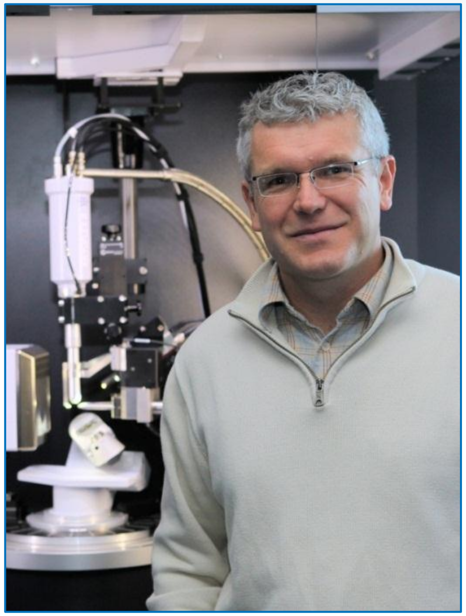
PHOTON 100:
Shutterless Data Acquisition with Continuous Scans

Michael Ruf and Roger Durst

October 8, 2013

Welcome



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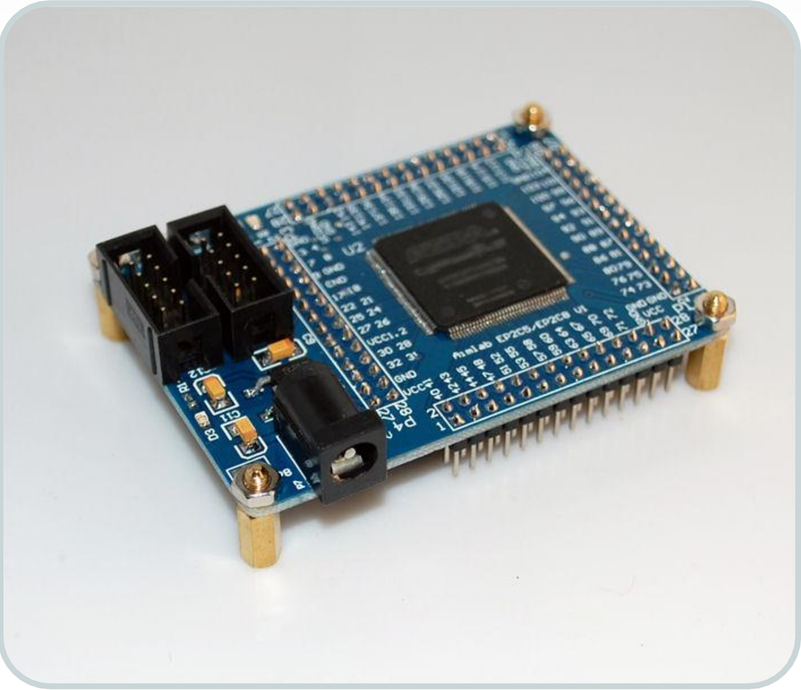
Shutterless data collection

- The PHOTON 100 shutterless data acquisition mode allows data collection in a fraction of the time compared to “shuttered” mode.
- Data quality is always matched or even exceeded and always can be improved further by collecting data with higher multiplicity.
- Compared to large-format CCD detectors, the factor for time saving can increase to a factor of up to eight.

PHOTON 100 detector

- Large 100-cm^2 sensor for fast and efficient data collection
- Low power consumption sensor for high reliability
- Air-cooled for low maintenance
- High sensitivity
- No glass fiber taper for superior spatial accuracy
- Optimized pixel size and point spread function for superior signal
- Large pixel volumes for best light conversion
- **Shutterless operation and continuous scan mode for best data acquisition efficiency**
- 3-year warranty

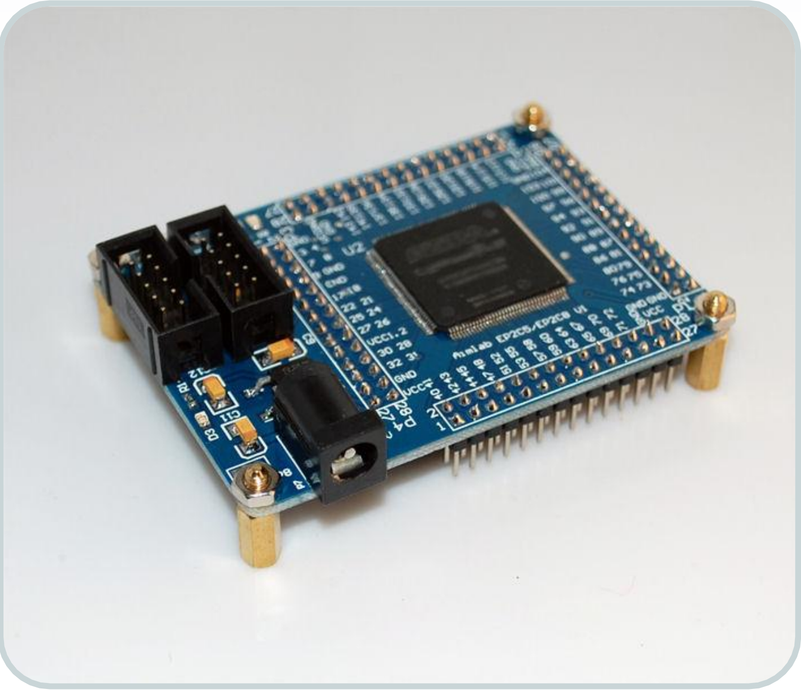
Shutterless data collection for unprecedented acquisition speed and data quality



On-camera data processing for best efficiency

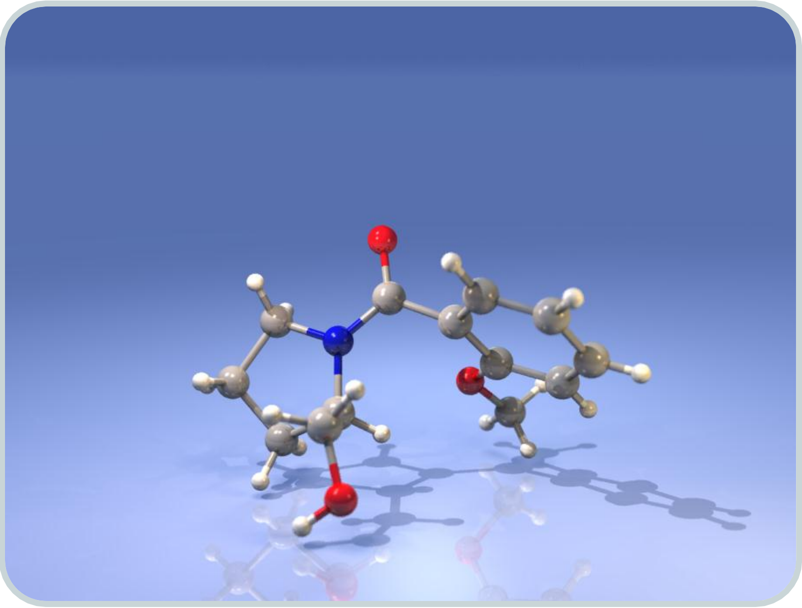
- All the necessary image corrections are applied in a special real-time processor in the camera electronics
- The output data are fully corrected
- Facilitates operation of the detector in a true dead-time-free shutterless mode with continuous sample rotation

FPGA - Field-programmable gate array



- Configured after manufacturing — hence "**field-programmable**"
- **Large resources** of logic gates and RAM blocks to implement complex digital computations
- Fine-grained **parallelism**
  - Doing 4 operations at once doesn't count; 1024 does
- Ideal for **pipelining**
  - A pipeline is a set of data processing elements connected in series, so that the output of one element is the input of the next one
  - Create a pipeline by dividing a complex operation into simpler operations

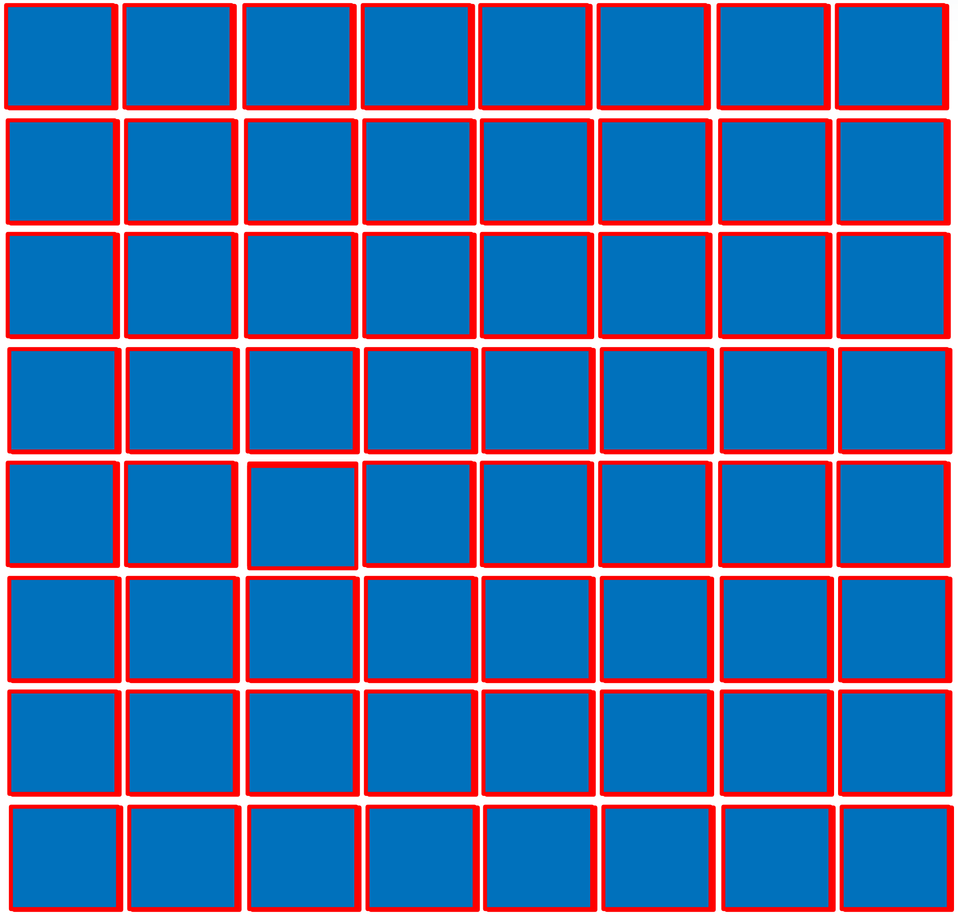
Shutterless data collection for unprecedented acquisition speed and data quality



Shutterless data acquisition for overhead-free data collection

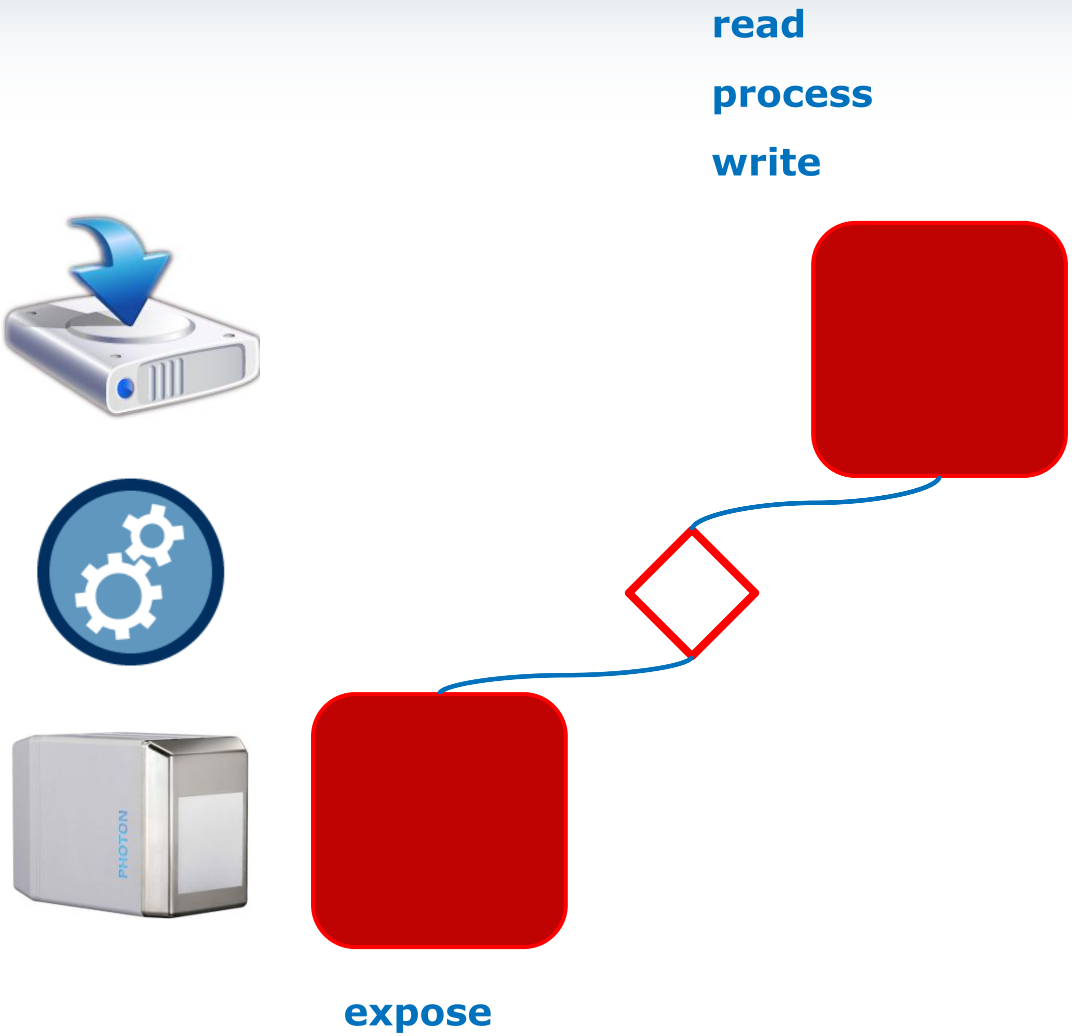
- Data is read out while the camera is exposed to X-rays
- Eliminates the need to open and close the X-ray shutter
- Eliminates the need to stop, reposition and start the goniometer
- Eliminates mechanical jitter
- In shutterless mode the sample is constantly exposed to X-rays and continuously rotated, which maximizes data acquisition efficiency
- **Superior data quality in less time is possible today**

