Pixel Array Detectors: Counting and Integrating

Roger Durst, Bruker AXS

October 13, 2016

The quest for a *perfect detector*

- There is, of course, no 'perfect' detector
  - *All available detector technologies have limitations*
  - ***The real question thus becomes which detector technology approaches an ideal detector most closely for a given experiment***
- For many applications, pixel array detectors currently come closer to ideal performance than any other available technology
- There are now two types of pixel array detectors:
  - Counting pixel array detectors
  - More recently, integrating pixel array detectors have been introduced
- ***What are the relative benefits and limitations?***

Advantages of photon-counting pixel array detectors

- High speed
  - Each pixel is essentially an independent detector
- High sensitivity
  - Single photon detection possible
- Very low dark current
  - Only limited by cosmic rays/scattered X-ray background
- Energy resolution

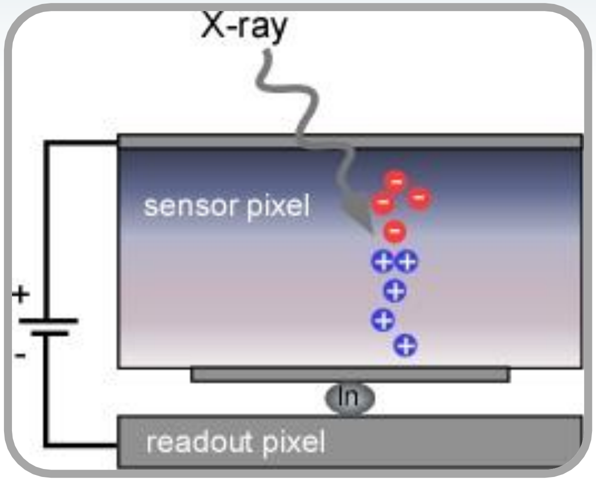
Limitations of photon-counting pixel detectors

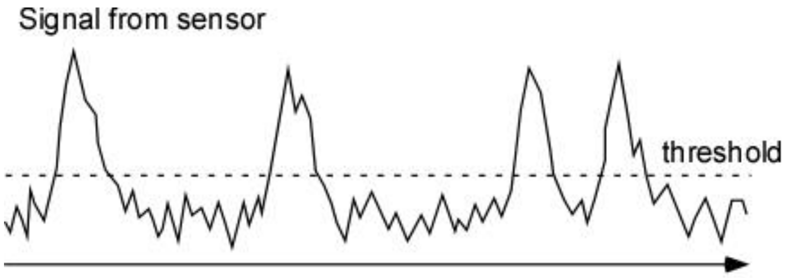
- Count rate saturation
  - Loss of counts at high count rates
- Charge sharing losses
  - Loss of counts at pixel boundaries

Photon-counting pixel array detector

How to make a “noise-free” detector

- An X-ray absorbed in the sensor produces a pulse of charge
- The height of this pulse is then compared to a threshold
- As long as the electronic noise is small compared to the threshold then the detection becomes effectively noise-free
    - No dark current, can integrate long exposures without loss of data quality
    - No read noise, better signal-to-noise for very weak reflections





The benefits and limitations of counting

- How many jelly beans are in this picture?
  - Please try to count them within 10 seconds

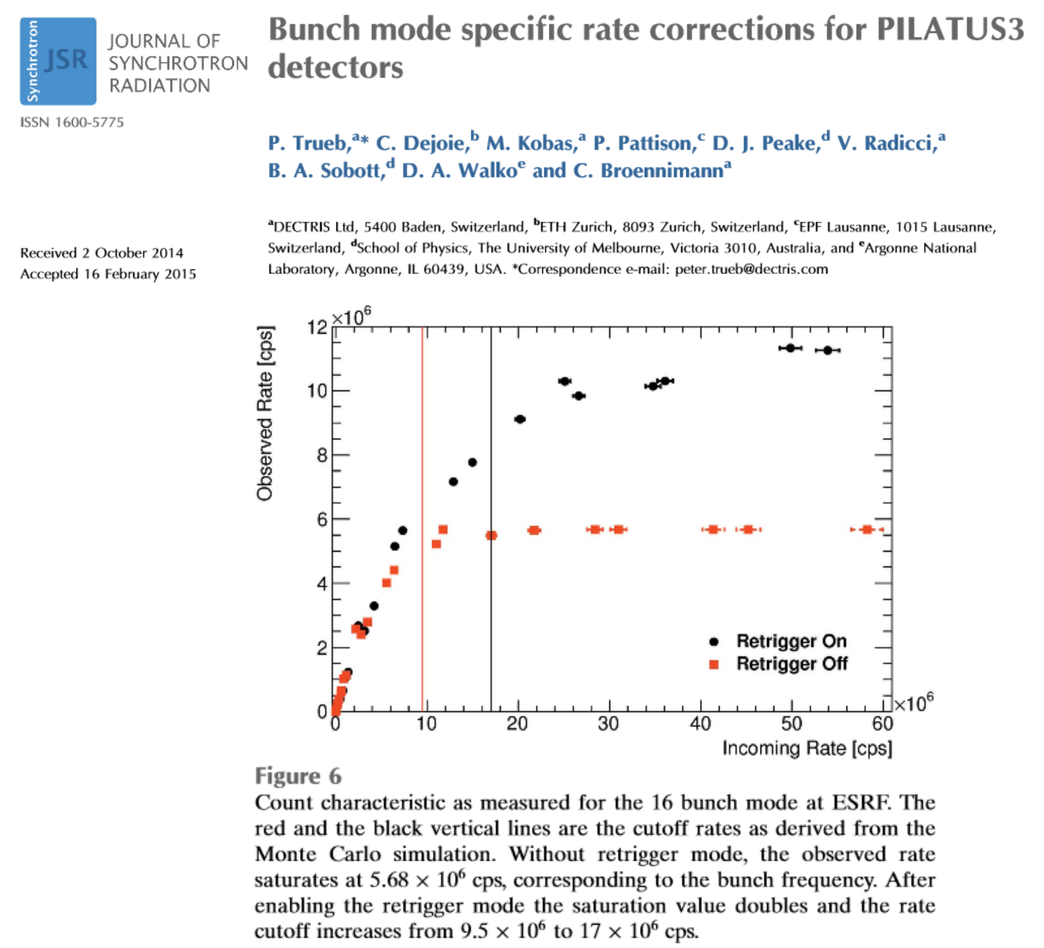
Count rate limit

- Now try to count these in 10 sec…
- This harder. *This is beyond the count rate limit of most humans*
- *Similarly, counting X-rays detectors also have count rate limits*
    - *At high count rates counts are lost*

Richard Souvign © 2011

Photon-counting PAD count rate limitations

- At high count rates counting photon-counting PADs saturate due to pulse pile up
  - Detector becomes increasingly non-linear
  - Typically limits operation to <1x10⁷ counts/sec-pixel
- Count rate saturation can be calibrated and corrected in software, but only approximately
- This limitation becomes more significant as source intensity increases



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Bunch mode specific rate corrections for PILATUS3 detectors

P. Trueb,[a]* C. Dejoie,[b] M. Kobas,[a] P. Pattison,[c] D. J. Peake,[d] V. Radicci,[a] B. A. Sobott,[d] D. A. Walko[e] and C. Broennimann[a]

[a]DECTRIS Ltd, 5400 Baden, Switzerland, [b]ETH Zurich, 8093 Zurich, Switzerland, [c]EPF Lausanne, 1015 Lausanne, Switzerland, [d]School of Physics, The University of Melbourne, Victoria 3010, Australia, and [e]Argonne National Laboratory, Argonne, IL 60439, USA. *Correspondence e-mail: peter.trueb@dectris.com

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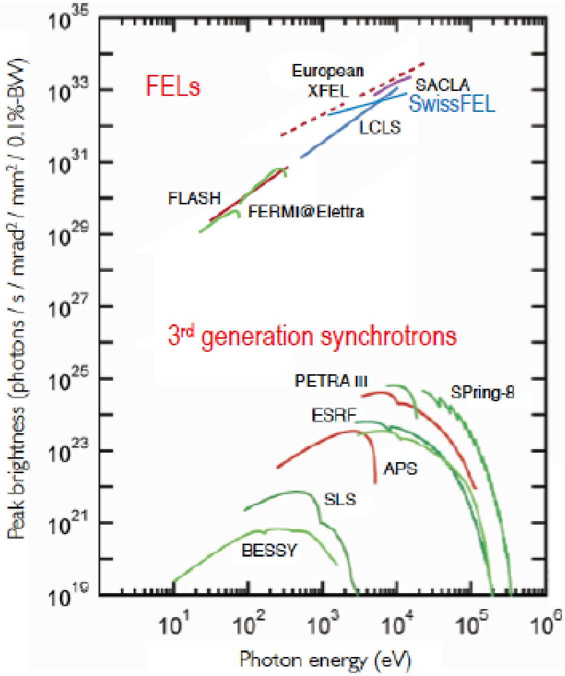
Figure 6

Count characteristic as measured for the 16 bunch mode at ESRF. The red and the black vertical lines are the cutoff rates as derived from the Monte Carlo simulation. Without retrigger mode, the observed rate saturates at 5.68×10^6 cps, corresponding to the bunch frequency. After enabling the retrigger mode the saturation value doubles and the rate cutoff increases from 9.5×10^6 to 17×10^6 cps.

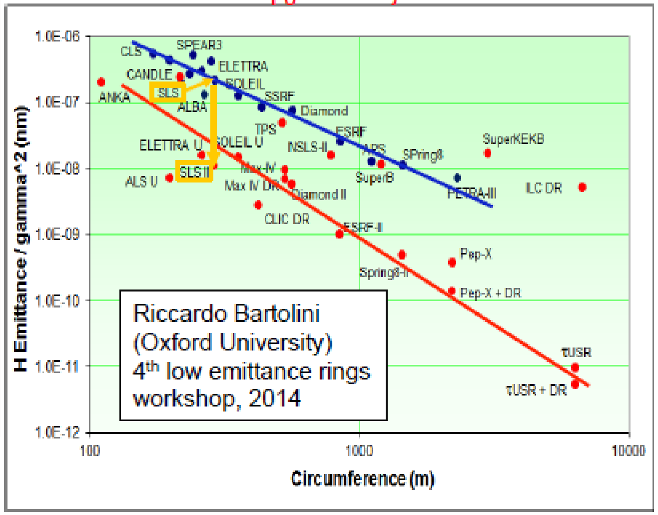
New sources:

Driving higher counting rates

- Count rate limitations become more significant for next-gen sources
  - It is unlikely that photon-counting detectors will be used for diffraction at next-gen, diffraction-limited synchrotrons (>100x brighter)
  - ***It is absolutely impossible to employ photon counting detectors at XFELs*** (>1,000,000x brighter)



Upgrade at synchrotrons:



Riccardo Bartolini
(Oxford University)
4th low emittance rings workshop, 2014

- A factor 10-100 lower horizontal emittance
- MAX IV (2015), SIRIUS (2016), ESRF-2 (2019), SLSII (>2021?) etc...

