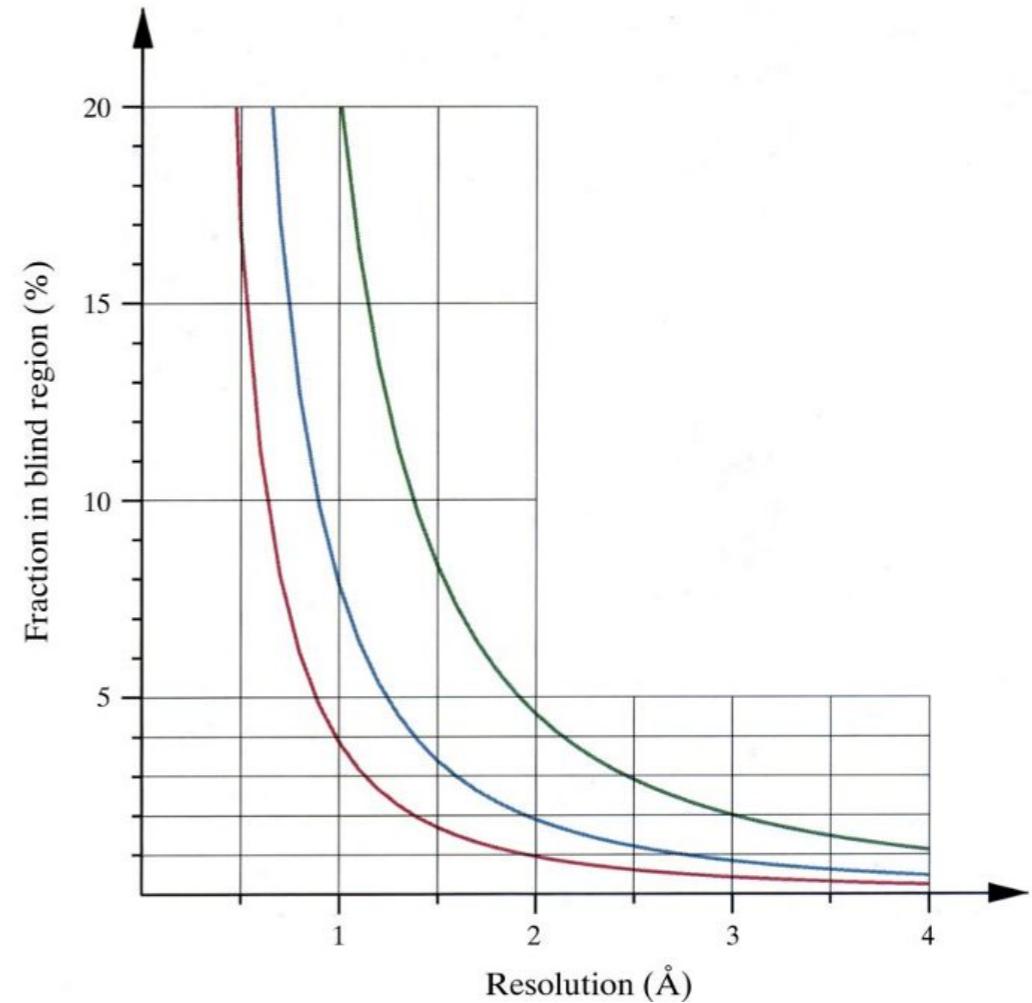
Completeness

Table 1

Rotation range ($^{\circ}$) required to collect a complete data set in different crystal classes.

The direction of the spindle axis is given in parentheses; *ac* means any vector in the *ac* plane.

Point group	Native data	Anomalous data
1	180 (any)	$180 + 2\theta_{\max}$ (any)
2	180 (<i>b</i>); 90 (<i>ac</i>)	180 (<i>b</i>); $180 + 2\theta_{\max}$ (<i>ac</i>)
222	90 (<i>ab</i> or <i>ac</i> or <i>bc</i>)	90 (<i>ab</i> or <i>ac</i> or <i>bc</i>)
4	90 (<i>c</i> or <i>ab</i>)	90 (<i>c</i>); $90 + \theta_{\max}$ (<i>ab</i>)
422	45 (<i>c</i>); 90 (<i>ab</i>)	45 (<i>c</i>); 90 (<i>ab</i>)
3	60 (<i>c</i>); 90 (<i>ab</i>)	$60 + 2\theta_{\max}$ (<i>c</i>); $90 + \theta_{\max}$ (<i>ab</i>)
32	30 (<i>c</i>); 90 (<i>ab</i>)	$30 + \theta_{\max}$ (<i>c</i>); 90 (<i>ab</i>)
6	60 (<i>c</i>); 90 (<i>ab</i>)	$60 + \theta_{\max}$ (<i>c</i>); $90 + \theta_{\max}$ (<i>ab</i>)
622	30 (<i>c</i>); 90 (<i>ab</i>)	30 (<i>c</i>); 90 (<i>ab</i>)
23	~ 60	~ 70
432	~ 35	~ 45