PHOTON 100 detector readout



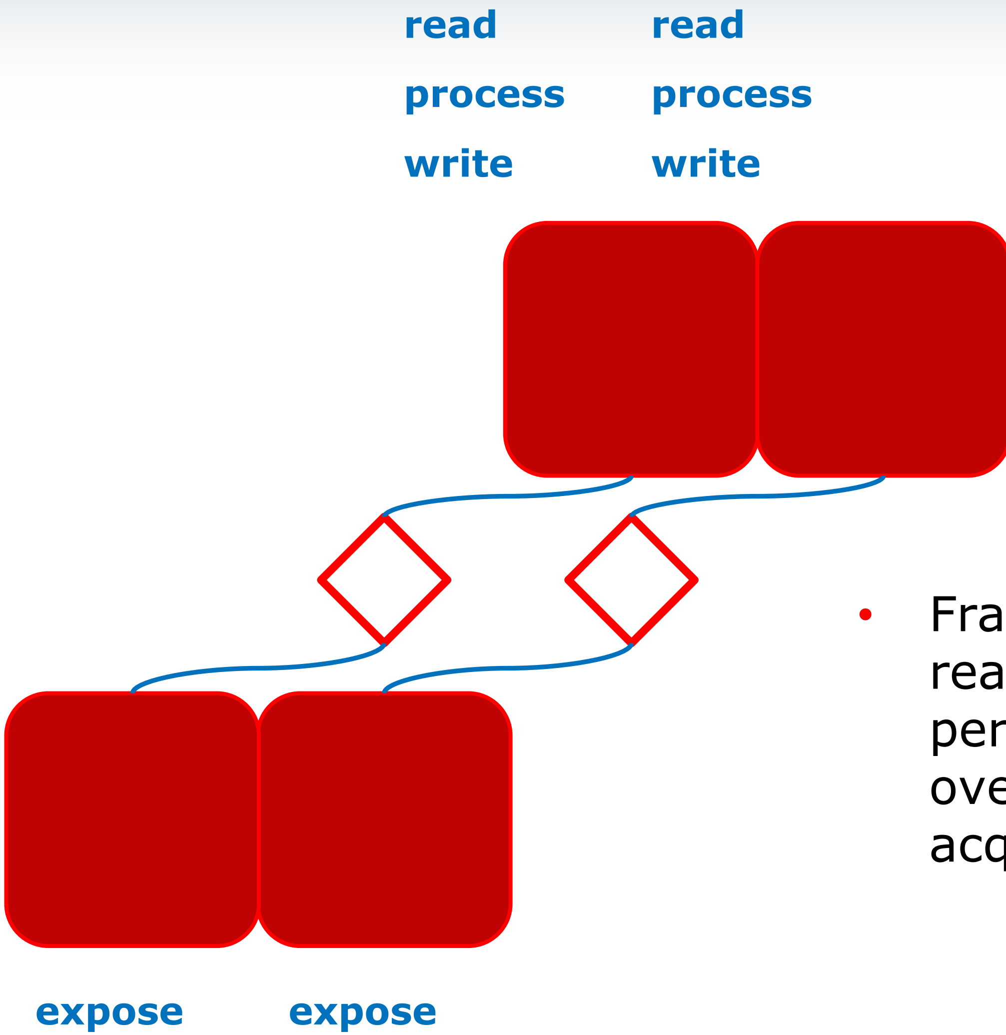
- Two sensors are read out in parallel
- Readout is pixel per pixel and row per row
- Readout of a 1024 × 1024 array takes 0.8 s
- Readout and on-camera processing are performed in less than 1 second

PHOTON 100 frame acquisition one cycle



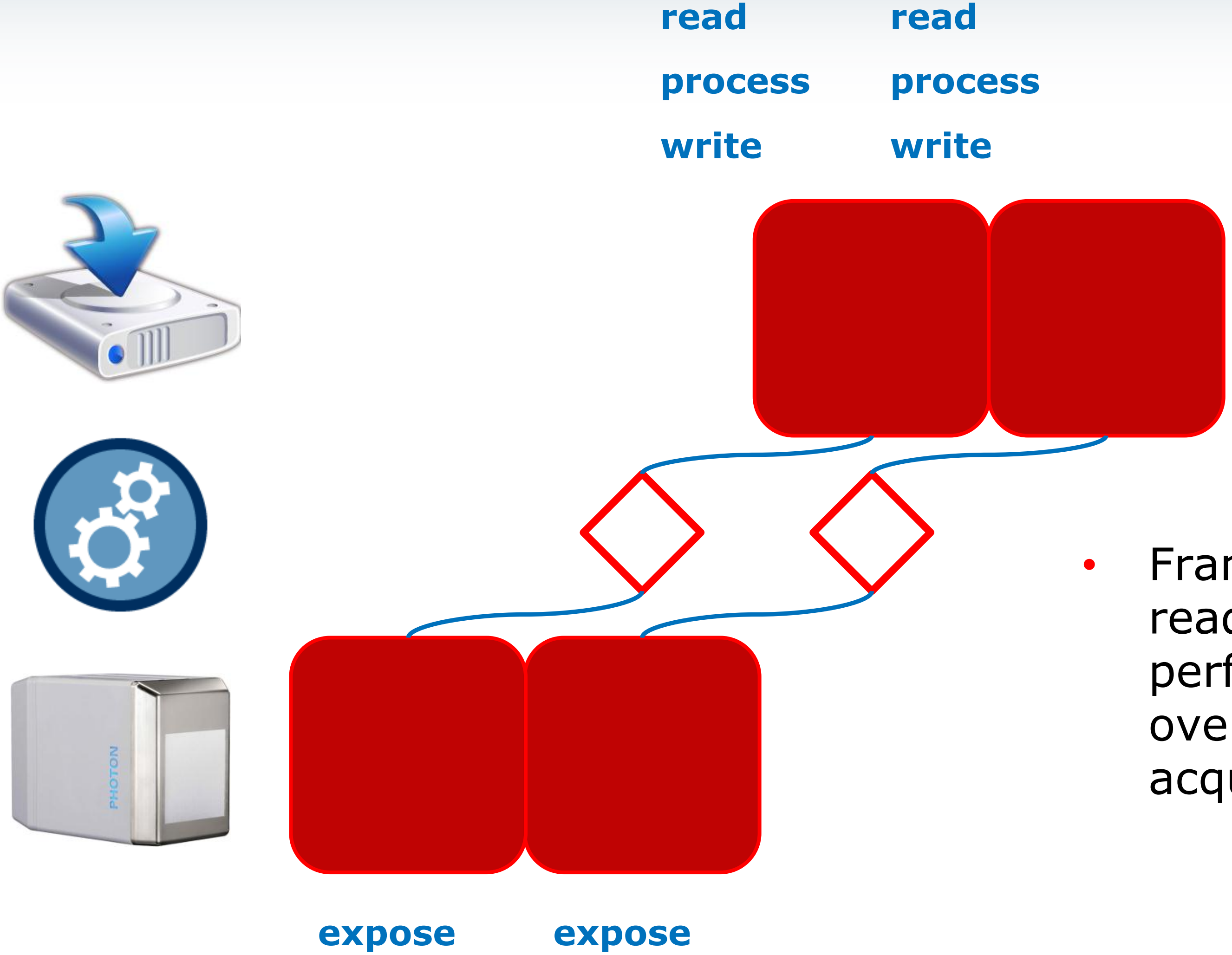
- On-camera frame processing pipeline for overhead-free data acquisition

PHOTON 100 shutterless frame acquisition two cycles



- Frame exposure and read-process-write are performed in parallel for overhead-free data acquisition

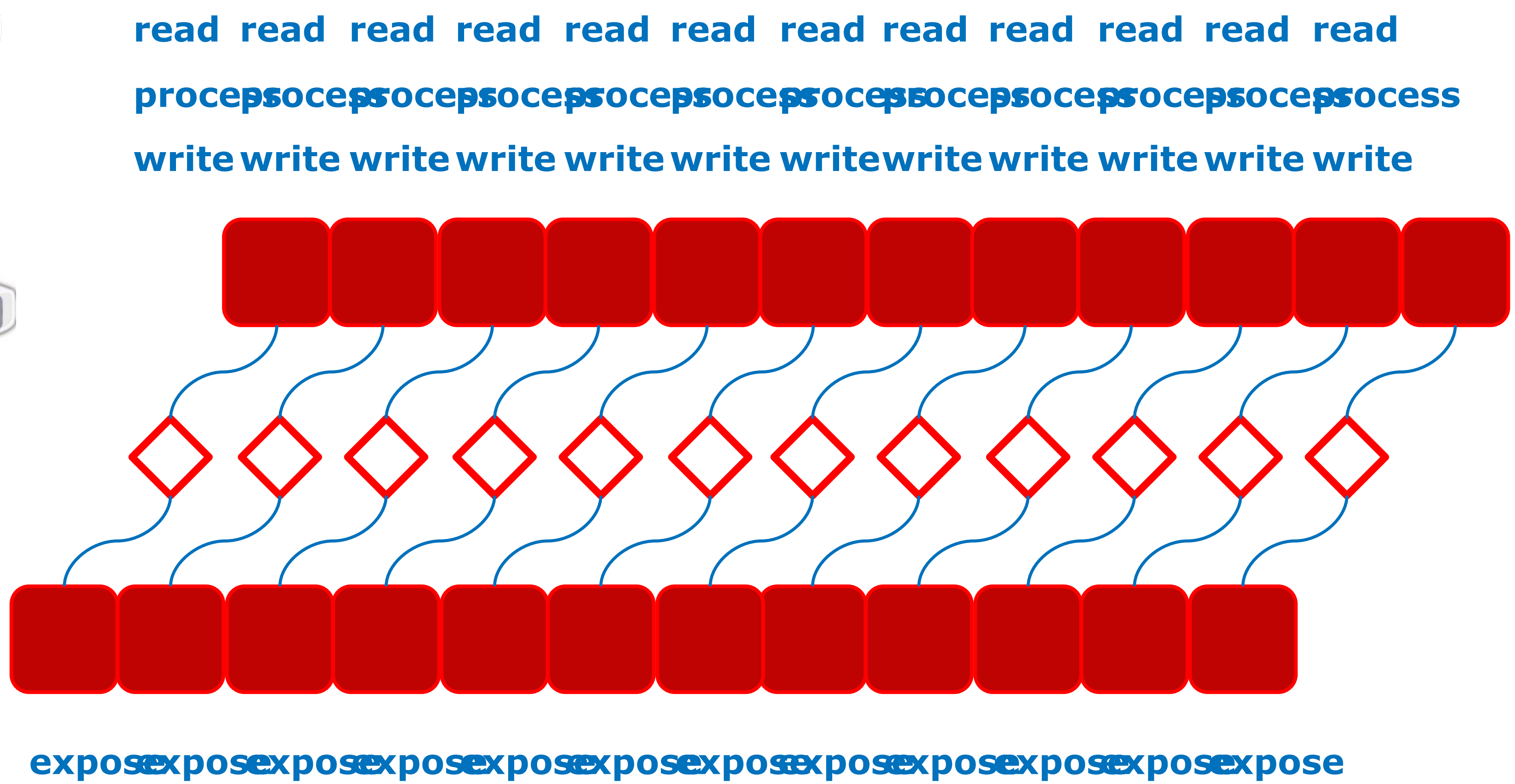
PHOTON 100 shutterless frame acquisition two cycles