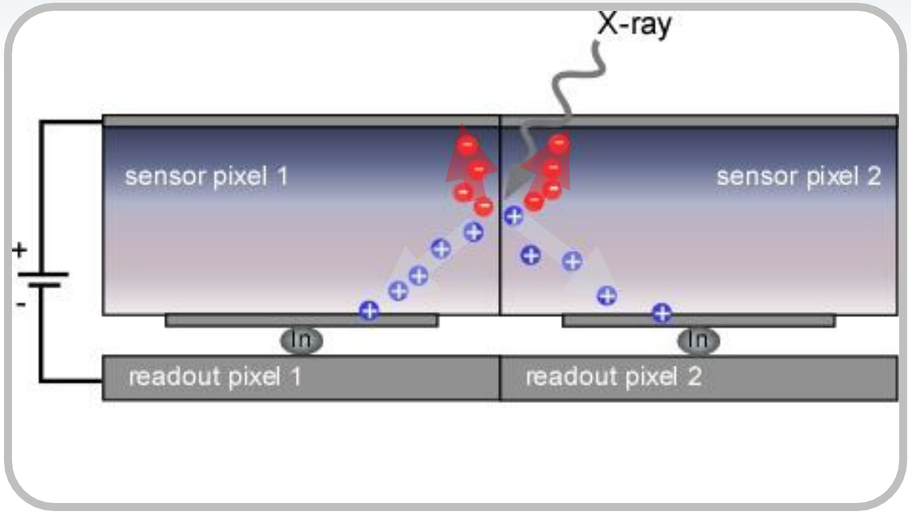
Counting errors:
Hidden/lost counts

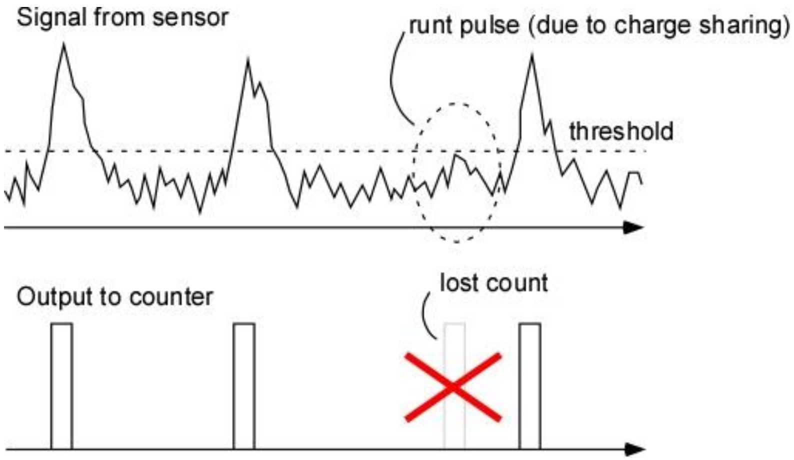
- Try to count the exact number of jelly beans in this jar
  - Take as long as you like…
- This is impossible to do exactly (without removing the beans) as *some of the beans are hidden from view*
  - ***Lost (hidden) counts*** can happen in an pixel detectors as well due to:
    - ***Charge sharing***
    - Gaps
    - Readout dead time

Photon counting pixel array limitations:
Charge sharing noise

- Charge produced by a single X-ray near a pixel boundary is shared between adjacent pixels
  - "Charge sharing" *
- ***Because of this, pulses near the edge of a pixel are smaller and can be lost***

*Journal of Instrumentation, Vol .10, Jan 2015, Looking at single photons using hybrid detectors, A. Bergamaschi, et al.,



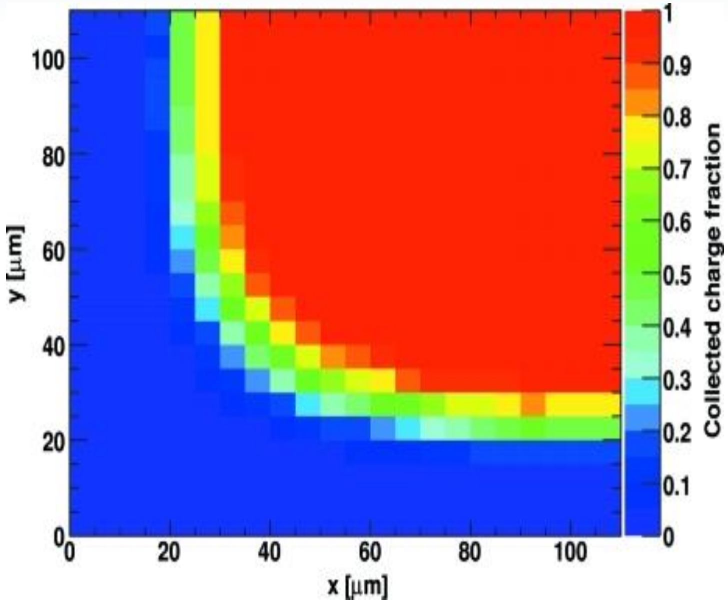


Photon loss due to charge sharing

- Each pixel has a 20 μm insensitive region at the edge due to charge diffusion
- Charge collected by pixel given by

$$I_{pix} = \int_{x_1}^{x_2} \int_{y_1}^{y_2} \frac{1}{2\pi\sigma_x\sigma_y} \exp\left(-\left[\frac{(x-x_0)^2}{2\sigma_x^2} + \frac{(y-y_0)^2}{2\sigma_y^2}\right]\right) \mathrm{d}x\mathrm{d}y$$

- If I_{pix} < threshold (typically 0.5) ***then the photon is lost***
- This happens in a thin strip along the edges and in the corners



*Charge collection in Pilatus Pixel**

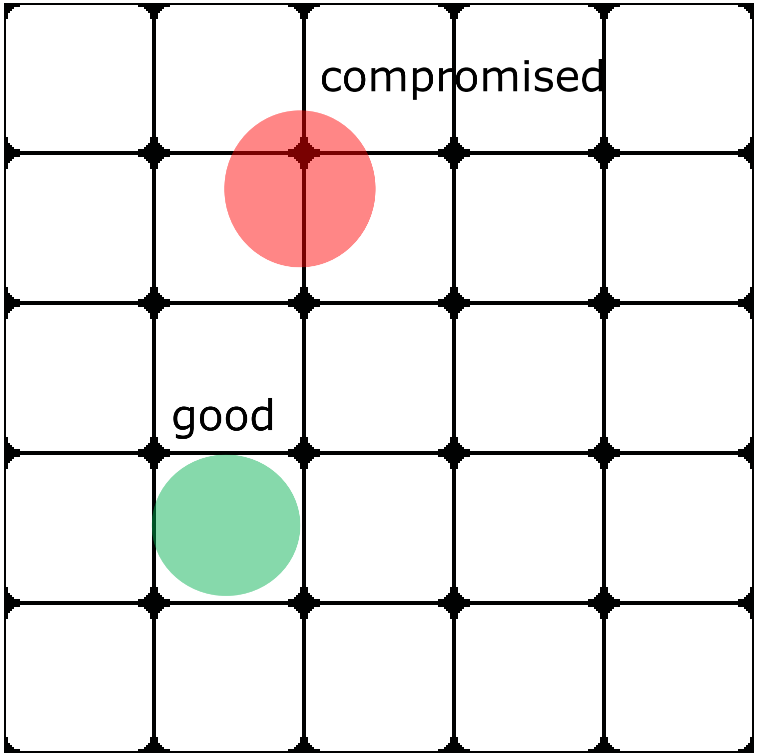
P. Trueb et al., J. Synchrotron Rad. (2012) 19, 347

**One corner shown*

5x5 pixel dead area map:
EIGER (ref. Shanks 2014)

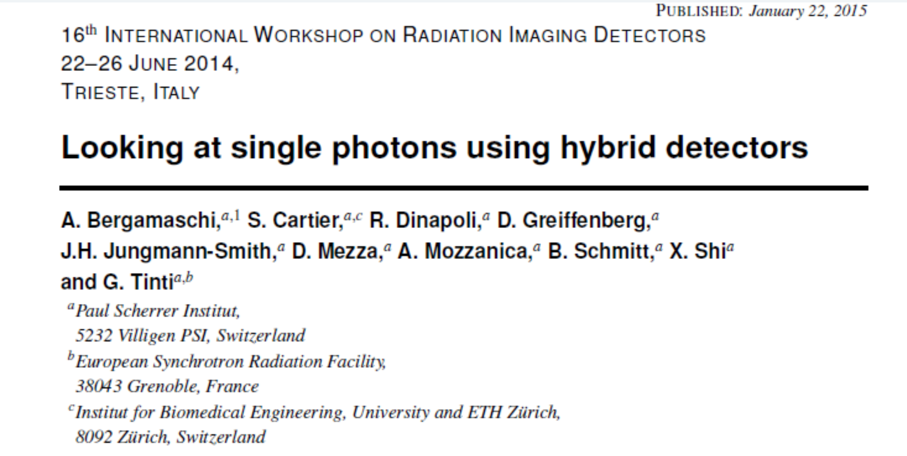
- If a reflection hits the edge or corner of a pixel then X-rays are lost
  - Causes errors in measured reflection intensities
- No accurate correction in software possible (because there is no profile information)

EIGER (75 µm pixels)



DEVELOPMENT OF LOW-NOISE DIRECT-CONVERSION X-RAY AREA DETECTORS FOR PROTEIN MICROCRYSTALLOGRAPHY
K. Shanks, 2014

Charge sharing:
How much of the pixel area is effected?