Z. Daughter, *ACTA Cryst D* 1999, 55, 1703.

Redundancy

symmetry equivalent reflections in **P2₁**,

$h \ k \ l$

$h -k \ l$

$-h \ k -l$

$-h -k -l$

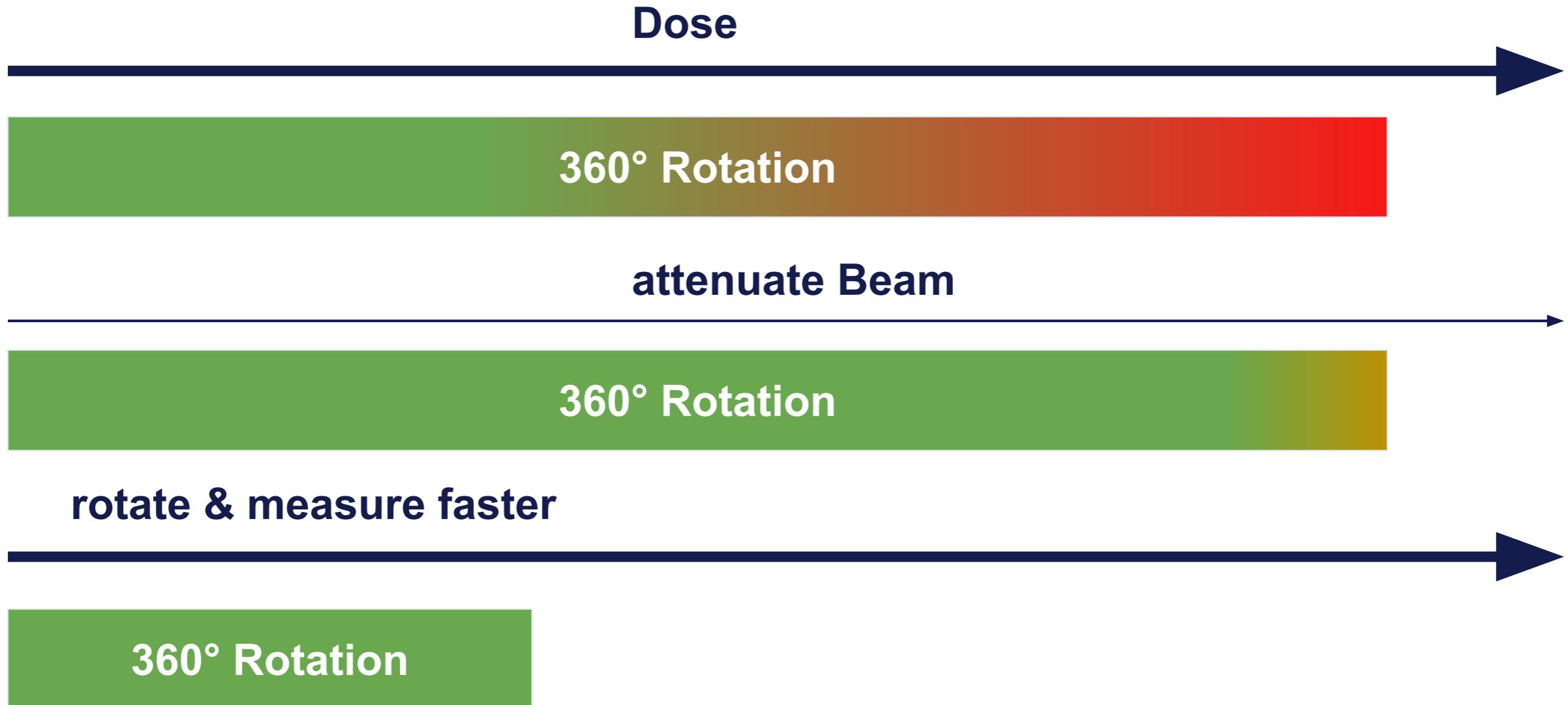
symmetry equivalent reflections in **P1**

$h \ k \ l$

$-h -k -l$

→ always get at least one full 360° rotation

Spread your Photons

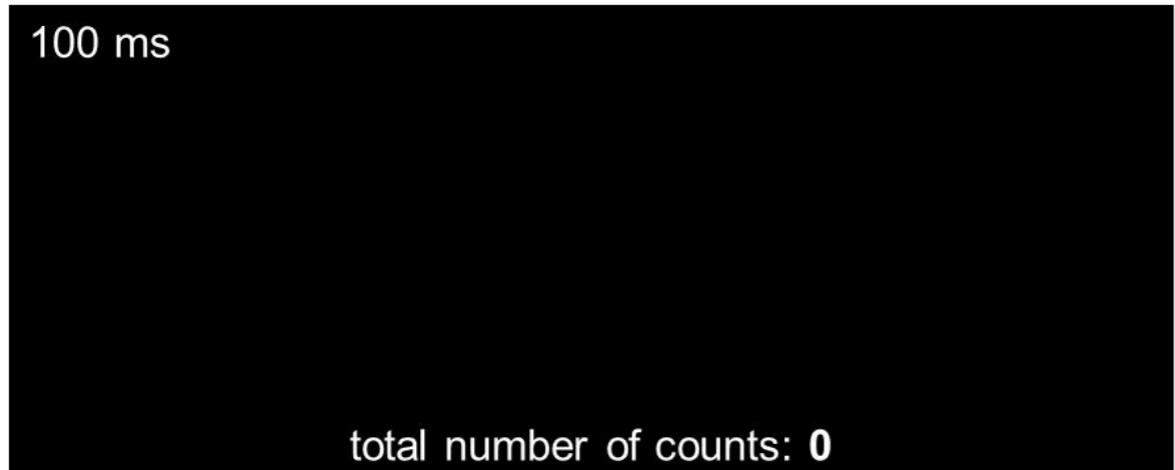


What does it take to get good MX data?