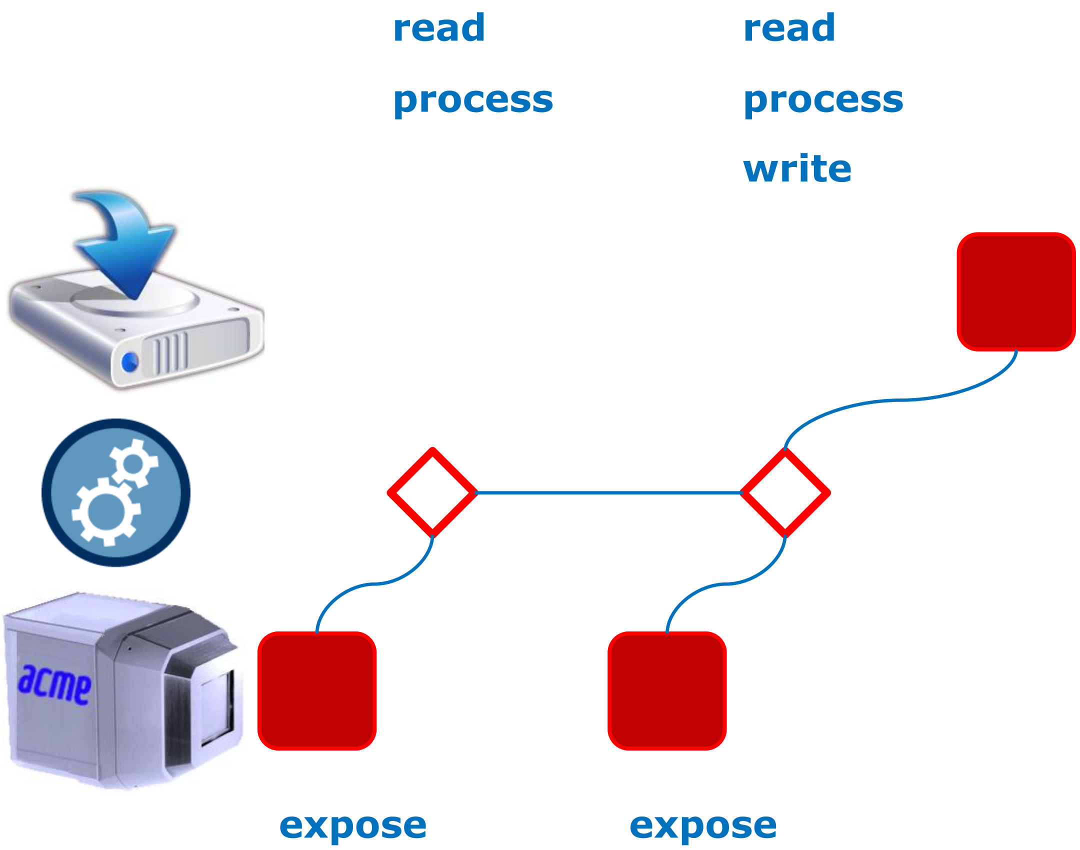
- Frame exposure and read-process-write are performed in parallel for overhead-free data acquisition

PHOTON 100 shutterless frame acquisition continuous

- 12 images collected and written in 13s

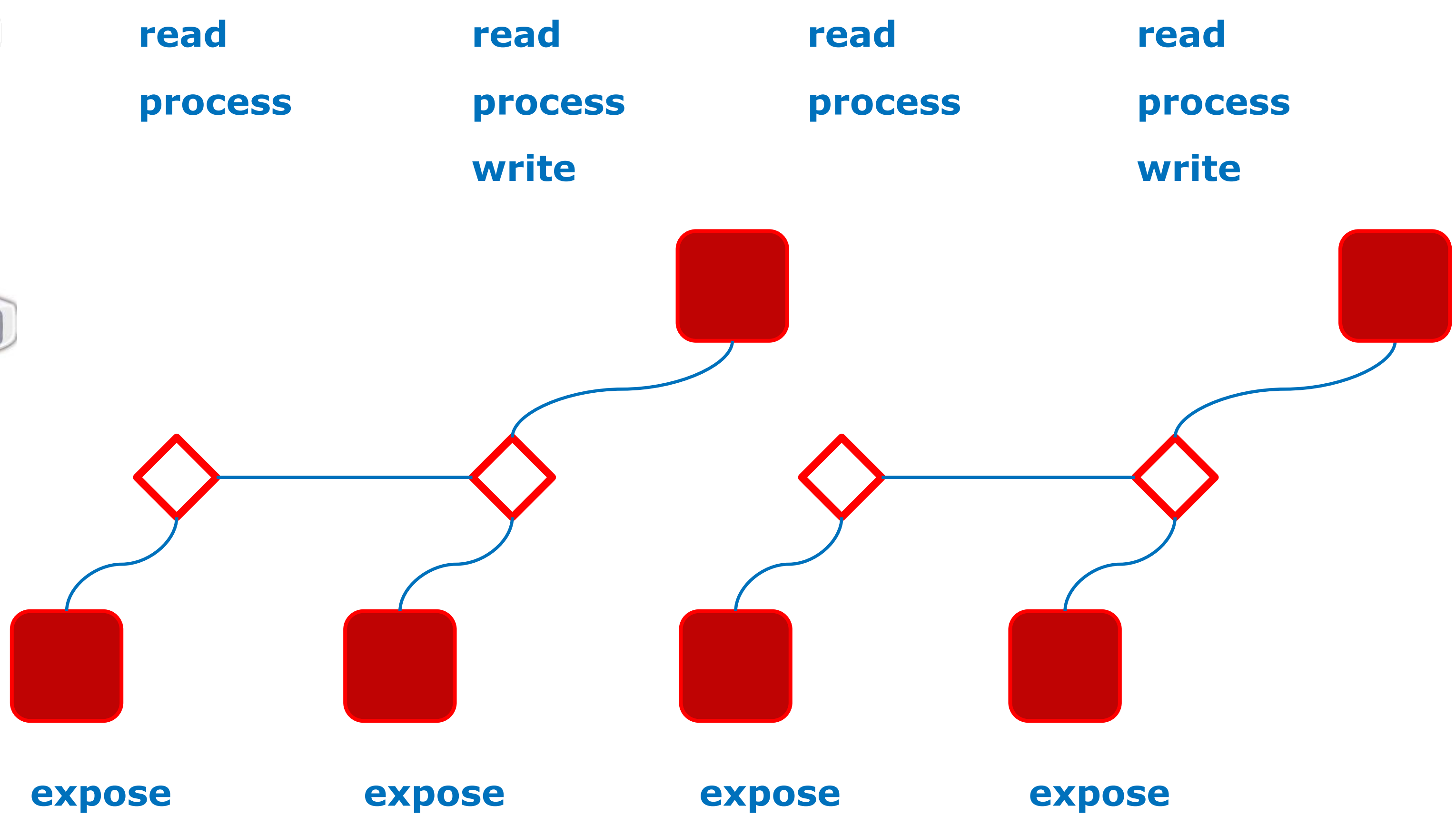


CCD correlated frame acquisition



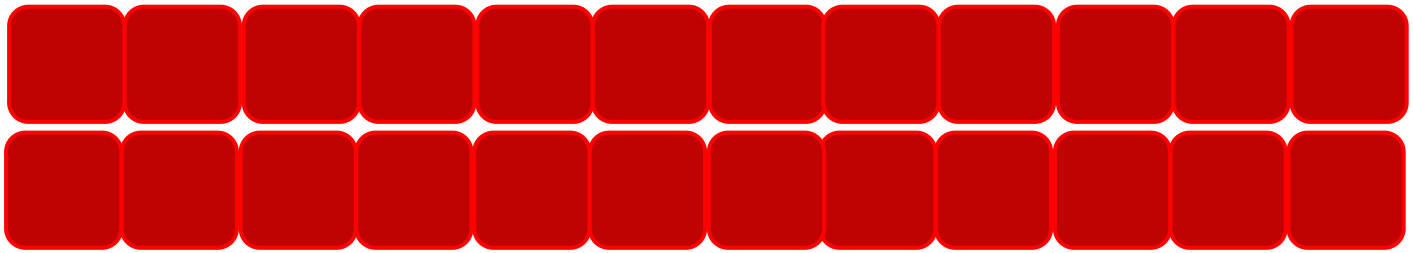
CCD correlated frame acquisition

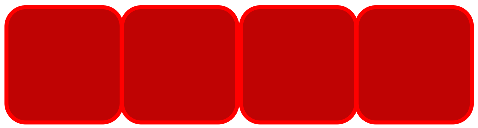
- 2 images collected and written in 12s



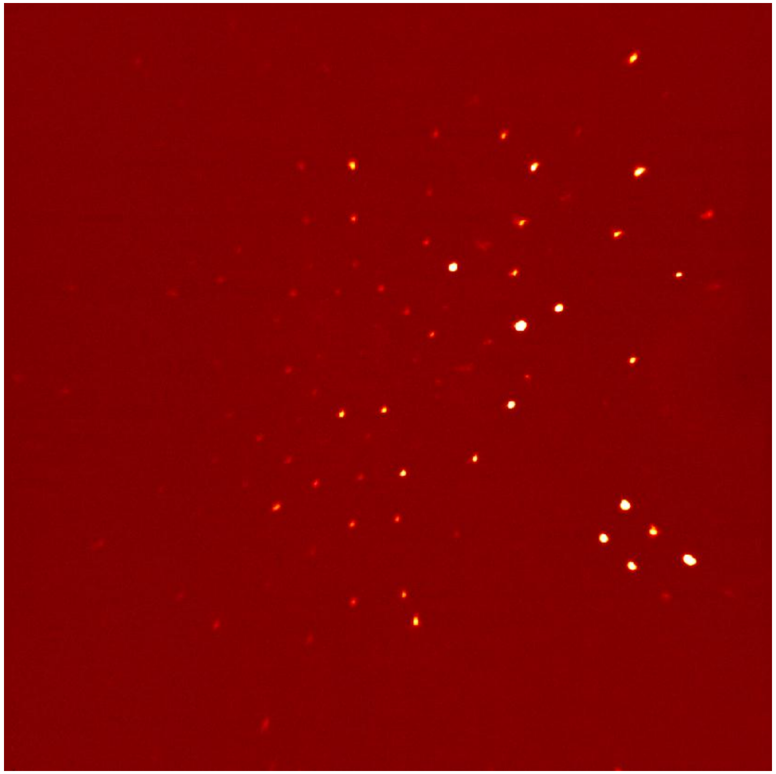
PHOTON 100 - fast and efficient

- 24 images collected with the PHOTON 100
- 4 images collected with a CCD detector



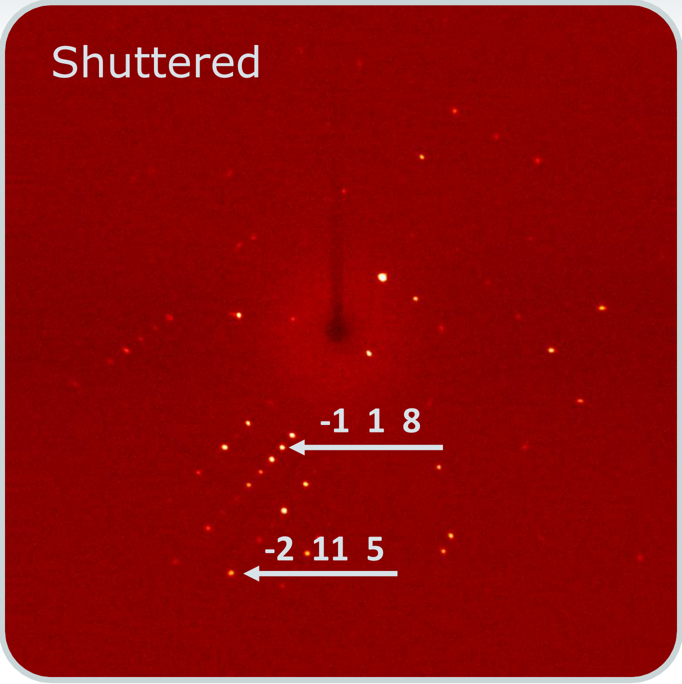


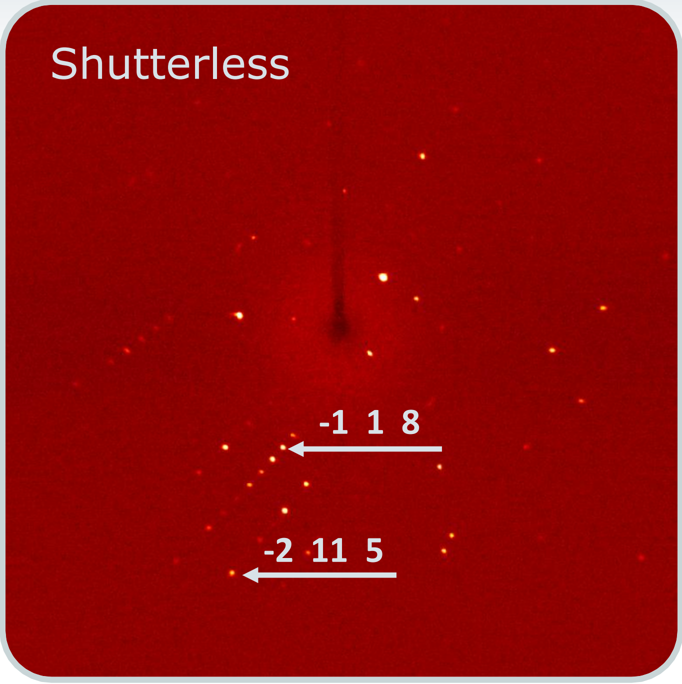
PHOTON 100 – how fast is fast?