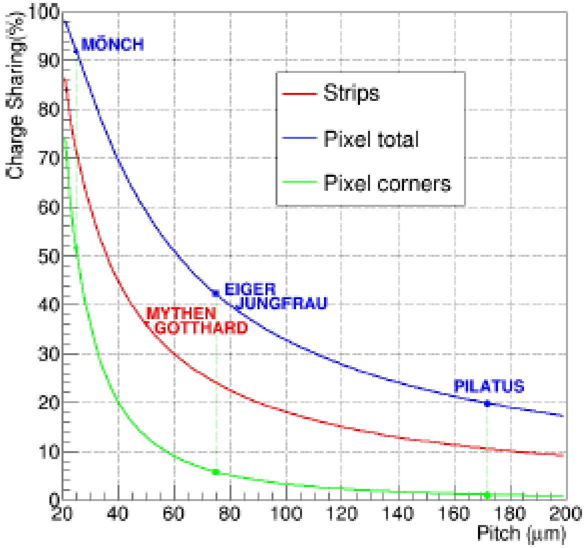
PUBLISHED: *January 22, 2015*

16th INTERNATIONAL WORKSHOP ON RADIATION IMAGING DETECTORS
22–26 JUNE 2014,
TRIESTE, ITALY

Looking at single photons using hybrid detectors

A. Bergamaschi,[a,1] S. Cartier,[a,c] R. Dinapoli,[a] D. Greiffenberg,[a] J.H. Jungmann-Smith,[a] D. Mezza,[a] A. Mozzanica,[a] B. Schmitt,[a] X. Shi[a] and G. Tinti[a,b]

[a] *Paul Scherrer Institut,*
5232 Villigen PSI, Switzerland
[b] *European Synchrotron Radiation Facility,*
38043 Grenoble, France
[c] *Institut for Biomedical Engineering, University and ETH Zürich,*
8092 Zürich, Switzerland



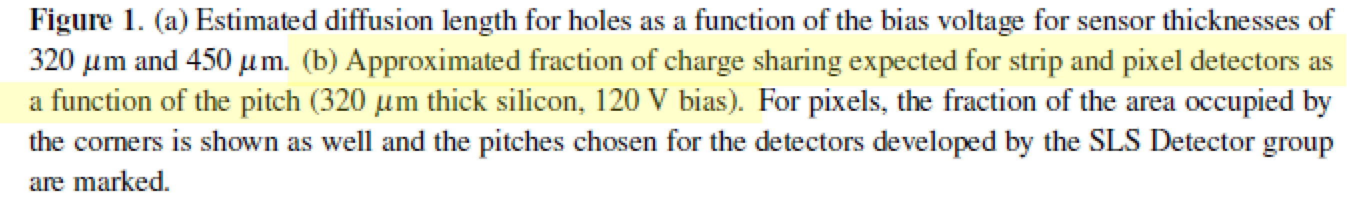
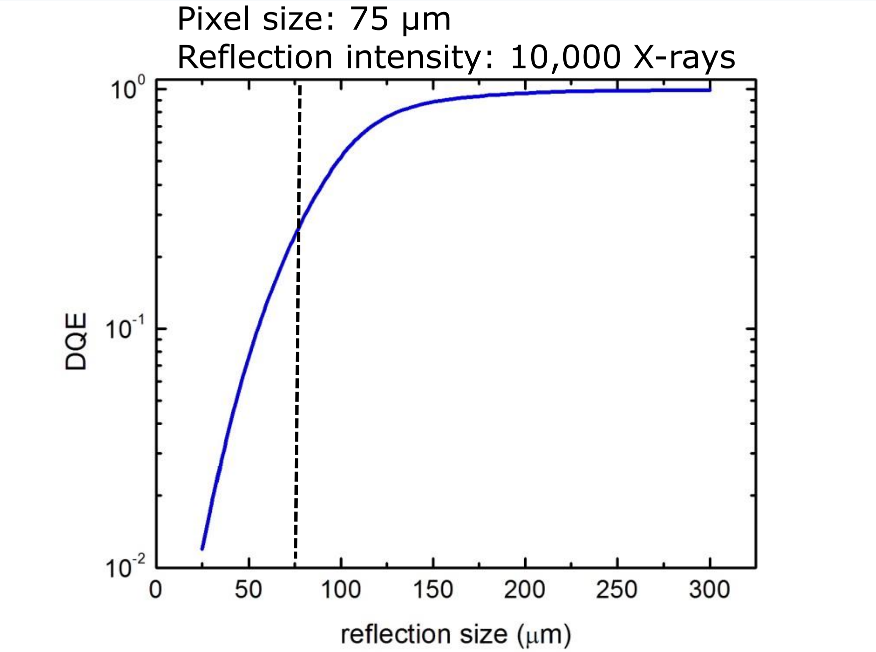


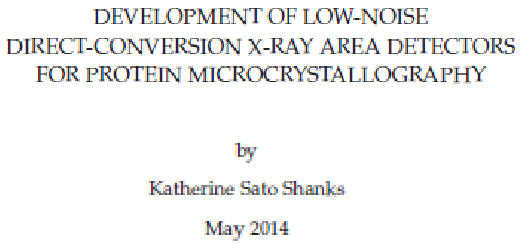
Figure 1. (a) Estimated diffusion length for holes as a function of the bias voltage for sensor thicknesses of 320 μm and 450 μm. (b) Approximated fraction of charge sharing expected for strip and pixel detectors as a function of the pitch (320 μm thick silicon, 120 V bias). For pixels, the fraction of the area occupied by the corners is shown as well and the pitches chosen for the detectors developed by the SLS Detector group are marked.

- Bergamaschi (2015) shows that charge sharing becomes worse for smaller pixels
  - For 172 µm pixels 20% of pixel area effected by charge sharing
  - For 75 µm pixels 43% of pixel area effected
  - ***For 25 µm pixels 100% of pixel is effected***

How does charge sharing impact DQE?

- Impact on DQE depends on the reflection size
  - Reflections large compared to the pixel size are not strongly effected (as the effect is ‘averaged out’)
- However, reflections smaller than the pixel size are significantly effected
  - E.g., a 50 micron spot with an intensity of 10,000 X-rays would be recorded with a DQE of only 10% (10 times lower than ideal, Shanks 2014)
- ***That is, significant information is lost for reflections comparable to or smaller than the pixel size***


Pixel size: 75 µm
Reflection intensity: 10,000 X-rays


DEVELOPMENT OF LOW-NOISE
DIRECT-CONVERSION X-RAY AREA DETECTORS
FOR PROTEIN MICROCRYSTALLOGRAPHY

by

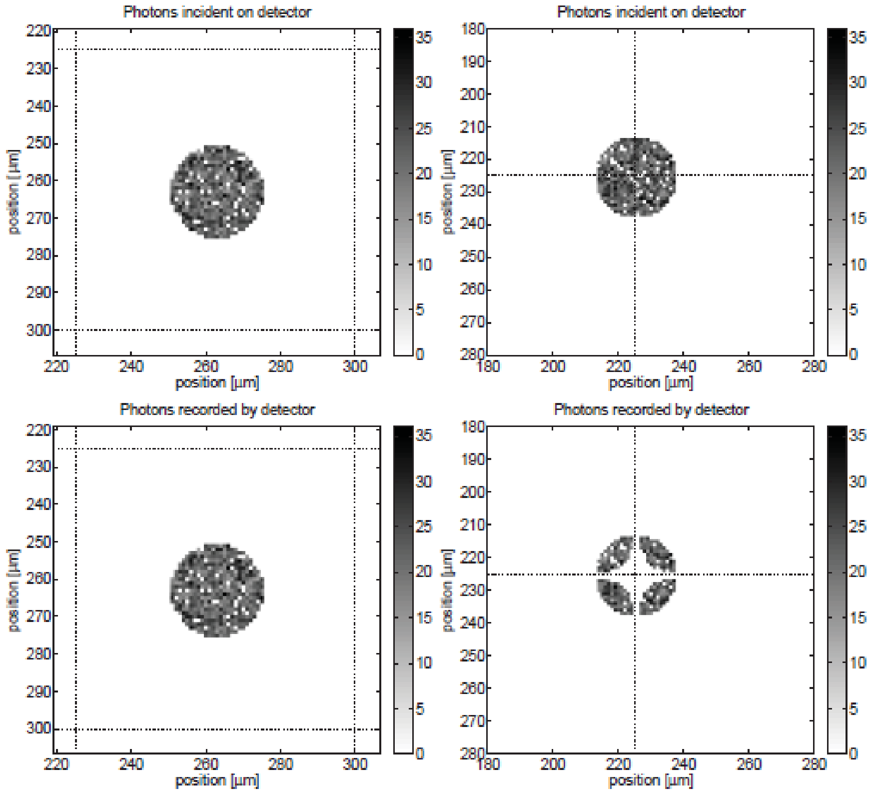
Katherine Sato Shanks

May 2014

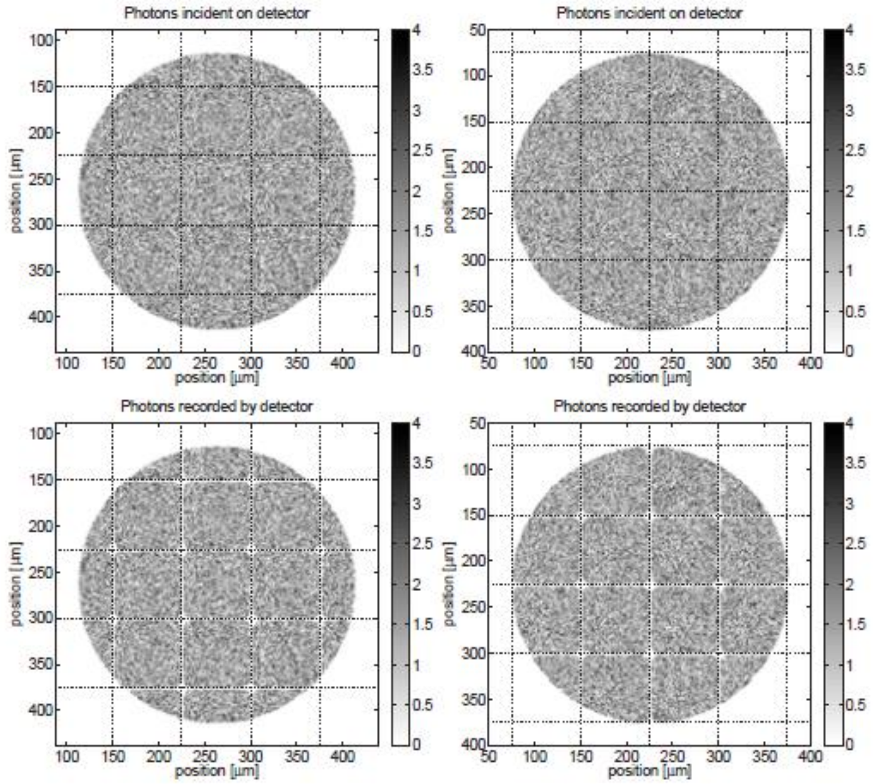
Charge sharing effect:

Information is lost for small reflections, but not for large

25 µm spot, 75 µm pixel



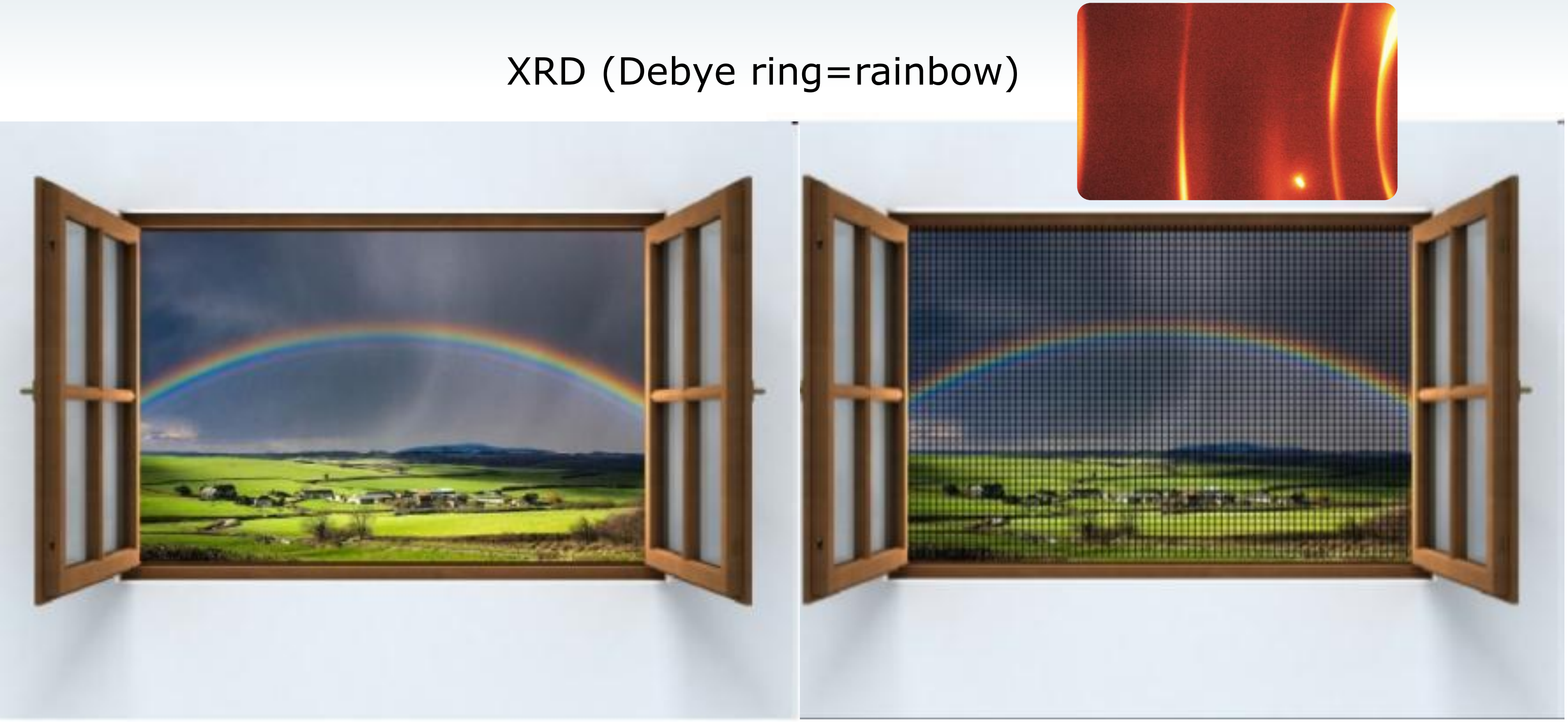
300 µm spot, 75 µm pixel



DEVELOPMENT OF LOW-NOISE DIRECT-CONVERSION X-RAY AREA DETECTORS FOR PROTEIN MICROCRYSTALLOGRAPHY
K. Shanks, 2014

Charge Sharing in XRD
Debye rings not affected

XRD (Debye ring=rainbow)



Window screen*=charge sharing

*Fensterfliegengitter

Photons are lost due to the wire screen (like charge sharing losses)
However, little information is lost as the rainbow covers many pixels

Charge Sharing in SC-XRD

Bragg reflections can be significantly effected

SC-XRD (Bragg reflections=stars)

Photons are lost due to the wire screen (like charge sharing losses)

Significant information is lost since stars are localized

Charge sharing in pixel detectors:
Other interesting references

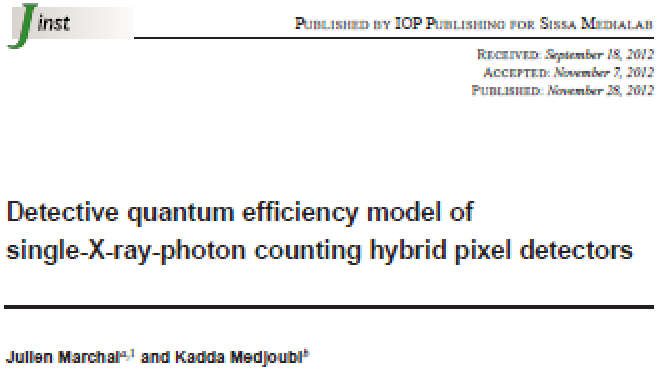
ELSEVIER Nuclear Instruments and Methods in Physics Research A 487 (2002) 113–122

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A

www.elsevier.com/locate/nima

Charge sharing in silicon pixel detectors

K. Mathieson[a,*], M.S. Passmore[b], P. Seller[c], M.L. Prydderch[c], V. O'Shea[a], R.L. Bates[a], K.M. Smith[a], M. Rahman[a]



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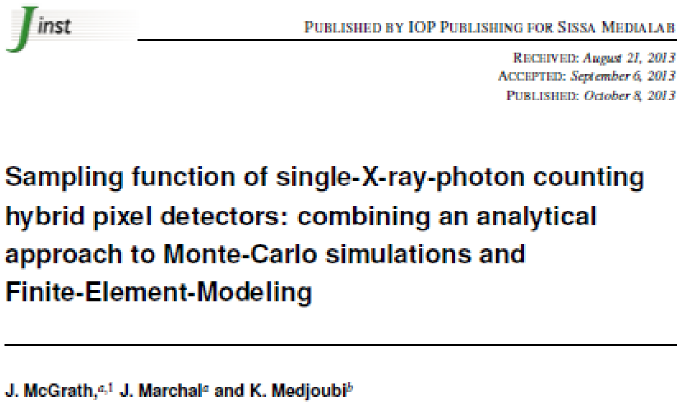
ACCEPTED: *November 7, 2012*
PUBLISHED: *November 28, 2012*

Detective quantum efficiency model of single-X-ray-photon counting hybrid pixel detectors

Julien Marchal[a,1] and Kadda Medjoubi[b]



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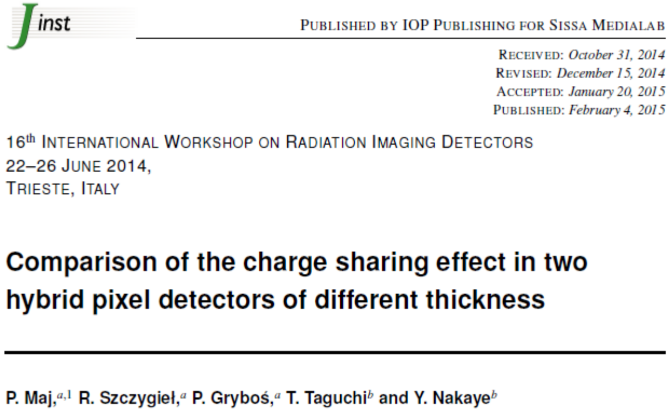
Sampling function of single-X-ray-photon counting hybrid pixel detectors: combining an analytical approach to Monte-Carlo simulations and Finite-Element-Modeling

J. McGrath,[a,1] J. Marchal[a] and K. Medjoubi[b]



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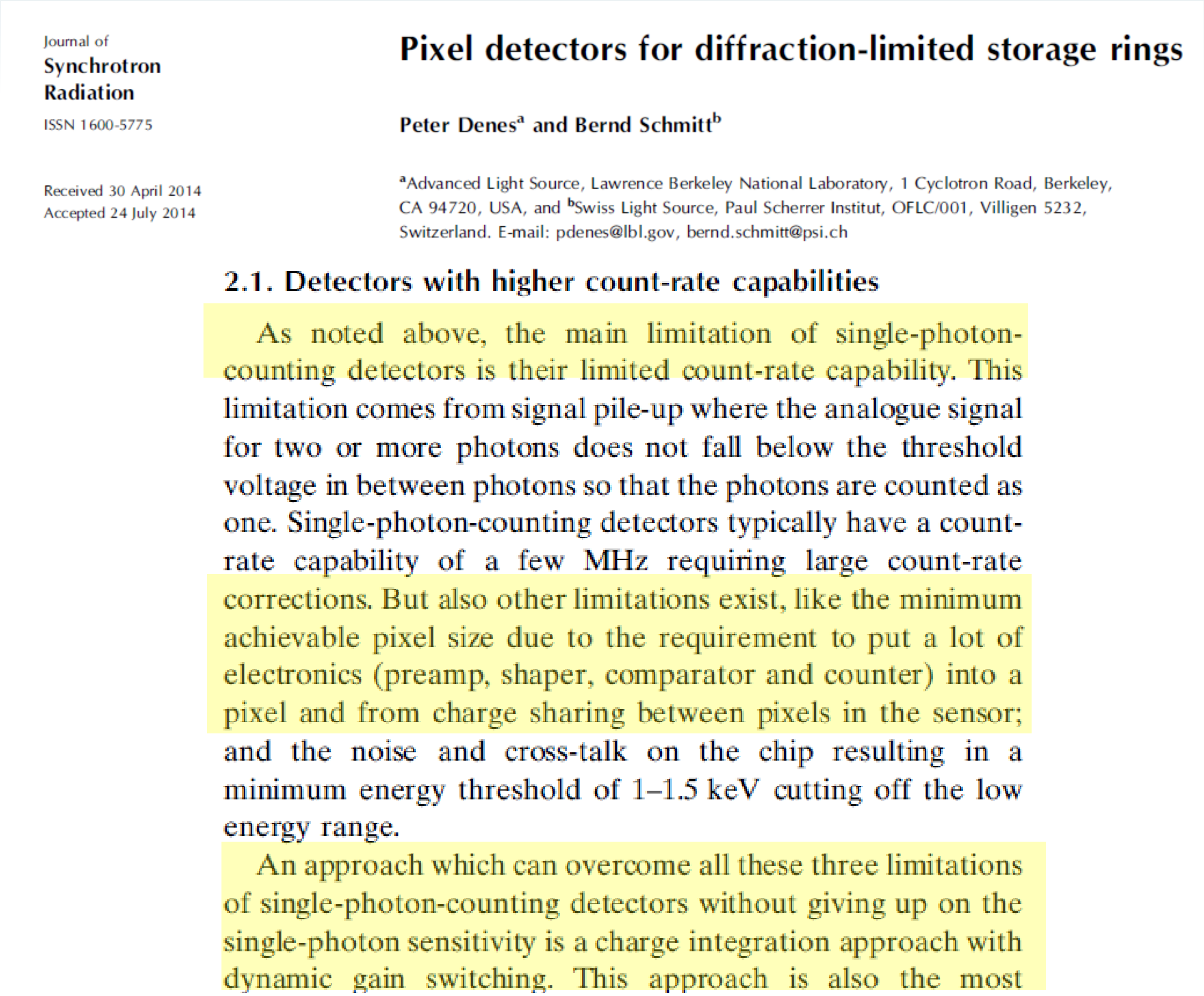
TRIESTE, ITALY

Comparison of the charge sharing effect in two hybrid pixel detectors of different thickness

P. Maj,[a,1] R. Szczygieł,[a] P. Gryboś,[a] T. Taguchi[b] and Y. Nakaye[b]

How can one do better?