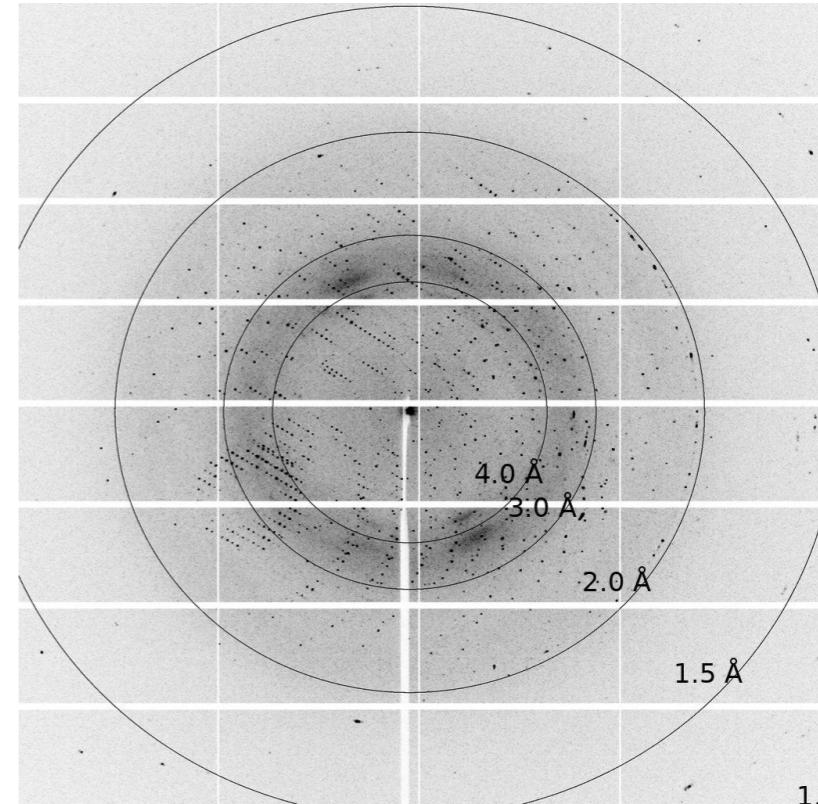
- low/no Radiation Damage ✓
- Completeness ✓
- Redundancy ✓
- No Noise and Low Background
- Scattering
- An Excellent Detector ✓