- Sealed tube with TRIUMPH
- Sucrose 1s images
- 0.45 × 0.50 × 0.73 mm
- Diffraction to 0.46Å
- R1 = 2.53% to 0.5 Å
- More on this experiment later

3s/3° shuttered and shutterless diffraction images

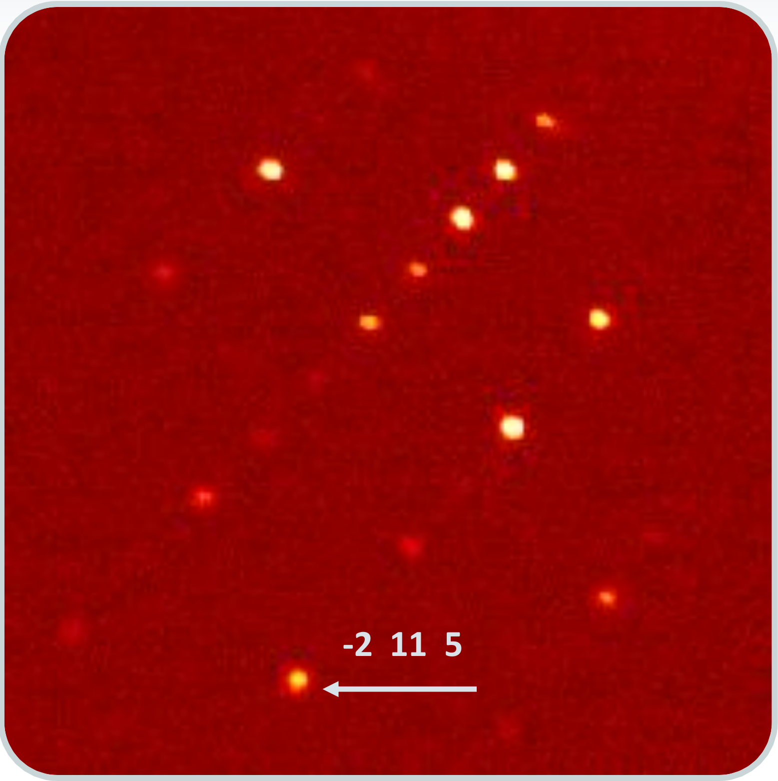




- -2 11 5 phi: 12° to 15°
- -1 1 8 phi: 12° to 15°

- -2 11 5 phi: 12.115° to 15.115°
- -1 1 8 phi: 12.182° to 15.182°

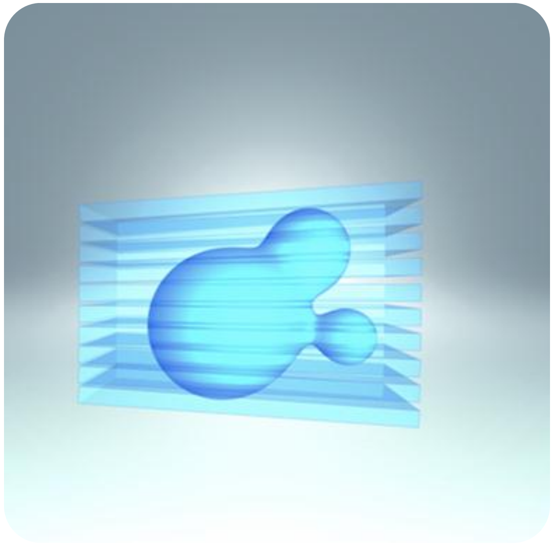
What about skew? – Not an issue!



- The skew for a reflection is negligible and orders of magnitude smaller than the crystal mosaicity
- For the extreme case to the left of 3s/3° the skew of a reflection is only 0.002°
- For a typical 10s/0.5° image the skew for a reflection is only about 0.0001°

Data processing

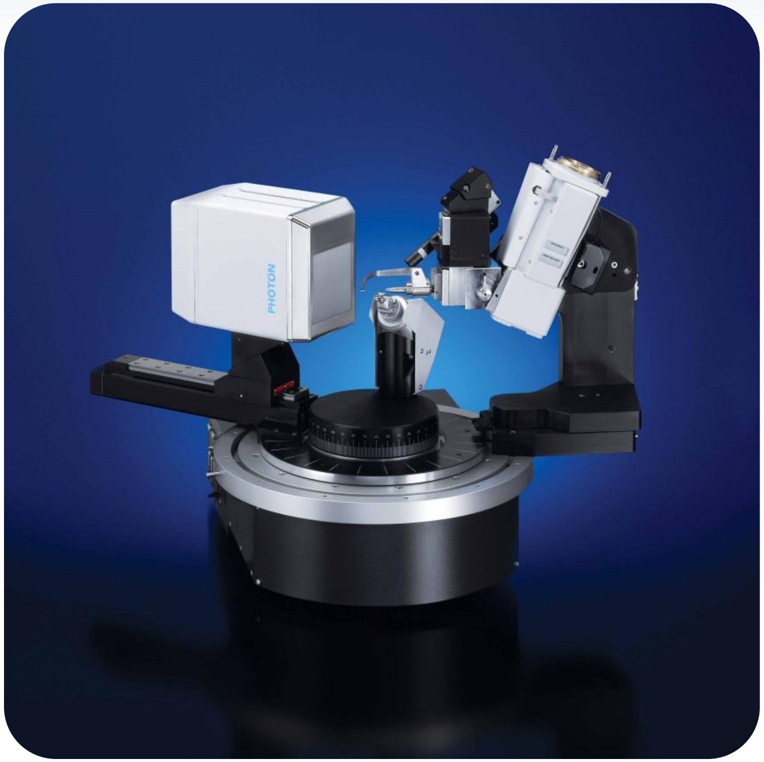
- Data acquisition and processing of shutterless data is completely transparent to the user
- Indexing routines have been modified to accommodate shutterless diffraction images
- Data integration has been adjusted to accommodate shutterless diffraction images



Examples of shutterless data

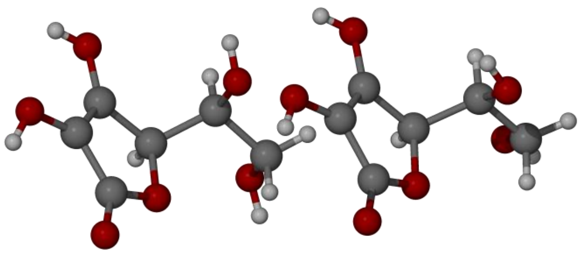
- Data collected on D8 QUEST with Mo source and TRIUMPH monochromator

- Predetermined strategy used
  - 170 degree sweep in omega by 1 degree frames
  - 2theta and omega fixed, phi rotated between sweeps
  - 3 runs for shuttered experiment
  - 3 or 6 runs for shutterless experiment



Summary of results for Vitamin C
8 second exposures

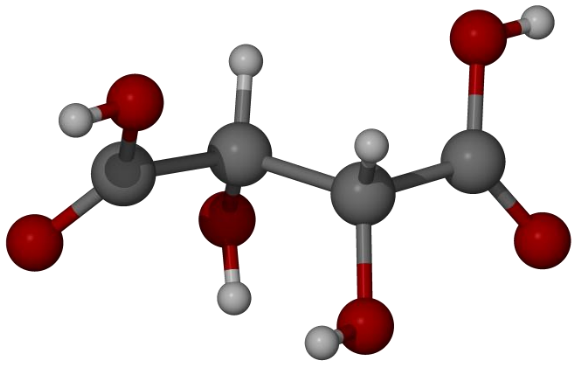
8 second exposures			
mode	Shutter	Shutterless	Shutterless, higher multiplicity
Experiment time	1h 54 min	1h 9 min	2h 17 min
Relative time	1.66	1	1.99
Refl. Total/Unique	8134/3262	8118/3263	16150/3329
Rint [%]	2.68	1.77	2.01
Rsig [%]	3.05	2.29	1.58
Rpim [%]	1.42	1.00	0.72
R1 [%]	3.22	2.91	2.76
wR2 [%]	7.95	7.71	7.48



- Ascorbic Acid (Vitamin C)
  - Crystal approximately 0.08 × 0.25 × 0.35 mm
  - Data collected with 8 seconds per exposure

Summary of results for Tartaric Acid 3 second exposures

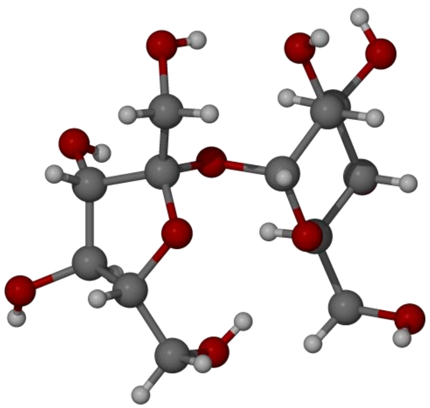
3 second exposures			
mode	Shutter	Shutterless	Shutterless, higher multiplicity
Experiment time	1h 4 min	26 min	52 min
Relative time	2.4	1.0	2.0
Refl. Total/Unique	3240/1348	3238/1347	6474/1367
Rint [%]	1.35	1.30	1.48
Rsig [%]	1.58	1.56	1.08
Rpim [%]	0.77	0.73	0.54
R1 [%]	2.14	2.13	2.06
wR2 [%]	5.51	5.62	5.55



- Tartaric Acid
  - Crystal approximately 0.2 × 0.2 × 0.2 mm
  - Data collected with 3 seconds per exposure

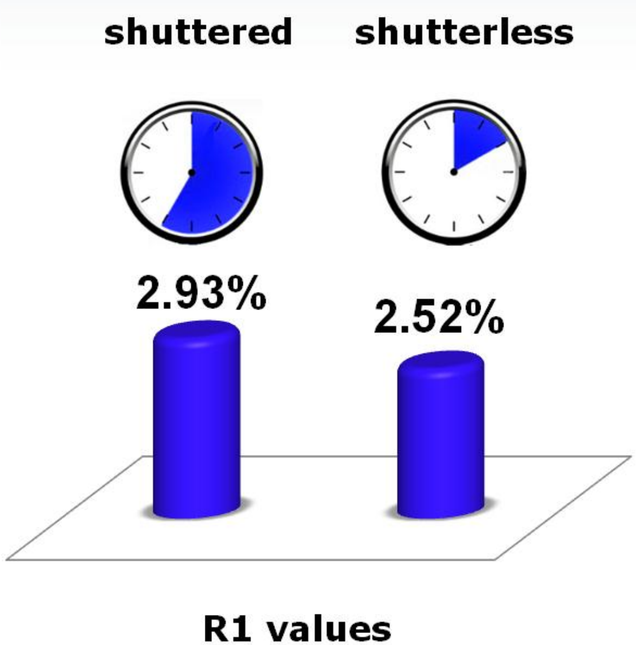
Summary of results for Sucrose
1 second exposures

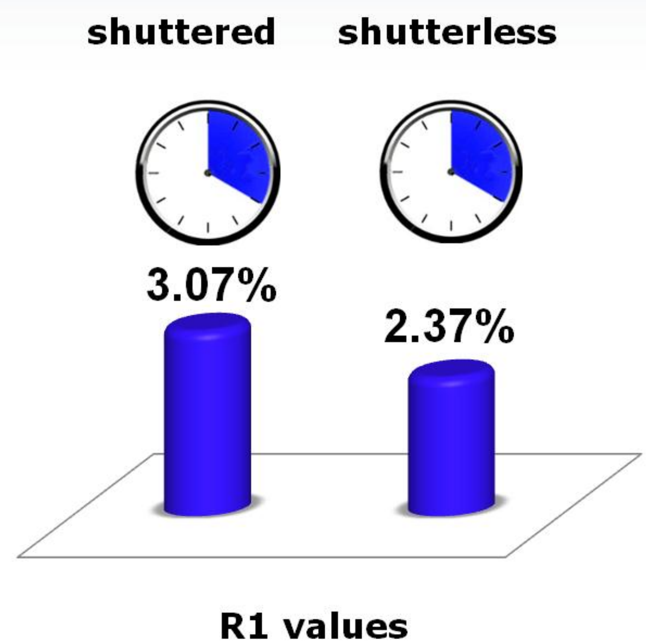
1 second exposures			
mode	Shutter	Shutterless	Shutterless, higher multiplicity
Experiment time	35 min	10 min	20 min
Relative time	3.5	1	2
Refl. Total/Unique	8315/3472	8431/3470	16873/3507
Rint [%]	2.99	1.73	1.87
Rsig [%]	3.82	2.03	1.35
Rpim [%]	1.61	0.90	0.63
R1 [%]	2.93	2.52	2.37
wR2 [%]	8.81	6.44	6.22



- Sucrose
  - Crystal approximately 0.5 × 0.5 × 0.4 mm
  - Data collected with 1 second per exposure