Charge integrating pixel array detectors



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Pixel detectors for diffraction-limited storage rings

Peter Denes[a] and Bernd Schmitt[b]

[a]Advanced Light Source, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA, and [b]Swiss Light Source, Paul Scherrer Institut, OFLC/001, Villigen 5232, Switzerland. E-mail: pdenes@lbl.gov, bernd.schmitt@psi.ch

2.1. Detectors with higher count-rate capabilities

As noted above, the main limitation of single-photon-counting detectors is their limited count-rate capability. This limitation comes from signal pile-up where the analogue signal for two or more photons does not fall below the threshold voltage in between photons so that the photons are counted as one. Single-photon-counting detectors typically have a count-rate capability of a few MHz requiring large count-rate corrections. But also other limitations exist, like the minimum achievable pixel size due to the requirement to put a lot of electronics (preamp, shaper, comparator and counter) into a pixel and from charge sharing between pixels in the sensor; and the noise and cross-talk on the chip resulting in a minimum energy threshold of 1–1.5 keV cutting off the low energy range.

An approach which can overcome all these three limitations of single-photon-counting detectors without giving up on the single-photon sensitivity is a charge integration approach with dynamic gain switching. This approach is also the most

Charge integrating pixel arrays

Advantages over photon counting pixel arrays

10th International Conference on
POSITION SENSITIVE DETECTORS

Contribution ID : **135**

Type : **Invited Paper**

(Invited) Jungfrau, Mönch and Eiger: Detector Development at the Swiss Light Source

Primary author(s) : Dr. SCHMITT, Bernd (Paul Scherrer Institut)

The detector group at the Swiss Light Source (SLS) is currently involved in several detector development projects both for synchrotrons and XFELs. In the presentation we give an overview of our developments… ***Jungfrau and Mönch are charge integrating systems which overcome several limitations of today's single photon counting detectors like count rate capability, pixel size or low energy limit.***

The detector is developed for SwissFEL (the XFEL currently being built at the Paul Scherrer Institute). However, with a frame rate of 1-2 kHz and a data quality similar to single photon counting detectors, ***it is also an excellent detector for applications at synchrotrons specifically those having a high photon rate (like protein crystallography or small angle scattering). (2015)***

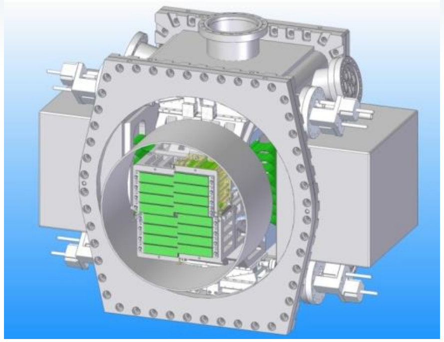
Why charge integration?

A better way to count jelly beans

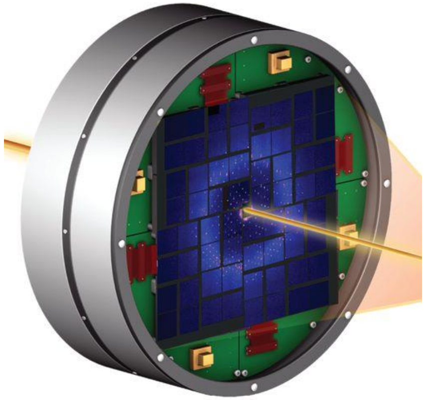
- Another way to ‘count’
  - Weight the beans
  - Divide by weight of a single jelly bean
- This is how a ***charge-integrating*** detector works
  - If the scale is very accurate (so that one can measure weights much smaller than a single bean) ***then it can accurately count a single bean (photon)***
  - That is, the measurement becomes essentially noise-free
    - Single photon (single jelly bean) sensitivity
  - ***This is first secret of CPADs***
- Benefits
  - No count rate saturation
  - Single photon sensitivity
- Limitation: upper count limit
  - ***Second secret of CPADS: Variable gain to achieve high dynamic range***

What is a Charge Integrating Pixel Array?

- A CPAD *is a pixel array* but has additional features:
  - **Full charge** is measured, not a simple threshold
  - Massively parallel readout to achieve high speed
  - Effective gain is ***variable*** to achieve high dynamic range
- CPAD detectors were recently developed for applications at 4th Gen beamlines*
  - CPADs include Jungfrau, Mönch (SwissFEL), AGIPD (European XFEL), CSPAD, ePIX (LCLS)
- CPADs are the most advanced detector technology available, they come closer to an ideal detector than any other technology



AGIPD (DESY)



CSPAD (LCLS)

*J Synch. Radiat. 2014 Sep 1; 21(Pt 5): 1006–1010, Pixel detectors for diffraction-limited storage rings, P. Denes and B. Schmitt

Charge sharing pixel arrays:
Dynamic gain switching

- By switching feedback capacitors pixel gain can be changed dynamically
  - High gain for weak signals
  - Low gain for stronger signals
- Allows detector to achieve simultaneously Poisson-limited (quantum-limited) performance and a large dynamic range

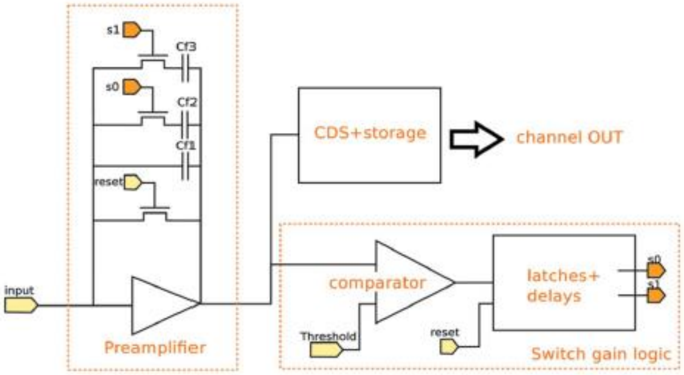


Figure 3
Dynamic gain-switching front-end. After reset a comparator monitors the output of the charge-integration stage and just before saturation switches in larger feedback capacitors to reduce the gain. In this way each pixel adjusts itself to the incoming number of photons.

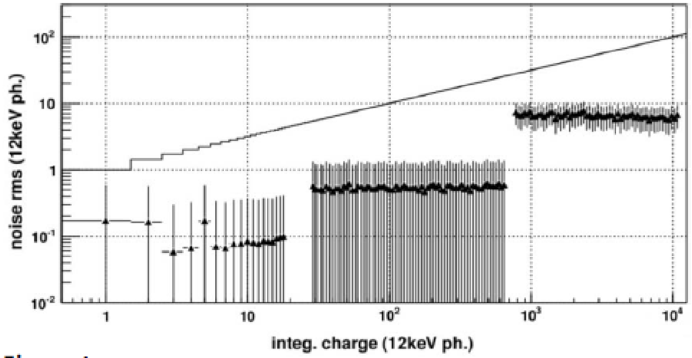
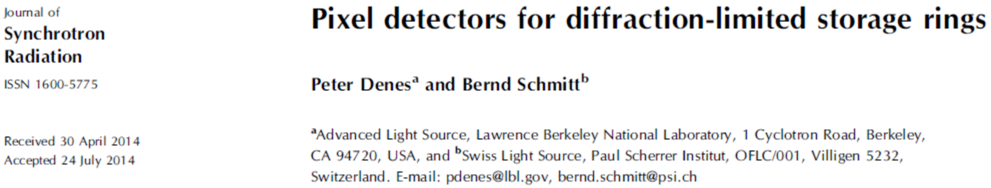


Figure 4
Noise (normalized to 12 keV photons) measured in Jungfrau as a function of the intensity over the entire dynamic range. At all intensities the noise is below the Poisson fluctuations shown as a black line. This means that the uncertainty of the data is limited by the Poisson fluctuations, *i.e.* the detector has the best possible data quality.



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Pixel detectors for diffraction-limited storage rings

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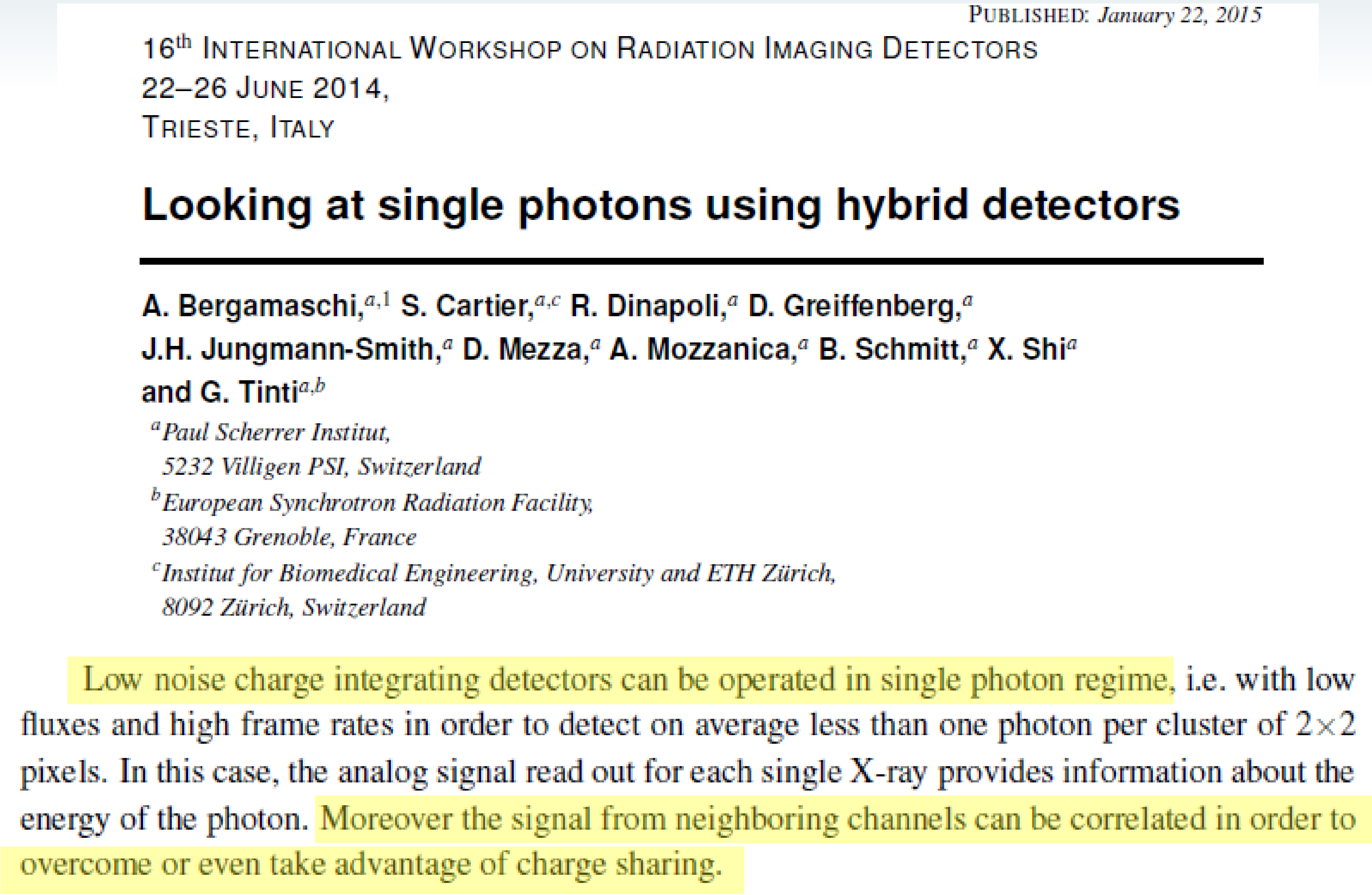
[a]Advanced Light Source, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA, and [b]Swiss Light Source, Paul Scherrer Institut, OFLC/001, Villigen 5232, Switzerland. E-mail: pdenes@lbl.gov, bernd.schmitt@psi.ch