Background Reduction



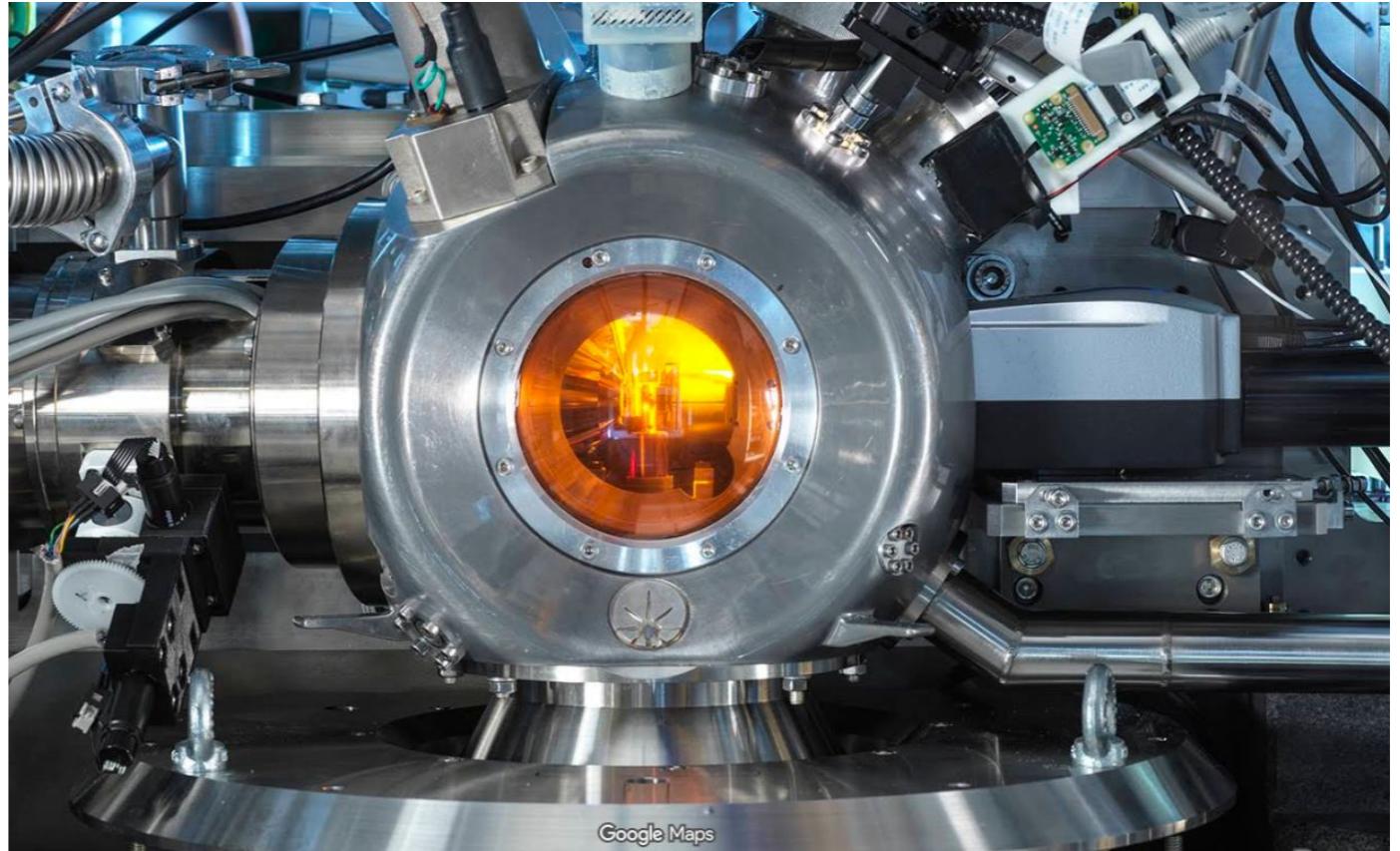
no detector background



but ALL matter scatters
loop, air, beamstop, crystal

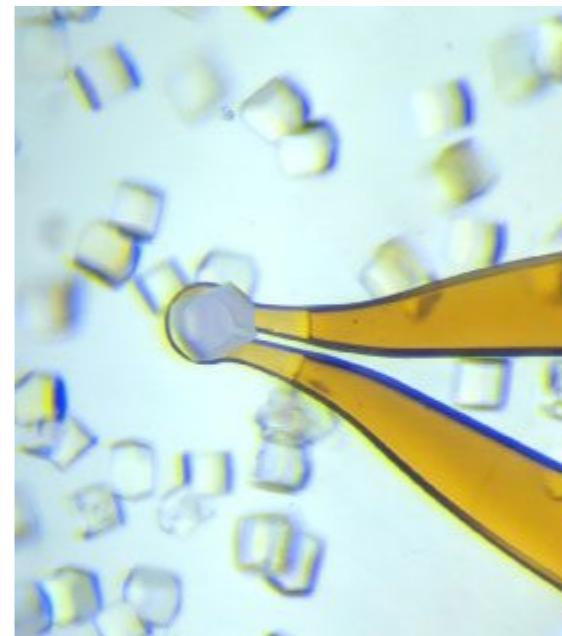
Background Reduction

measure in vacuum
at DLS :)