Summary of results for Sucrose
1 second exposures



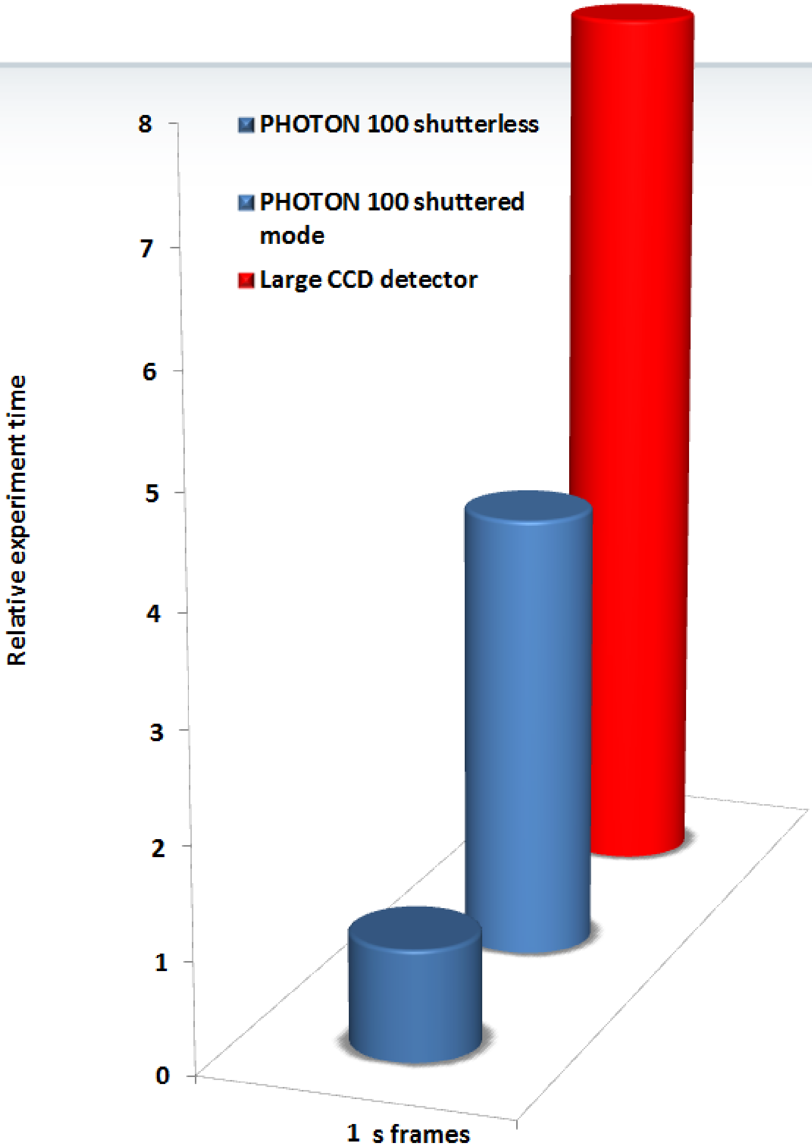


- Similar data were collected in shuttered and shutterless mode
- Although collected in about a fourth of the time, shutterless data are of better quality

- Data were collected for the same experiment time in shuttered and shutterless mode
- Shutterless data with higher multiplicity are significantly better

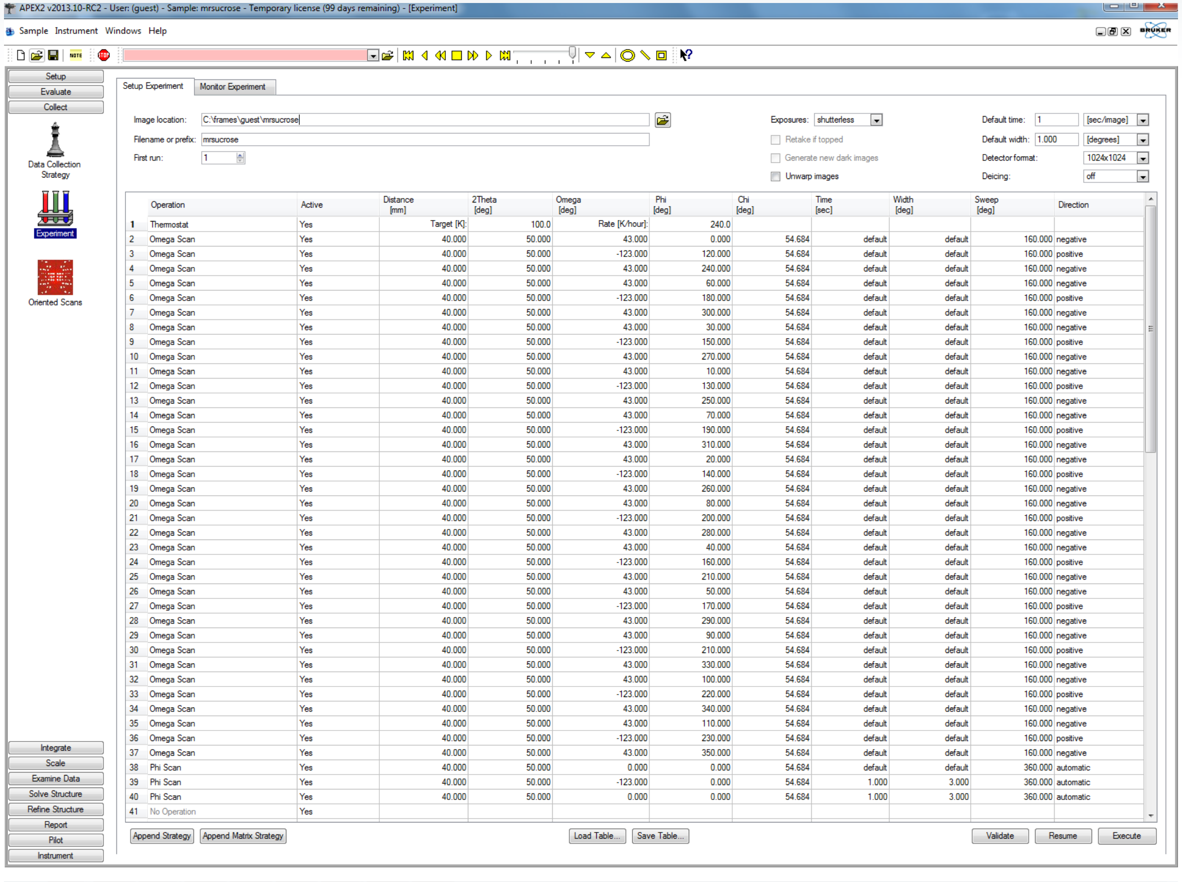
Tremendous time savings

- Shutterless acquisition provides dramatic time savings for shorter exposure times, up to 8 times faster compared to a large CCD



Shutterless data and multiplicity
How far can we push this?

- How long does it take to collect a 15 fold redundant data set of sucrose in P2(1) complete to 0.5Å?
- 40 runs of data
- **2.8 h!!!**

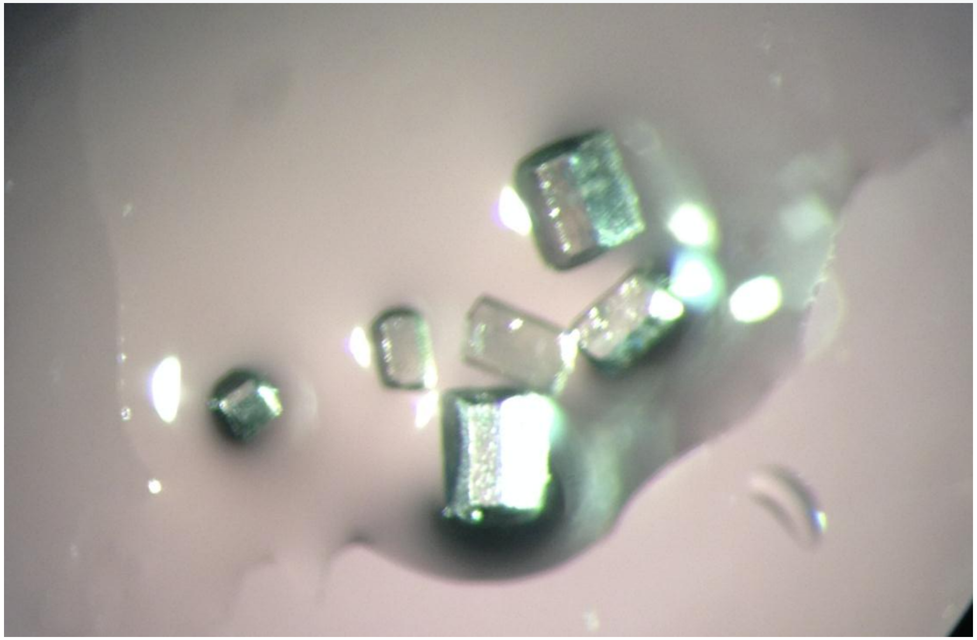


	Operation	Active	Distance [mm]	2Theta [deg]	Omega [deg]	Phi [deg]	Chi [deg]	Time [sec]	Width [deg]	Sweep [deg]	Direction
1	Thermostat	Yes	Target [K]:	100.0	Rate [K/hour]:	240.0					
2	Omega Scan	Yes	40.000	50.000	43.000	0.000	54.684	default	default	160.000	negative
3	Omega Scan	Yes	40.000	50.000	-123.000	120.000	54.684	default	default	160.000	positive
4	Omega Scan	Yes	40.000	50.000	43.000	240.000	54.684	default	default	160.000	negative
5	Omega Scan	Yes	40.000	50.000	43.000	60.000	54.684	default	default	160.000	negative
6	Omega Scan	Yes	40.000	50.000	-123.000	180.000	54.684	default	default	160.000	positive
7	Omega Scan	Yes	40.000	50.000	43.000	300.000	54.684	default	default	160.000	negative
8	Omega Scan	Yes	40.000	50.000	43.000	30.000	54.684	default	default	160.000	negative
9	Omega Scan	Yes	40.000	50.000	-123.000	150.000	54.684	default	default	160.000	positive
10	Omega Scan	Yes	40.000	50.000	43.000	270.000	54.684	default	default	160.000	negative
11	Omega Scan	Yes	40.000	50.000	43.000	10.000	54.684	default	default	160.000	negative
12	Omega Scan	Yes	40.000	50.000	-123.000	130.000	54.684	default	default	160.000	positive
13	Omega Scan	Yes	40.000	50.000	43.000	250.000	54.684	default	default	160.000	negative
14	Omega Scan	Yes	40.000	50.000	43.000	70.000	54.684	default	default	160.000	negative
15	Omega Scan	Yes	40.000	50.000	-123.000	190.000	54.684	default	default	160.000	positive
16	Omega Scan	Yes	40.000	50.000	43.000	310.000	54.684	default	default	160.000	negative
17	Omega Scan	Yes	40.000	50.000	43.000	20.000	54.684	default	default	160.000	negative
18	Omega Scan	Yes	40.000	50.000	-123.000	140.000	54.684	default	default	160.000	positive
19	Omega Scan	Yes	40.000	50.000	43.000	260.000	54.684	default	default	160.000	negative
20	Omega Scan	Yes	40.000	50.000	43.000	80.000	54.684	default	default	160.000	negative
21	Omega Scan	Yes	40.000	50.000	-123.000	200.000	54.684	default	default	160.000	positive
22	Omega Scan	Yes	40.000	50.000	43.000	280.000	54.684	default	default	160.000	negative
23	Omega Scan	Yes	40.000	50.000	43.000	40.000	54.684	default	default	160.000	negative
24	Omega Scan	Yes	40.000	50.000	-123.000	160.000	54.684	default	default	160.000	positive
25	Omega Scan	Yes	40.000	50.000	43.000	210.000	54.684	default	default	160.000	negative
26	Omega Scan	Yes	40.000	50.000	43.000	50.000	54.684	default	default	160.000	negative
27	Omega Scan	Yes	40.000	50.000	-123.000	170.000	54.684	default	default	160.000	positive
28	Omega Scan	Yes	40.000	50.000	43.000	290.000	54.684	default	default	160.000	negative
29	Omega Scan	Yes	40.000	50.000	43.000	90.000	54.684	default	default	160.000	negative
30	Omega Scan	Yes	40.000	50.000	-123.000	210.000	54.684	default	default	160.000	positive
31	Omega Scan	Yes	40.000	50.000	43.000	330.000	54.684	default	default	160.000	negative
32	Omega Scan	Yes	40.000	50.000	43.000	100.000	54.684	default	default	160.000	negative
33	Omega Scan	Yes	40.000	50.000	-123.000	220.000	54.684	default	default	160.000	positive
34	Omega Scan	Yes	40.000	50.000	43.000	340.000	54.684	default	default	160.000	negative
35	Omega Scan	Yes	40.000	50.000	43.000	110.000	54.684	default	default	160.000	negative
36	Omega Scan	Yes	40.000	50.000	-123.000	230.000	54.684	default	default	160.000	positive
37	Omega Scan	Yes	40.000	50.000	43.000	350.000	54.684	default	default	160.000	negative
38	Phi Scan	Yes	40.000	50.000	0.000	0.000	54.684	default	default	360.000	automatic
39	Phi Scan	Yes	40.000	50.000	-123.000	0.000	54.684	1.000	3.000	360.000	automatic
40	Phi Scan	Yes	40.000	50.000	0.000	0.000	54.684	1.000	3.000	360.000	automatic
41	No Operation	Yes									

Shutterless data and multiplicity
How far can we push this?