Charge integrating pixel array detector

Elimination of charge sharing noise



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Looking at single photons using hybrid detectors

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[a] *Paul Scherrer Institut,*
5232 Villigen PSI, Switzerland
[b] *European Synchrotron Radiation Facility,*
38043 Grenoble, France
[c] *Institut for Biomedical Engineering, University and ETH Zürich,*
8092 Zürich, Switzerland

Low noise charge integrating detectors can be operated in single photon regime, i.e. with low fluxes and high frame rates in order to detect on average less than one photon per cluster of 2×2 pixels. In this case, the analog signal read out for each single X-ray provides information about the energy of the photon. Moreover the signal from neighboring channels can be correlated in order to overcome or even take advantage of charge sharing.

PHOTON II

CPAD technology for the homelab

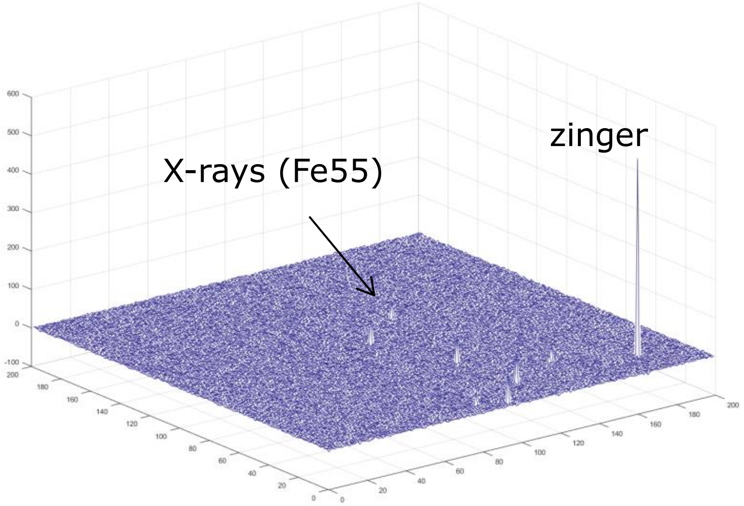
- The PHOTON II is the first CPAD detector offered for home lab applications
- Similar technology to CPAD technology developed for 4th Gen XFEL beamlines
  - Large active area (140 x 100 mm^2)
  - Single photon sensitivity (SPDC 0.99)
  - No charge sharing noise
  - No count rate saturation
  - High dynamic range
  - Negligible parallax (<1 pixel at 24 KeV)
  - High speed (70 frames/sec)
  - Readout dead time 0 sec (dual port readout buffer)
  - Excellent DQE >0.9 from 5 to 24 keV

Size

- PHOTON II features the largest monolithic silicon sensor currently available: 10 x 14 cm^2
  - No gaps
  - 135 µm pixel size
- **Benefit: collect more data faster**

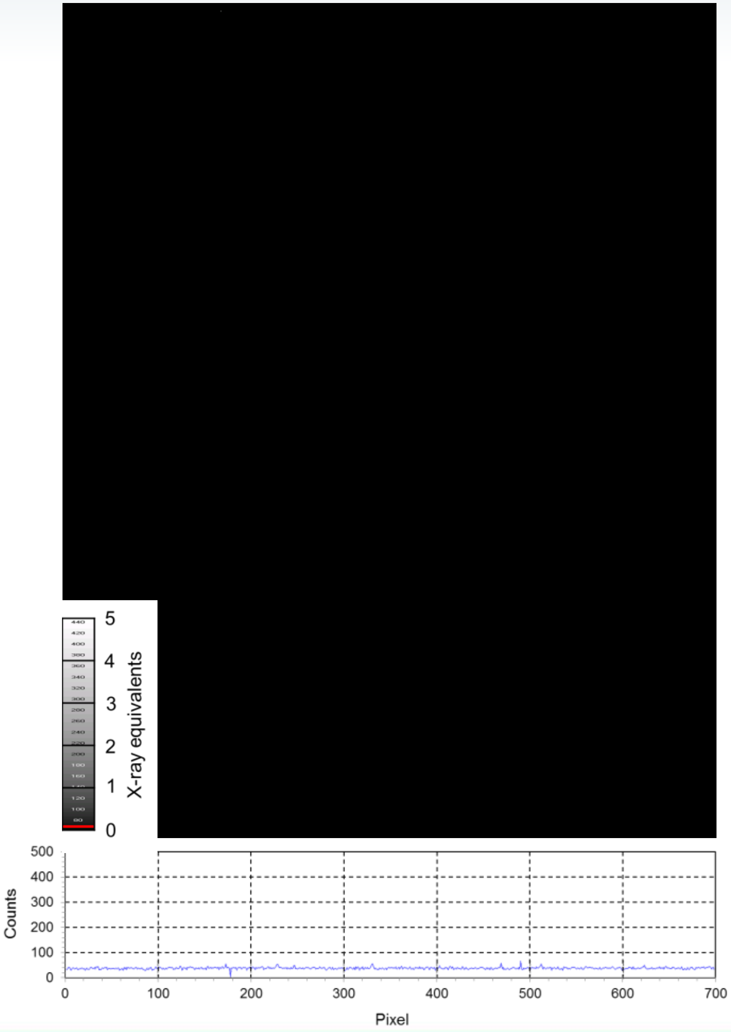
PHOTON II sensitivity

- The PHOTON II achieves 20 electrons read noise typical at 70 fps
  - Integrated noise on 4 pixels 40 electrons
- The conversion gain at 8.1 keV is 180 electrons typical
- Therefore, the single photon detection confidence is
  - erf(180/40)>0.99
- The PHOTON II achieves single photon sensitivity across the entire operating energy range: 8-24 keV
- Energy resolution is also used for real time 'zinger' rejection
- **Benefit: Better data quality for weak reflections, long exposures**



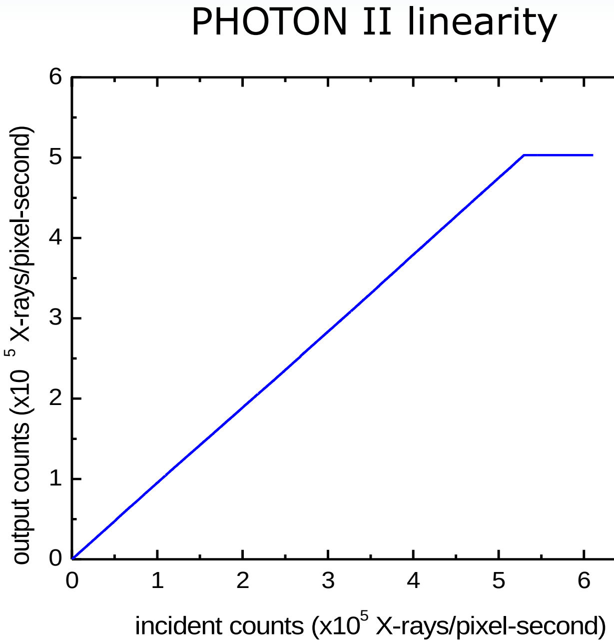
Dark signal

- Integrating detectors suffer from accumulation of thermal dark current
- However, cooling to -15 C suppresses dark current
- Energy resolution used to filter 'zinger' noise
  - Cosmic rays and natural radiation
- Dark frame after 300 sec shows essentially no intrinsic detector noise
  - Noise <0.17 photon rms



Linearity

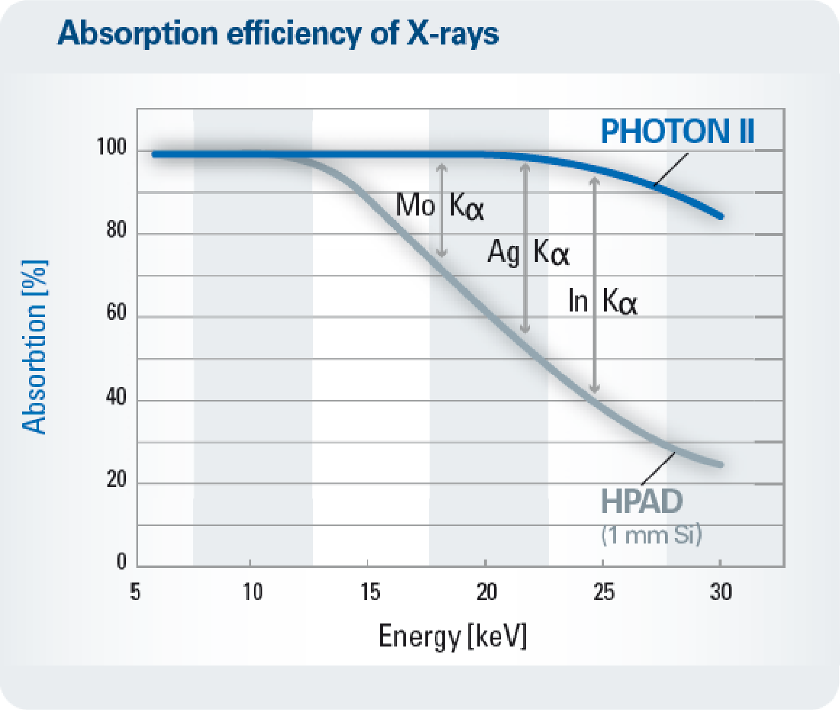
- PHOTON II has essentially no nonlinearity at high count rates
  - At 5×10^5 counts per second per pixel PHOTON II nonlinearity is >0.2%
- **Benefit: Better data for strong diffractors**