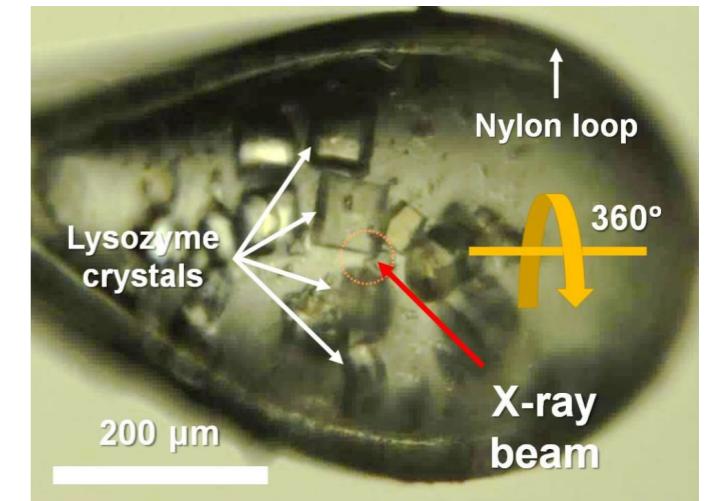


Background Reduction

mount samples carefully



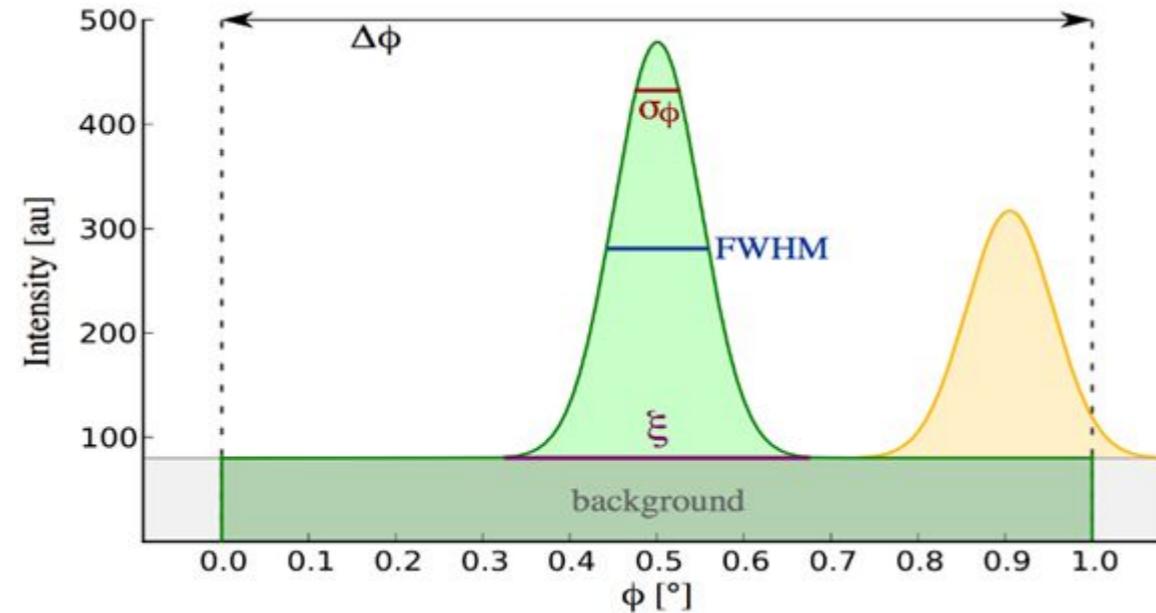
do :)