- In 3.5h I had screened 6 crystals by collecting complete data sets and had collected and processed a 15-fold data set

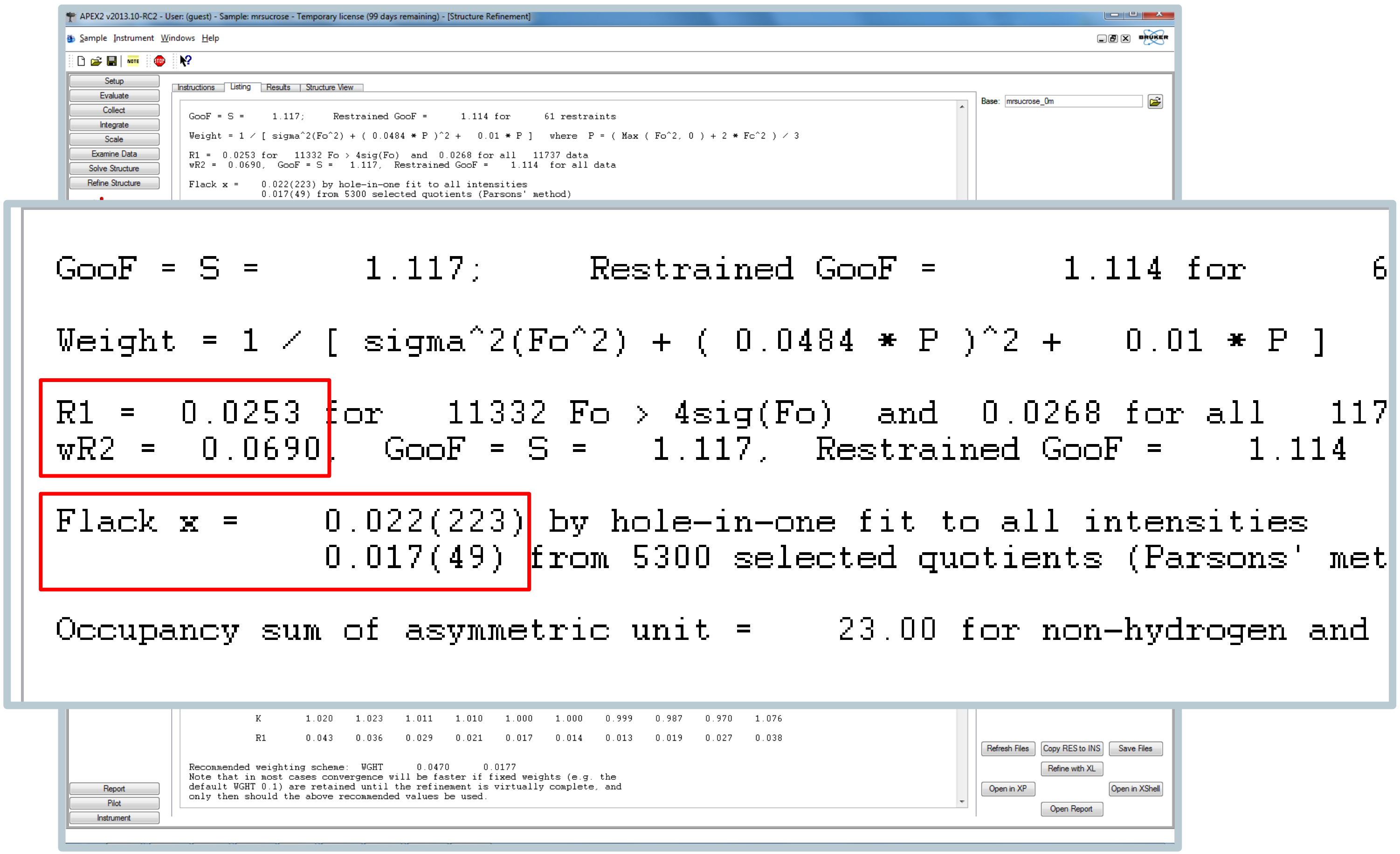
- Why?



screened sucrose crystals

Shutterless data and multiplicity
How far can we push this?

- Absolute configuration from Mo-data?



Shutterless data collection

- The PHOTON 100 shutterless data acquisition mode allows data collection in a fraction of the time compared to “shuttered” mode

- Data quality is always matched or even exceeded and always can be improved further by collecting data with higher multiplicity

- Compared to large-format CCD detectors the factor for time saving can increase to a factor of up to eight

- **The shutterless data acquisition mode of the PHOTON 100 will start a paradigm shift from “improving data quality through increased exposure time” to “increasing data quality through increased multiplicity”**

Supporting material

Product Sheet SC-XRD 47

PHOTON 100 CMOS Detector

For Small Molecule Crystallography

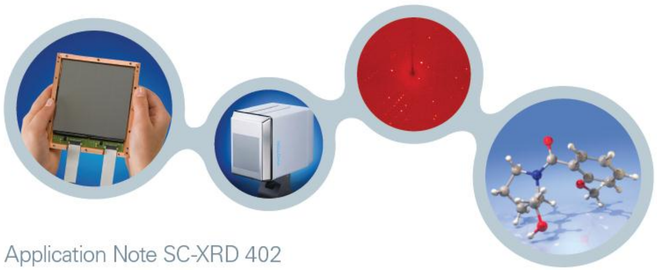
To take full advantage of today's very-high-flux sources requires modern detectors with compatible characteristics – namely high sensitivity, speed, resolution, and reliability. First seen at synchrotron beamlines, these features are also crucial for modern in-house systems.

CMOS (Complementary Metal Oxide Semiconductor) technology has undergone an impressive wave of advancement, and is now the perfect solution for high-performance crystallography. CMOS technology pioneers the implementation of advanced on-chip electronics and very large sensors, unachievable with CCD manufacturing processes.

The PHOTON 100 is the premier CMOS active pixel sensor detector for crystallography with proven performance and reliability with all the features to meet the requirements of cutting-edge crystallographic data acquisition:

PHOTON 100, the premier CMOS active pixel sensor detector for X-ray crystallography

- Large sensor for fast and efficient data collection
- High quantum gain for highest sensitivity and performance
- Taperless design for best spatial resolution
- No gaps for superior data
- Air-cooled for low maintenance
- High reliability
- 3-year warranty
- On-Camera processing for best efficiency
- Continuous scans for reduced systematic error
- Shutterless data collection for unprecedented acquisition speed and data quality



Application Note SC-XRD 402

PHOTON 100 Detector in Shutterless Mode

Faster data acquisition and improved data quality

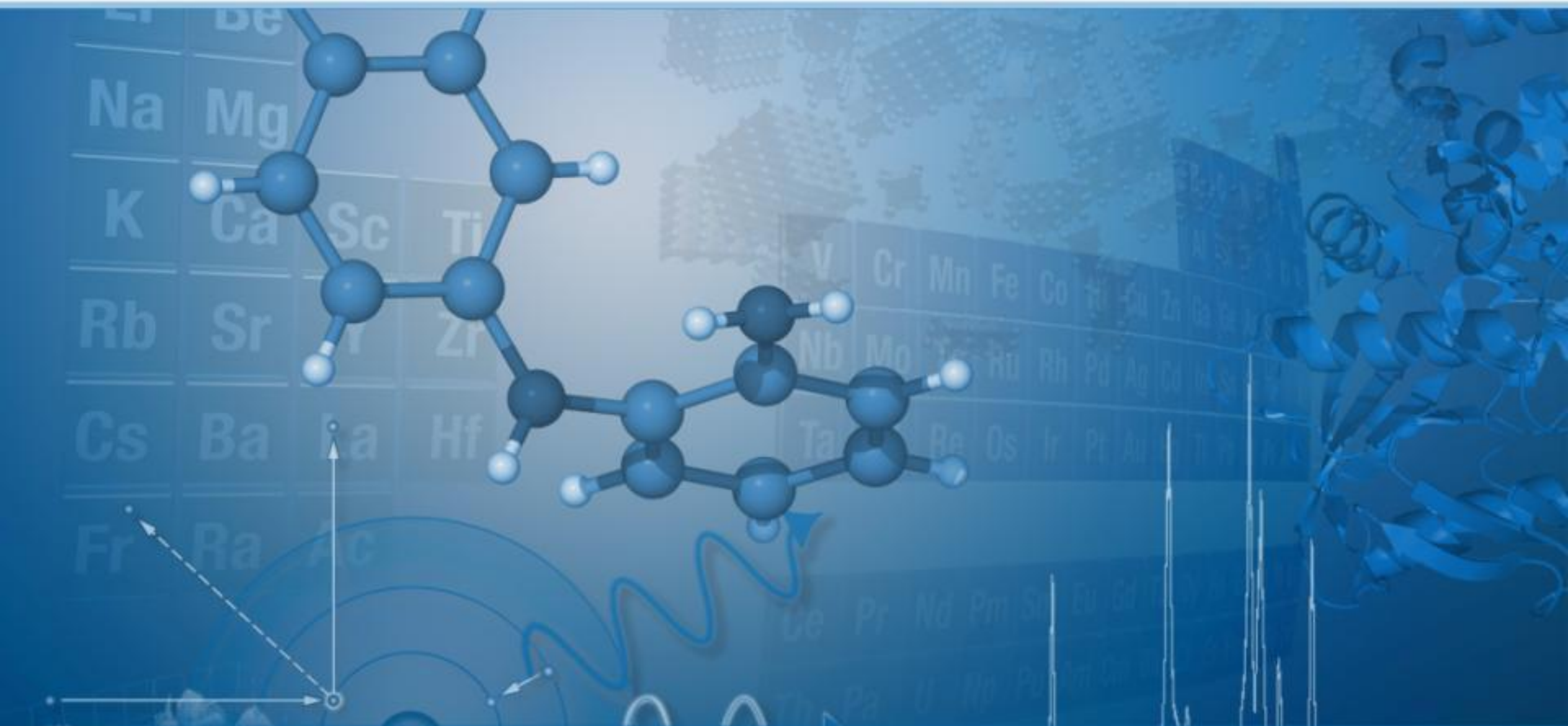
Large active area, high sensitivity, and low maintenance are the most obvious advantages of the PHOTON 100 CMOS detector. These features make the PHOTON 100 ideal for chemical crystallography, which encounters a wide variety of samples, from very small and weakly diffracting crystals, to large, well-diffracting samples. CMOS technology allows for the implementation of advanced features that are not available for older imagers like CCDs. On-chip electronics provide the unique opportunity to apply all necessary corrections in a real-time processor, resulting in fully corrected output data. This approach eliminates frame-to-frame dead time and is a prerequisite for operation of a detector in a shutterless, dead-time-free mode, employing continuous sample rotation. In practice, the PHOTON 100 imager design permits data to be read out while the camera is exposed to X-rays, eliminating the need to close and re-open the X-ray shutter and to stop, reposition and re-start the goniometer. In shutterless mode, the sample is constantly exposed to X-rays and continuously rotated, which maximizes data acquisition efficiency and, even more importantly, eliminates mechanical jitter, resulting in superior data quality, faster.

D8 QUEST with Mo sealed X-ray source and TRIUMPH monochromator

This application note compares data that were collected with the PHOTON 100 in conventional mode, i.e. closing and re-opening the shutter between each frame ("shuttered" mode), with data obtained in shutterless mode. Three crystalline samples of small organic compounds, ascorbic acid, tartaric acid and sucrose, were investigated.

Shutterless data collection: Hybrid Pixel Arrays versus CMOS Active Pixel Sensors