PHOTON II absorption efficiency

- The advanced scintillator screens employed in the PHOTON II features high absorption at higher energies
  - Up to twice the efficiency of Silicon sensors
- Because of this the PHOTON II has higher DQE and also essentially no parallax

- **Benefit: Better data, especially for high energies (Mo, Ag, In)**



D8 VENTURE METALJET

State-of-the-art in-house

- Flux density comparable with 2nd generation synchrotron beamlines
- Smallest X-ray beams available on in-house source
- No anode deterioration – always 100% performance
- Extremely stable beam
- KAPPA goniometer
- PHOTON II CPAD detector

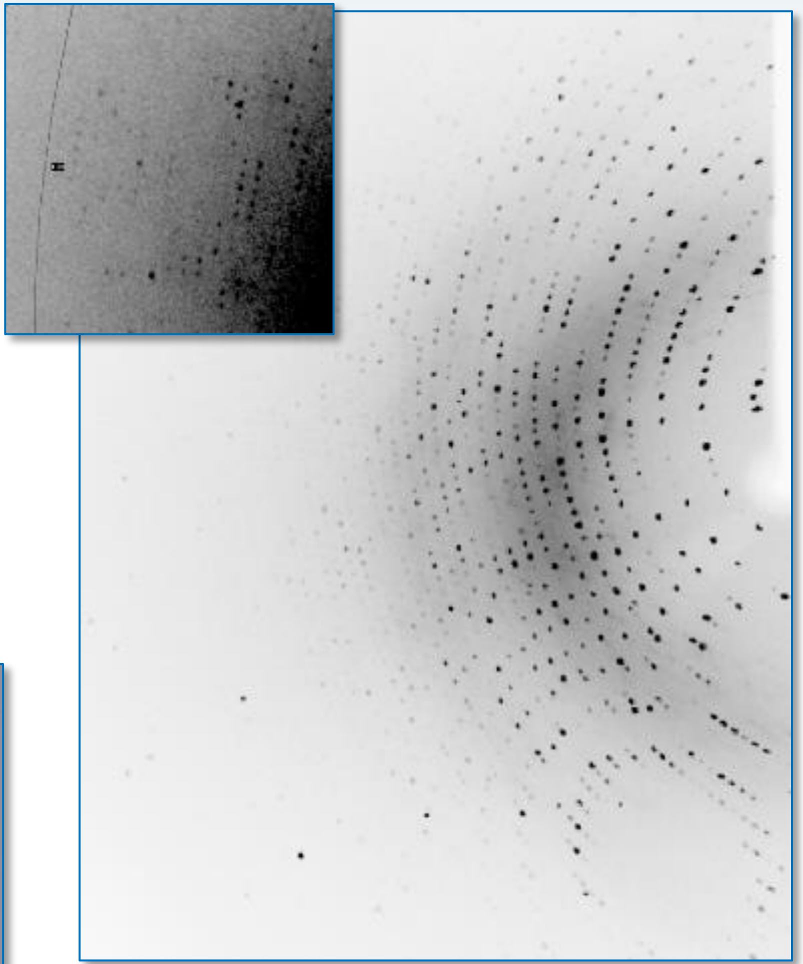
P Tautomerase on METALJET w. PHOTON II

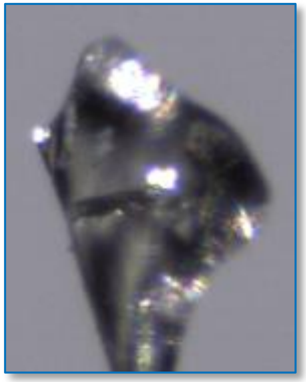
Data collection

Space group	$P2_12_12_1$
Data collected	340°, 135°*
Exposure time	100, 10 sec/°
Divergence	7.6 mrad
DX	75 mm
Rotation angle	0.2°, 0.5°
Wall time	10 hrs
Max resolution	1.25 Å

- Crystal dimensions
  - 0.125 x 0.142 x 0.175 mm

* Parameters for the high and low resolution scans





P Tautomerase

Comparison with beamline data

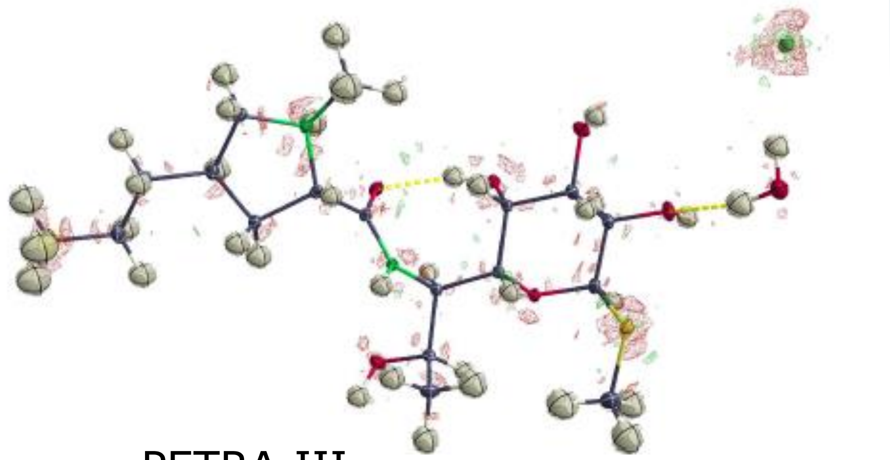
The high intensity of the METALJET allows the same diffraction limit to be acquired but the greater beam stability combined with the enhanced accuracy and sensitivity of the PHOTON II allows the D8 VENTURE to produce much better data.

	D8 VENTURE METALJET	**X25 NSLS (published data)**
Resolution limit (Å)	1.25	1.25
R_{merge}	0.039 (0.448)	0.101 (0.498)
$I/\sigma I$	17.12 (2.38)	17.5 (2.27)
Multiplicity	4.92 (3.09)	4.6 (4.4)
Completeness (%)	99.9 (99.8)	99.0 (96.9)
Detector	PHOTON II	PILATUS 6M

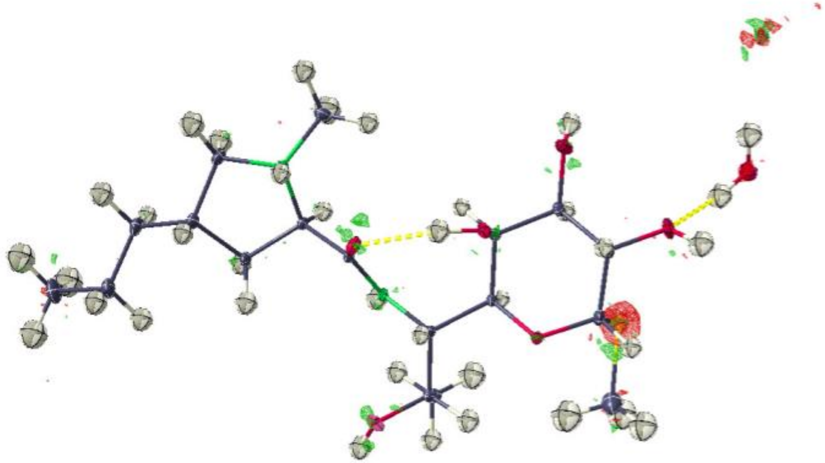
Charge density comparison

Lincomycin

- Charge density measurements are one of the 'acid tests' of system performance
  - Requires sub-atomic resolution
  - Light atom targets are especially challenging
- Charge density comparison: Lincomycin
- Top PILATUS 6M at PETRA III P11 (beamline). J. Lübben, DGK 2014
- Bottom PHOTON II data in home lab with microfocus source