don't :(

K. H. Nam, *Crystals* 2022, 12, 103.

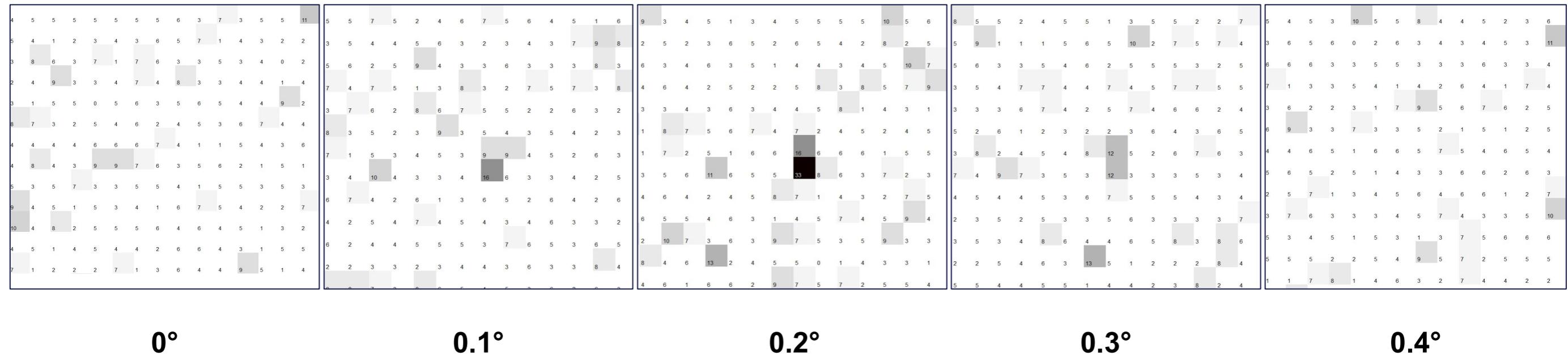
Background Reduction - fine slicing



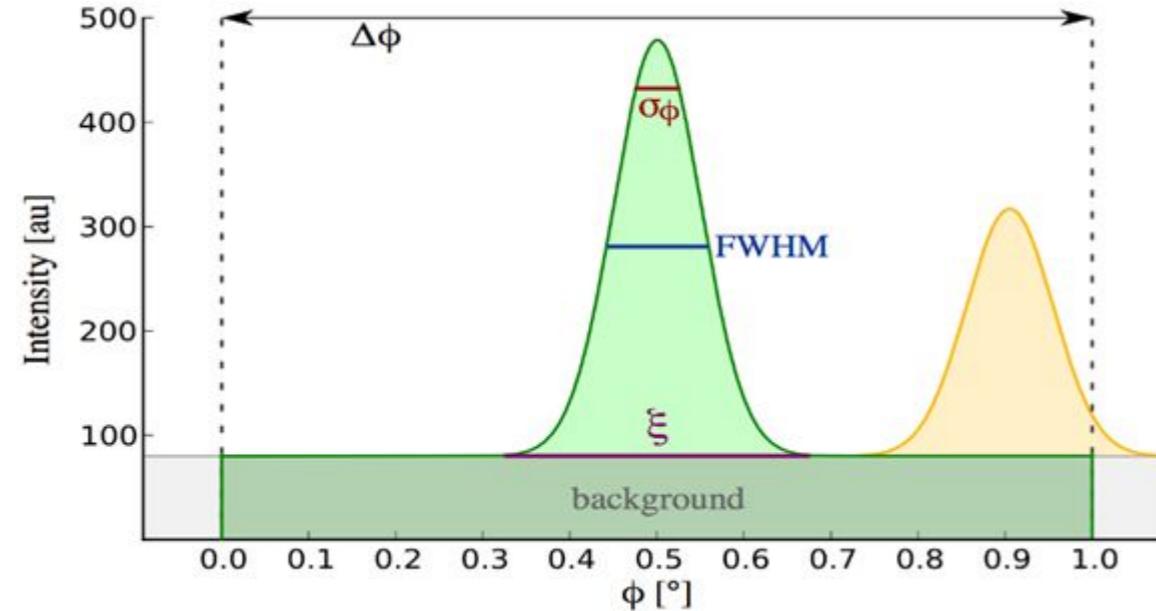
Wide ϕ -slicing

- $\Delta\phi > \xi$
- Lots of background
- Few images