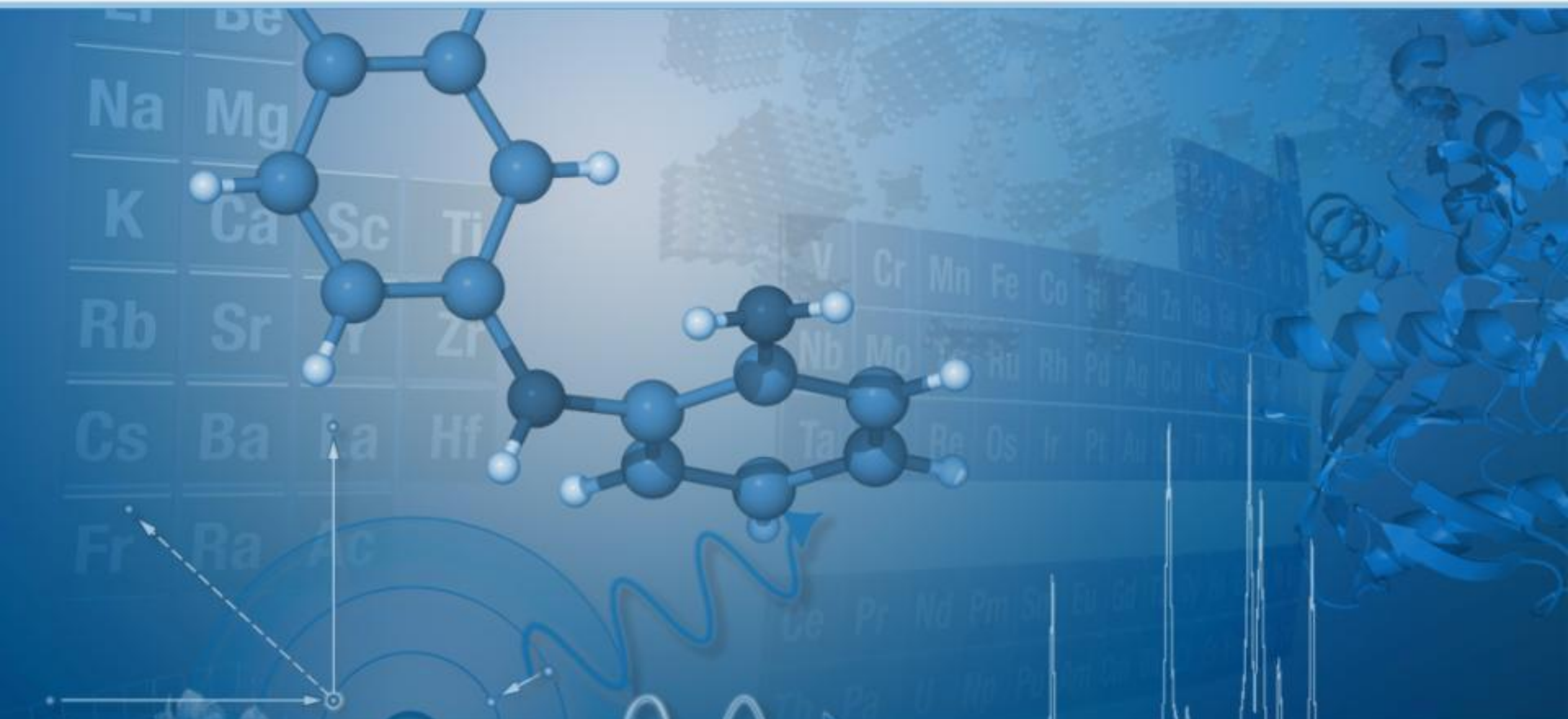
R. Durst



Shutterless data collection: photon counting vs integrating detectors

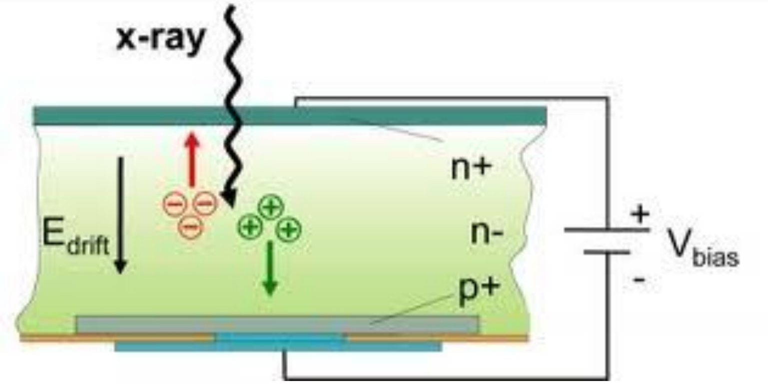
- There are now two detector technologies which support shutterless data collection
  - ***Hybrid pixel array detectors*** (H-PADs) have become the detector of choice for 3rd gen synchrotron X-ray experiments
    - H-PADs are the leading *photon-counting* technology
  - ***CMOS Active Pixel Sensors*** (CMOS APS) are the detector of choice for next gen medical radiography as well for 4th gen beamlines
    - CMOS APS is the leading *integrating* detector
- Both are available for home lab crystallography
- What are the pros and cons of these two technologies?

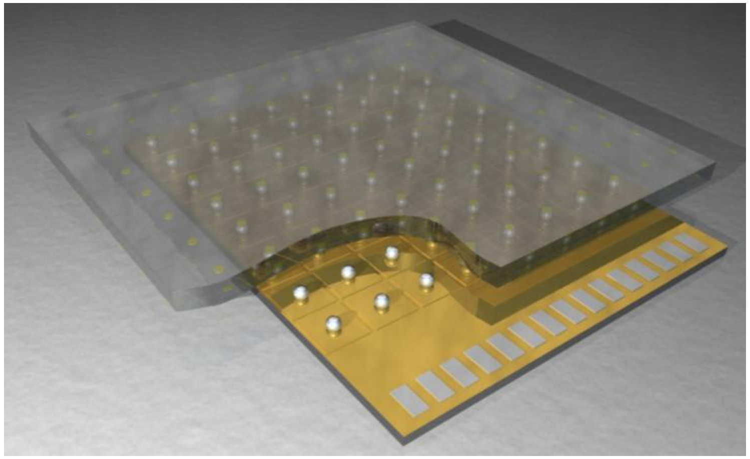
Pixel array detectors



What is a hybrid pixel array?

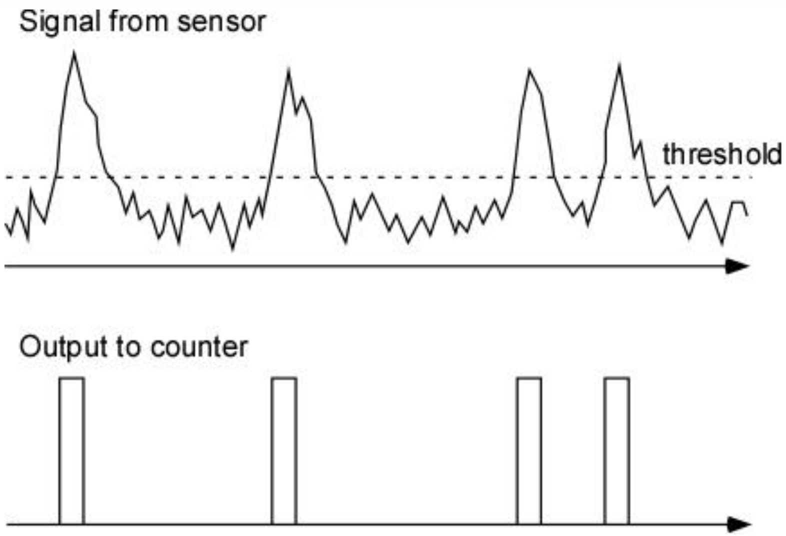
- X-rays produce pulse of electron-hole pairs in a fully depleted Si (or GaAs or CdZnTe) sensor
- Holes drift to a counting circuit
  - Bump-bonded to sensor
- If pulse exceeds a threshold, an X-ray is counted





Photon counting:
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



Pixel array technology

A number of groups and companies are now working on hybrid pixel array technologies including:

- PILATUS, EIGER (PSI): Commercialized by Dectris
- MEDIPIX3 (CERN): Commercialized by Panalytical PIXCEL
- XPAD (ESRF): Commercialized by IMXPAD

Advantages of pixel array detectors

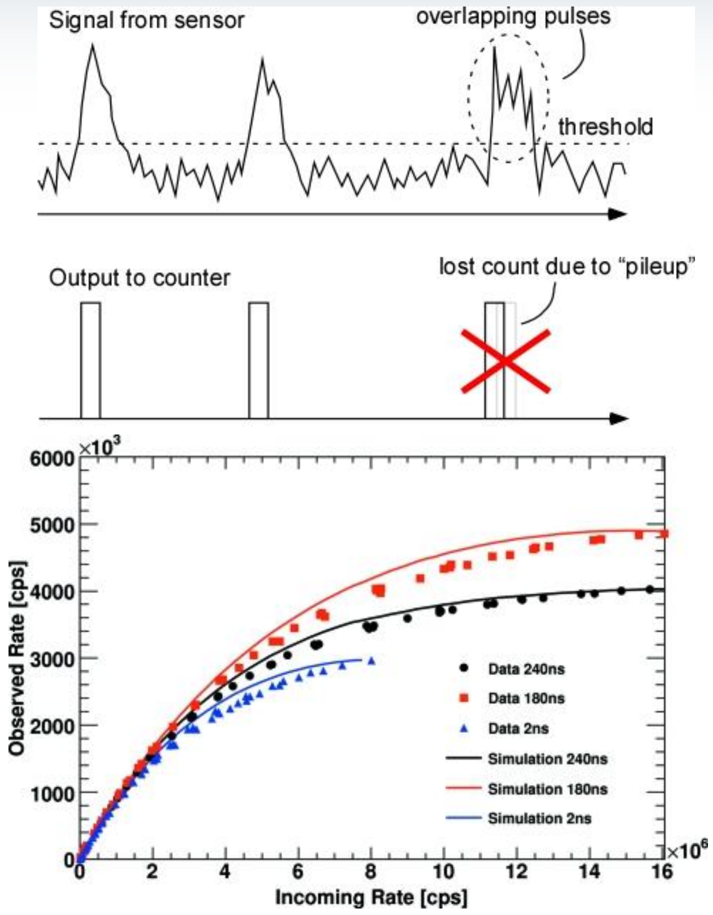
- Speed and dynamic range
  - Up to 20 Hz frame rate
  - Up to 10^6 dynamic range
- High sensitivity
  - Single photon detection confidence 0.9
- Low dark current
  - Only limited by cosmic rays/scattered X-ray background
  - Can take very long exposures if needed (although in most beamline experiments, this capability is rarely needed)

Limitations of hybrid pixel array detectors

- Cost
  - High cost per unit area
  - The sensor chip is manually bonded to the readout chip; this is an expensive procedure
- Chips cannot be tiled seamlessly
  - Typically gaps of about 5% of active area
- Data quality limited due to:
  - Counting nonlinearities
  - ***Charge sharing effects***

Hybrid pixel array limitations: Count rate saturation

- Photon counting detectors have non-linearity at high counting rates
- If pulses overlap too closely they cannot be distinguished
  - Leads to loss of counts for strong reflections
- This effect can be corrected in software (but not perfectly)
  - Mainly an effect for strong reflections

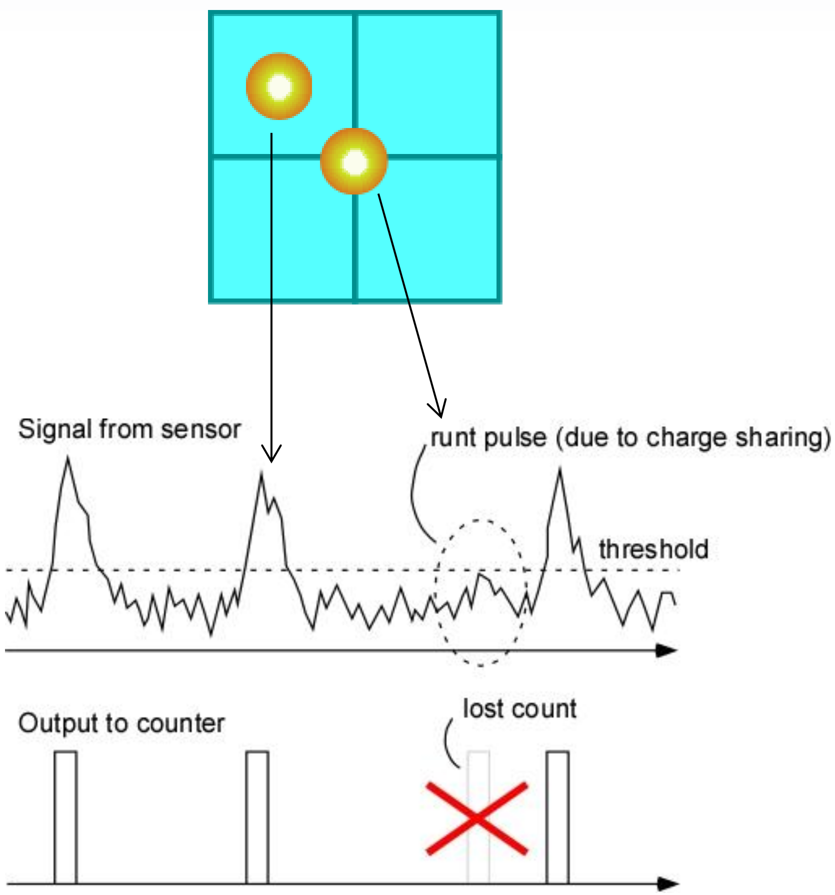


Count rate non-linearity in Pilatus detector

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

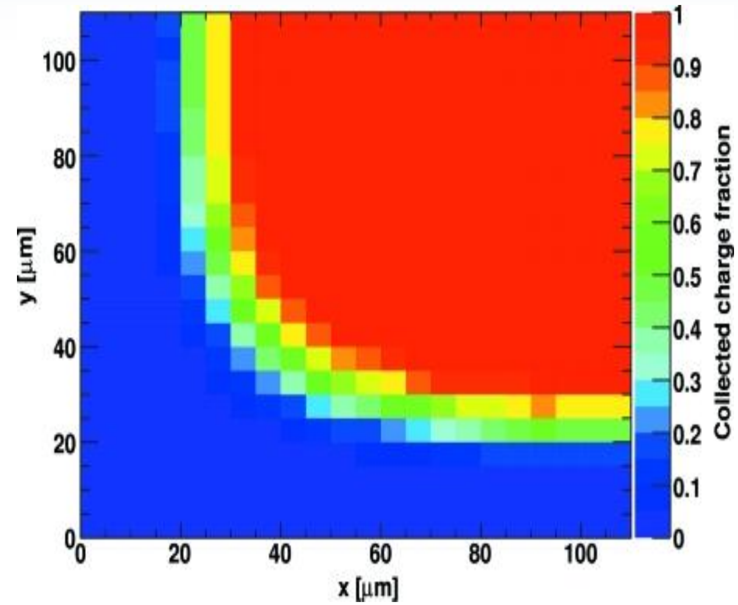
Hybrid pixel array limitations: Charge sharing noise

- Charge produced by a single X-ray near a pixel boundary is shared between adjacent pixels
  - "Charge sharing"
- Because the charge is split between two pixels (or four near the corners) X-ray counts can be lost near the pixel boundaries
  - These lost counts distort the measured reflection intensities
  - In essence this is a new noise source
- ***This is a fundamental limitation of pixel array detectors***



Effect of charge sharing: simulation

- Each PILATUS pixel has an insensitive region at the edge
  - Effective 30-40 μm ‘gap’ between pixels
- This can have a significant impact on H-PAD data quality
- This depends on sample size:
  - Samples larger than the pixels size are not strongly effected because data is average over several pixels
  - Data from samples comparable to or smaller than the pixel size will be significantly *degraded*