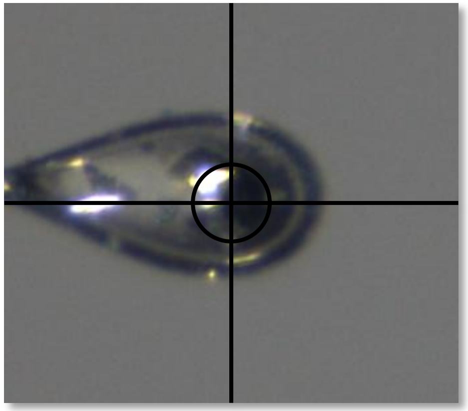
PETRA III

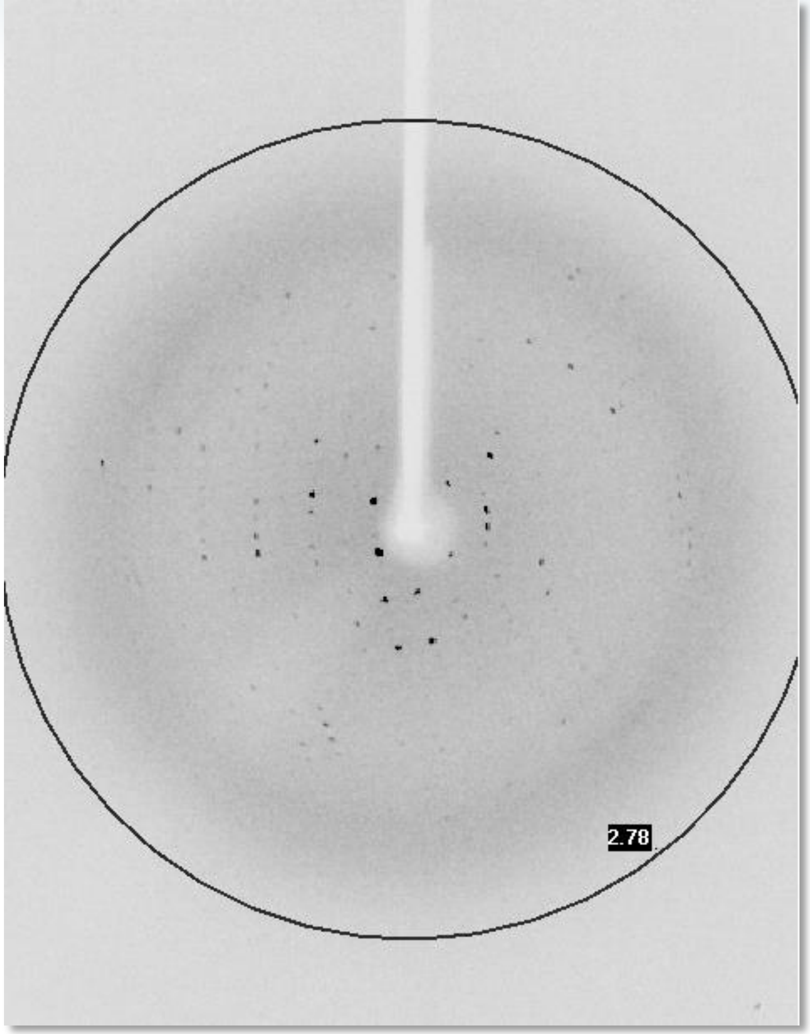


PHOTON II

Ox_1R-StaR data collection

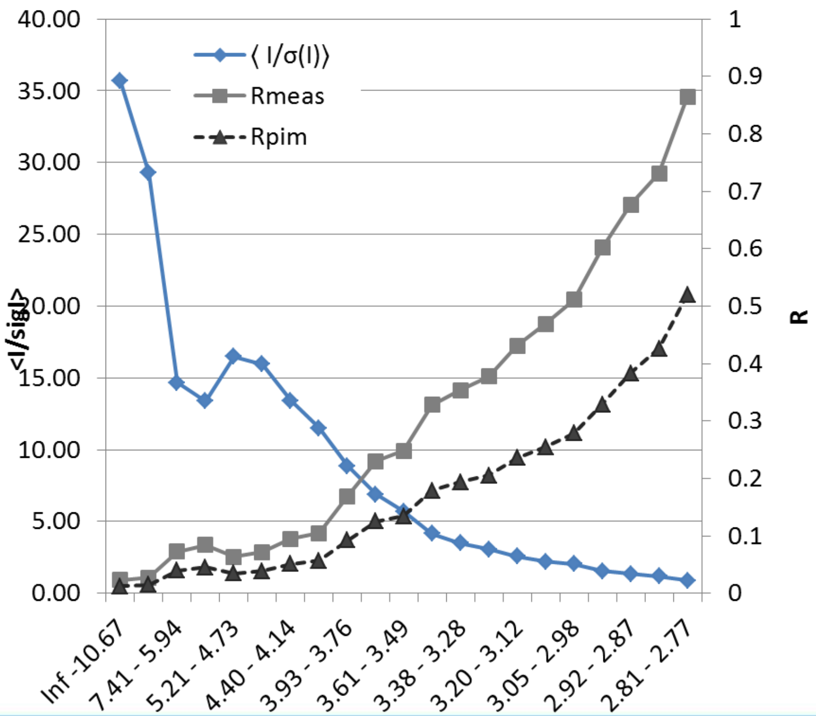
Crystal dimensions, µm	80 x 80 x 50
Space group	$P2_1$
a, *b*, *c* (Å)	59.575 146.433 71.724
α, β, γ (°)	90.00 112.38 90.00
Mosaicity (°)	0.41
Rotation range per image (°)	0.1
Exposure time per image (s)	6
Total degrees collected	162°
TOTAL MEASUREMENT TIME	**2.7 hrs**





Ox_1R-StaR data statistics

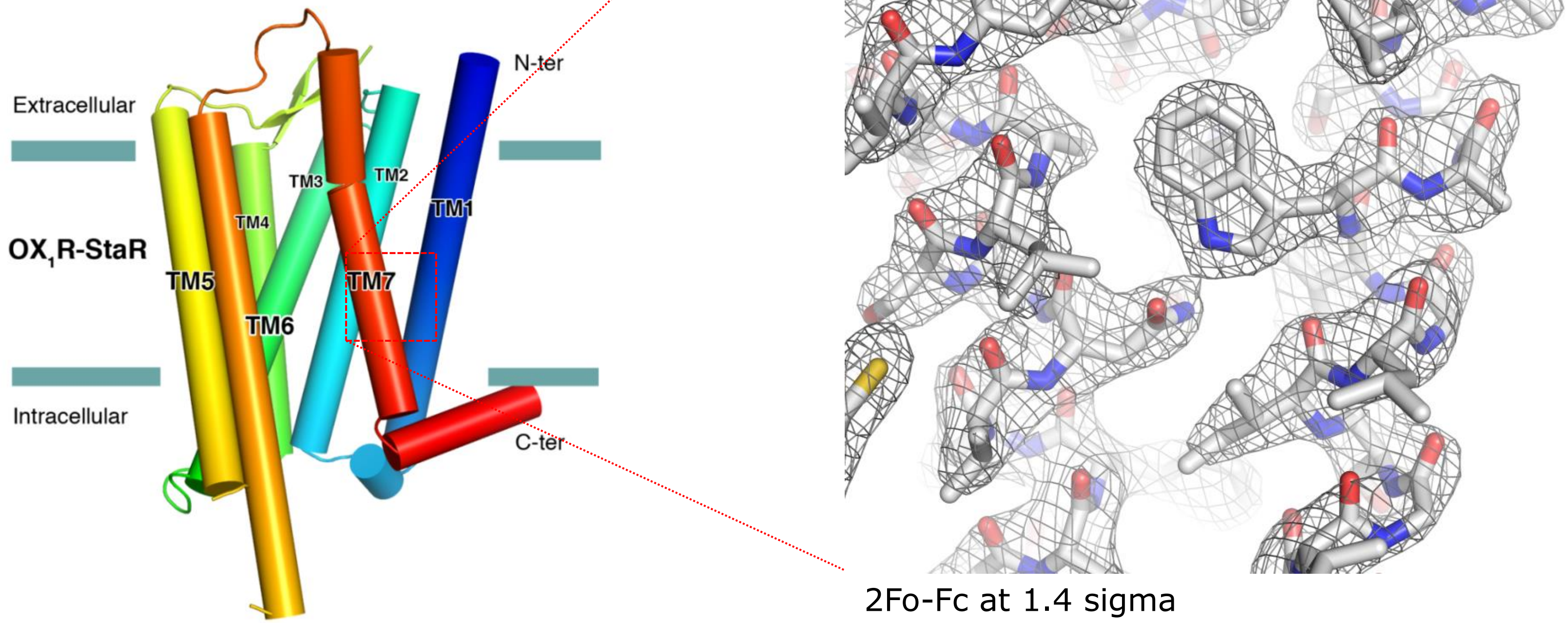
Data processing	**PROTEUM3**
Integration	SAINT+
Scaling, absorption correction	SADABS
Statistics	XPREP
High Resolution (Å)	2.87 – 2.77
Total No. of reflections	92207
No. of unique reflections	28725
Completeness (%)	99.3 (97.9)
Redundancy	3.21 (2.62)
$\langle I/\sigma(I) \rangle$	8.05 (1.05)
$R_{\text{r.i.m.}}$	13.91 (77.46)
$R_{\text{p.i.m.}}$	7.62 (45.68)
CC ½ at cut-off	50%



Ox_1R-StaR structure

Solved in-house using D8 VENTURE METALJET

- Structure determined by MR using PHASER
- Model Ox_1R-StaR structure unpublished
- Refinement using REFMAC5
- R_{work} / R_{free} = 0.2444 / 0.2721

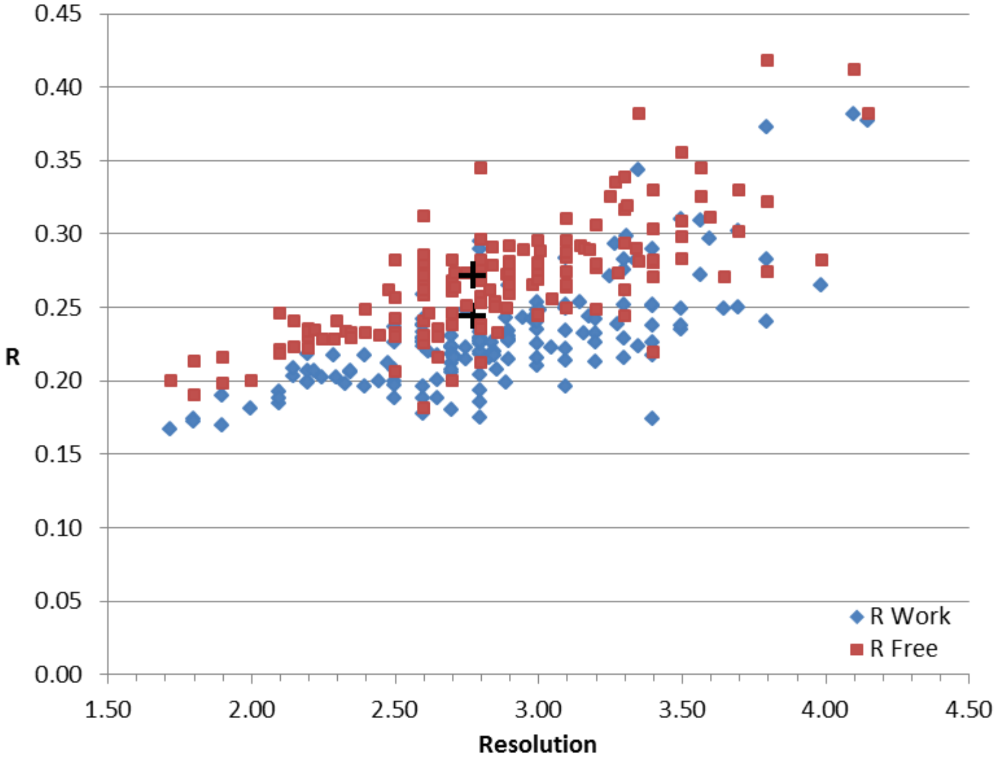


2Fo-Fc at 1.4 sigma

Ox$_1$R-StaR

World’s first in-house GPCR structure

- Refinement statistics for 159 GPCR structures retrieved from PDB
  - 155 at synchrotron
  - 4 XFEL
- Ox$_1$R-StaR collected on D8 VENTURE METALJET is world’s first reported in-house GPCR structure
- Structure resolution and refinement statistics consistent with those solved using synchrotron data



Summary:
Features and benefits of charge integrating pixel array detectors

- The key advantages of photon-counting pixel arrays include
  - High speed
  - Low noise, high sensitivity
- Charge integrating pixel array detectors (CPADs) have these same high speed and low noise characteristics but also offer unique advantages:
  - No charge sharing noise
  - Smaller pixel size possible
  - ***No count rate saturation***
- For single-crystal X-ray diffraction CPADs thus offer significant advantages
  - ***Especially for next-gen, ultra-high intensity sources***
- The PHOTON II is the first CPAD available for home laboratory use

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