Background Reduction - fine slicing

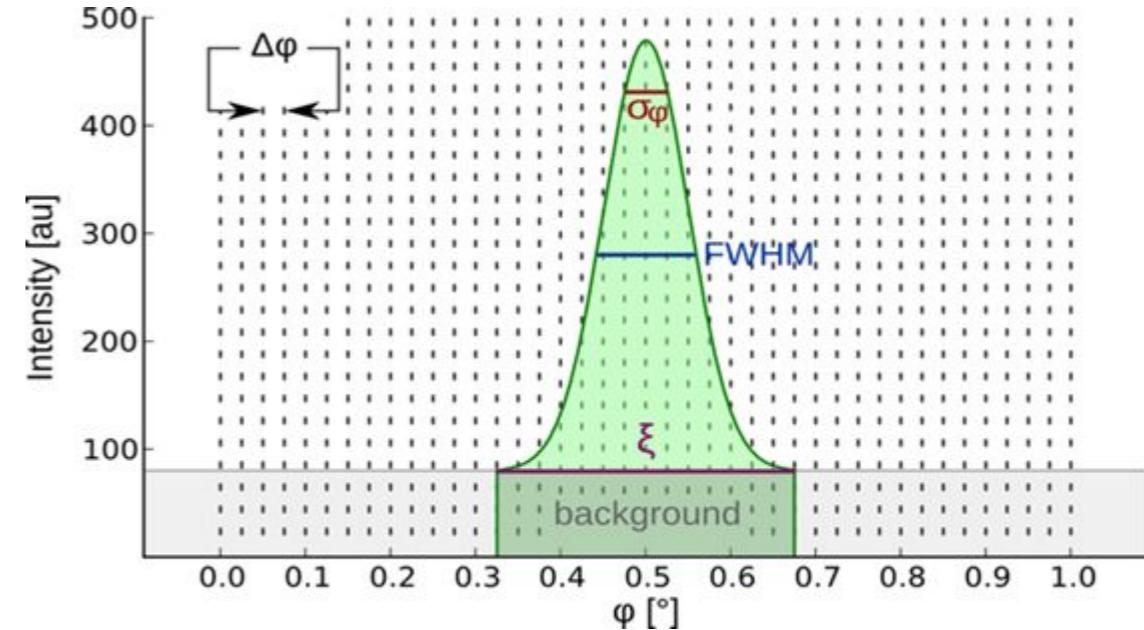


Background Reduction - fine slicing



Wide ϕ -slicing

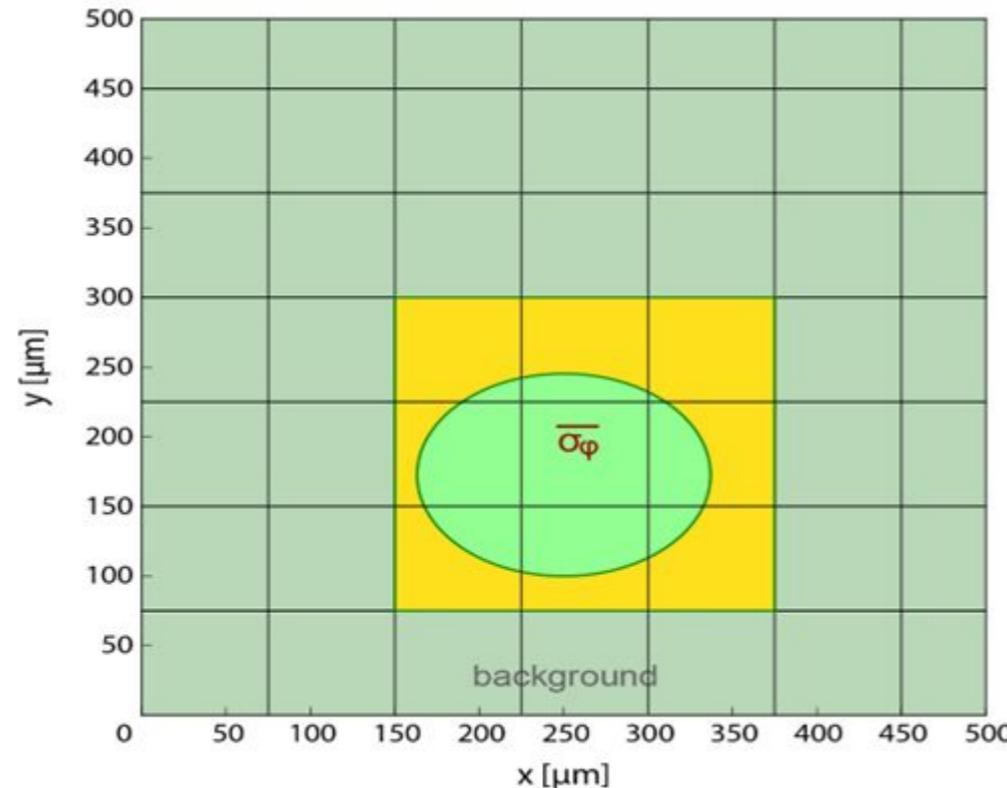
- $\Delta\phi > \xi$
- Lots of background
- Few images