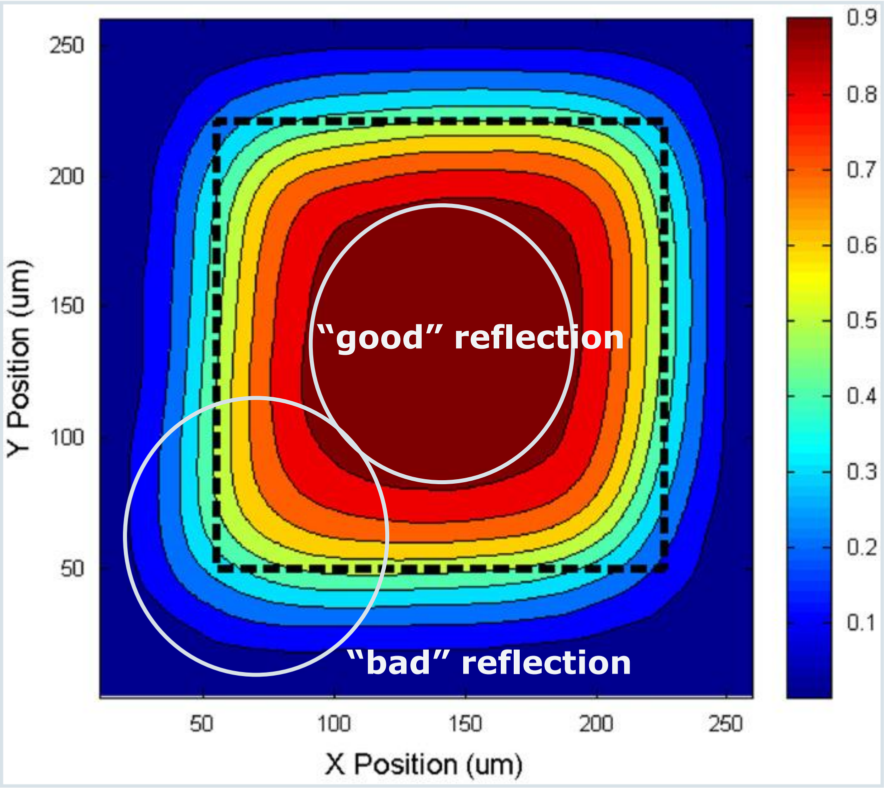
*Charge collection in Pilatus Pixel**

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

**One corner shown*

Experimental measurement of PILATUS pixel efficiency

- In agreement with theoretical calculations, experimental efficiency highest in center of pixel, 90%
- Efficiency drops to 30% in corners
- Intensity of small reflections (comparable or smaller than pixel size of 172 microns) are thus strongly effected by position on pixel
  - Effect smaller for larger reflections



*Charge collection in Pilatus Pixel**

A. Schubert, et al, Radiation Physics and Chemistry 79 (2010) 111.

Comparison: CCD vs PILATUS data (SLS)
Effect of charge sharing effect on data quality

"The experiment was repeated with the Mar CCD165 detector, installed at beamline X06SA, using identical experimental parameters but a different thaumatin crystal (#3). This crystal did not diffract as well as the one used in the experiment with the pixel detector. This can be seen in the lower completeness of 68.4% in the highest resolution shell. ***However, the reliability factor and the signal to noise ratio of the data set are more than a factor of two better for the CCD detector.***"

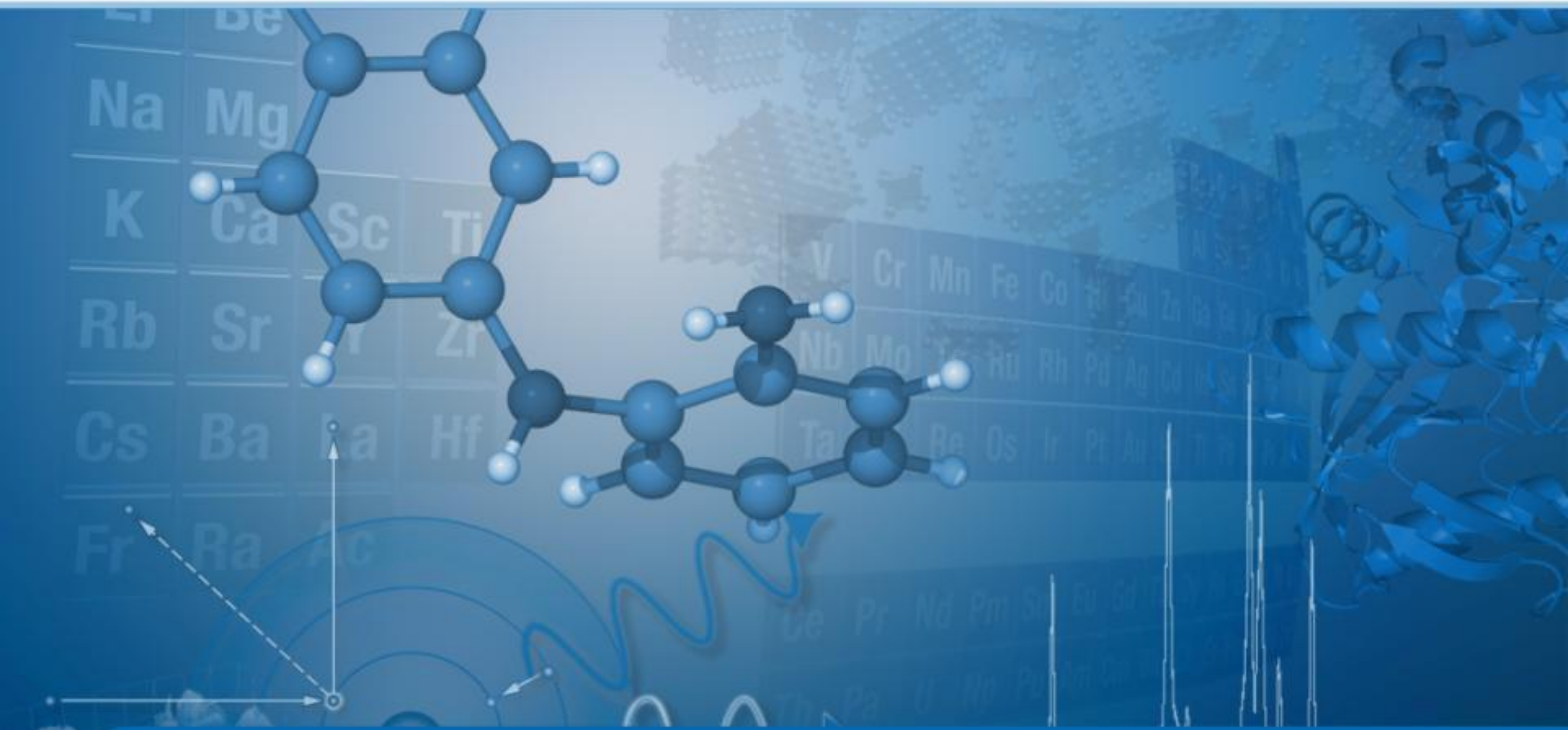
Results of the analysis of thaumatin data for the coarse ϕ-sliced experiments using two detector systems and a rotation increment $\Delta\phi$ = 0.5° per image.

The performance of the detectors in the highest resolution shell is listed in parentheses.

Detector	PILATUS 1M	Mar CCD165
Crystal	#1	#3
Crystal size (μm)	300 × 150 × 100	
Space group	92 ($P4_12_12$)	
Unit-cell a, c (Å)	57.50, 150.89	57.78, 150.06
Diffraction statistics		
Resolution (Å)	70–1.6 (1.7–1.6)	
Completeness (%)	99.9 (99.9)	94.8 (68.4)
Unique reflections	34320 (5579)	32580 (3817)
Total observed reflections	258324 (41040)	300251 (29070)
Redundancy	7.53 (7.36)	9.22 (7.62)
σ_{spot} (pixel)	0.50	0.32
R_{merge} (%)	9.5 (36.0)	4.6 (13.0)
Mean $I/\sigma(I)$	13.02 (5.17)	33.78 (13.35)
Refinement statistics		
R_{cryst} (%), working set	19.40	19.74
R_{free} (%), free set	21.20	21.05

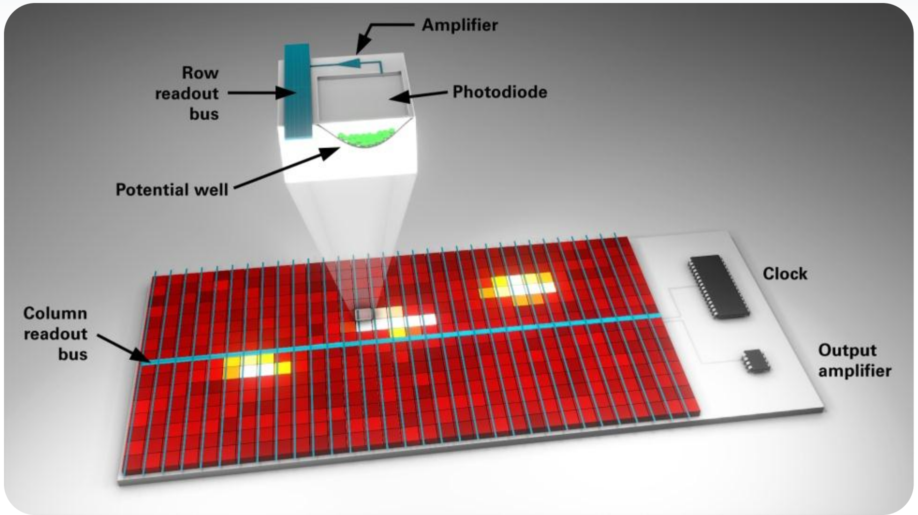
G. Huelsen, J. Appl. Cryst. (2006). 39, 550–557

CMOS Active Pixel Sensors



CMOS APS technology

- Active Pixel Sensors are integrating detectors
  - More similar to CCDs
- *Like pixel detectors, they can be run in shutterless mode*
- *Compared to HPADs, CMOS APS's are somewhat slower*
  - *CMOS APS <1 fps*
  - *HPAD 20 fps*
- *However, the APS offers a larger, gap-free active area*
- Also, CMOS APS's do not suffer from the data quality limitations of pixel arrays
  - *No charge sharing effects*
  - *No count rate saturation*



How to make a noise-free integrating detector

- Integrating detector sensitivity can be written as

$$SPDC = erf\left(\frac{g}{n_{tot}}\right)$$

Where g is the quantum gain of the detector and n_{tot} is the total noise (read plus dark current)

- PHOTON 100 can achieve $g/n_{tot} = 1,\ SPDC = 0.7$
  - *Compared to 0.9 for HPAD*
  - Statistically very close to ideal single photon sensitivity

Comparison: pixel array detector versus active pixel sensors

Detector type	CMOS APS	HPAD (typical)	Advantage
Active area (mm^2)	<100 x 100	<84 x 70	CMOS APS
Pixel size (μm)	96	172	CMOS APS
Single-photon sensitivity	0.7	0.9	HPAD
Frame rate (Hz)	**1**	**20**	**HPAD**
Shutterless data	Yes	Yes	-
Charge sharing noise	**No**	**Yes**	**CMOS APS**
Count rate saturation	**No**	**Yes**	**CMOS APS**
Dynamic range	10^5	10^6	HPAD
Gaps	None	Yes (5%)	CMOS APS
Cost	**$$**	**$$$$**	**CMOS APS**

Summary

- Both HPAD's and APS's are now available which can collect shutterless data
- HPAD's offer high speed and high sensitivity
  - However, data quality is limited by count rate saturation and charge sharing artifacts (for smaller samples)
- CMOS APS's offer several advantages
  - Large, gap-free active area
  - Single photon sensitivity
  - No count rate saturation
  - ***No charge sharing artifacts***

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Feb 26, 2013 **Advanced Crystallography: Data Collection and Data Reduction Techniques for Modulated Structures**	Drs. Michael Ruf and Charles Campana give a one-hour presentation demonstrating the steps required to collect and process data for modulated structures. Specific topics include: how to recognize modulated structures; introduction to q-vectors; APEX2 software tools; preparation of files for JANA2006; and examples of the solution of modulated structures from single-crystal diffraction data. View recording Download slides
Dec 05, 2012 **PROTEUM2 and Foreign Frame Formats**	View this 45-minute webinar to learn about Bruker's PROTEUM software, a suite of crystallographic data integration and reduction tools for macromolecules. Dr. Matt Benning and Dr. Michael Ruf will discuss how to reduce data from various detectors and show results from synchrotron beamlines. View recording Download slides
Nov 13, 2012 **Advanced Crystallography: Refinement of Disordered Structures**	Dr. Charles Campana gives a one-hour presentation demonstrating the steps required to refine disordered crystal structures. Along with specific examples, topics covered include SHELXL, SHELXTL, free variables, PART n and –n instructions, constraints vs restraints, and advanced refinement instructions. View recording Download slides
Dec 06, 2011 **High-Pressure Crystallography**	Dr. Francesca Fabbiani of Georg-August-Universität Göttingen takes you through the steps for performing a high-pressure single-crystal X-ray diffraction experiment with a diamond-anvil cell (DAC). You will learn DAC loading techniques and useful strategies for data collection, data reduction, and structure refinement. View recording Download slides
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