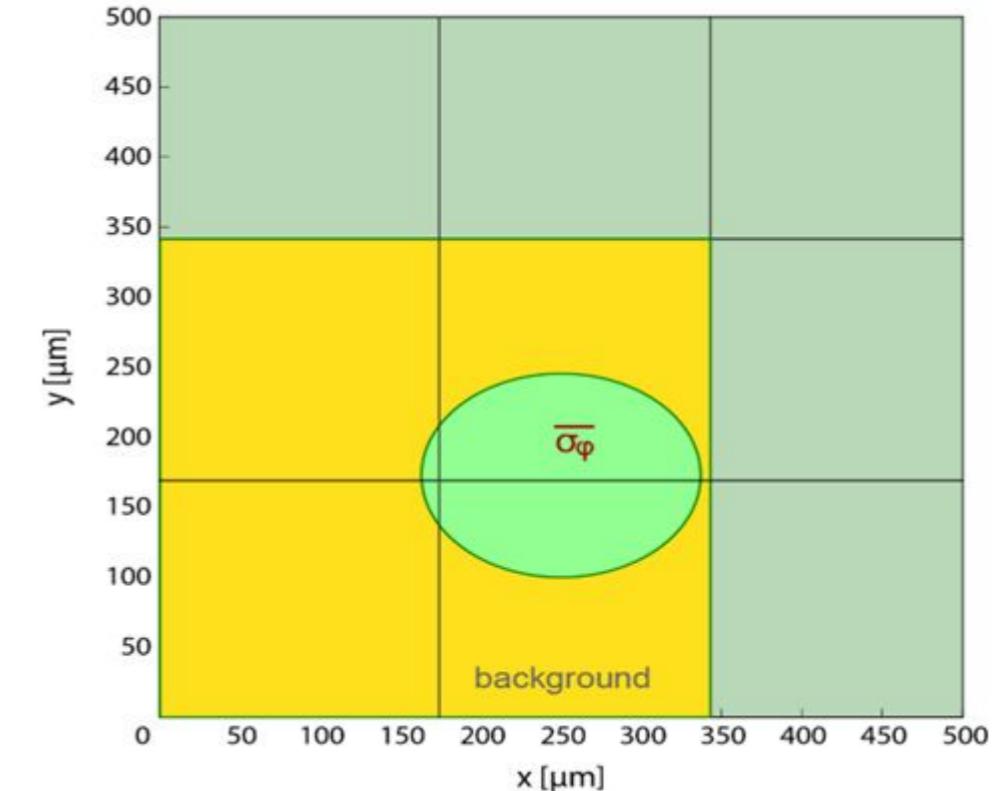
Fine ϕ -slicing

- $\Delta\phi \ll \xi$
- Minimal background
- Many images

Background Reduction - smaller pixels



EIGER



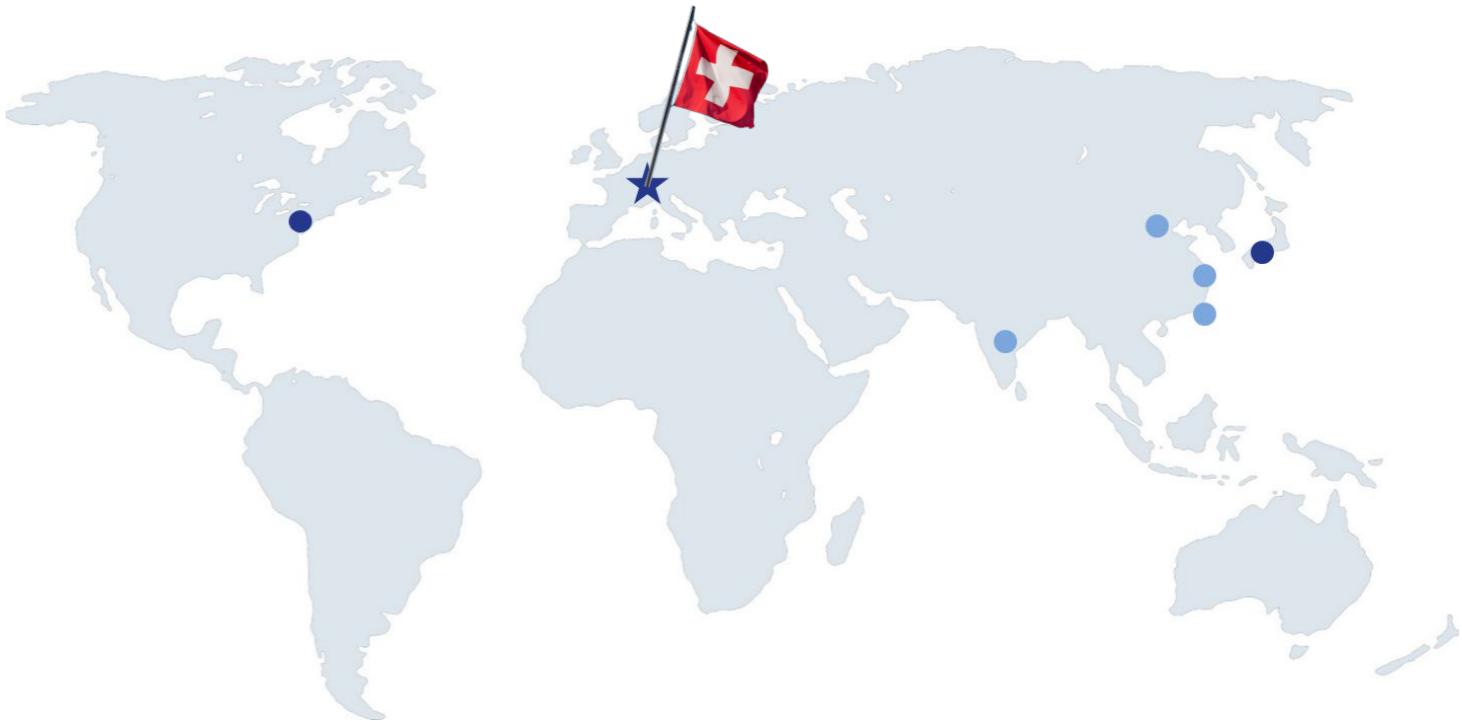
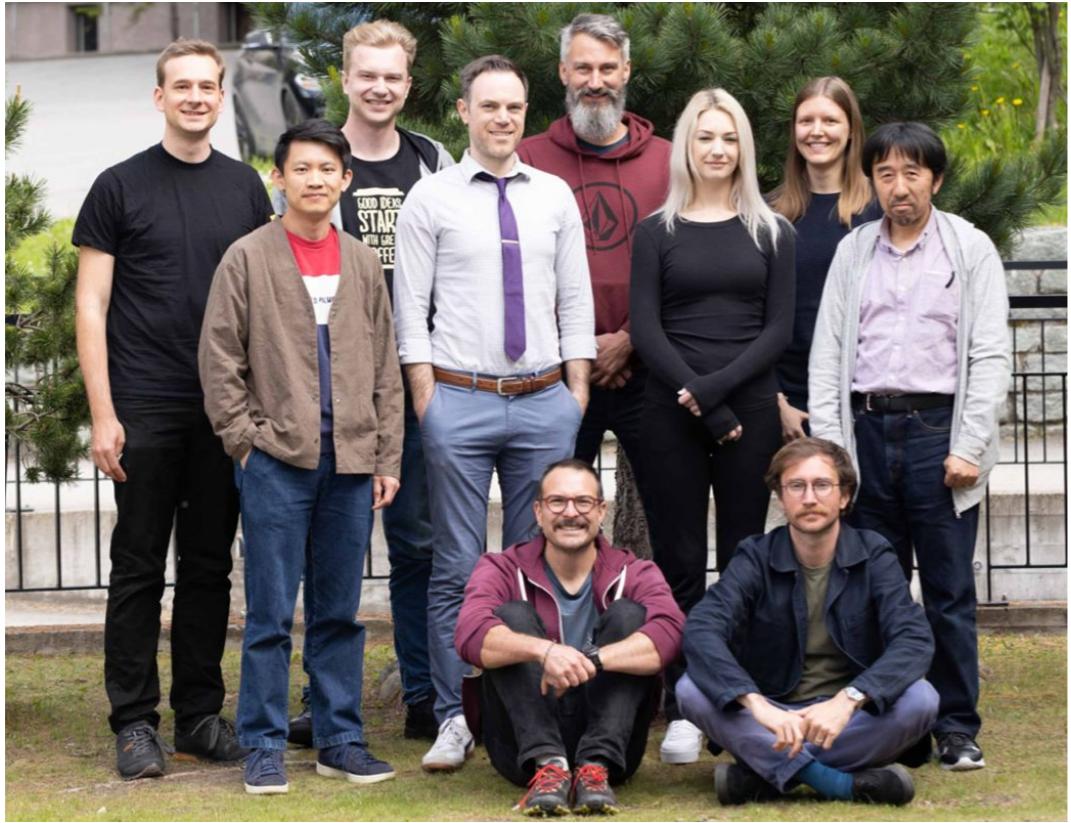
PILATUS

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- Redundancy ✓
- No Noise and Low Background
Scattering ✓
- An Excellent Detector ✓



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